Supplemental information for:

Identification of sulfur tolerant bimetallic surfaces using DFT parameterized models and atomistic thermodynamics

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Supplemental information

A summary of each DFT calculation performed in this manuscript follows this description. The calculations are organized in groups of host metals. A summary of the computational parameters used for in each calculation is provided, along with the geometry, maximum force on each atom, and the name of the pseudopotential used for each atom. A small figure illustrates the surface of each slab.

The clean surfaces are presented first, then the sulfur-poisoned surfaces. The contents of this file can be navigated using the pdf bookmarks.

CLEAN SURFACE STRUCTURES

Structures with Fe as the substrate:

Fe overlayer:

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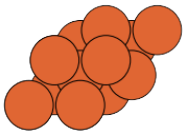
---------------------------------
Dacapo calculation from Fe-subs/Fe-layer/Fe111-sub+Fe-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -13307.987456 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9144  0.0000  0.0000] 4.91
a1 [ 2.4572  4.2560  0.0000] 4.91
a2 [ 0.0000  0.0000  18.0252] 18.03
No stress calculated.
Volume = 377.01 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Fe  [  0.000  0.000  0.000]   4   0.597  Fe_us_gga_d2.1.8.pseudo
 1    Fe  [  2.457  0.000  0.000]   4   0.597  Fe_us_gga_d2.1.8.pseudo
 2    Fe  [  1.229  2.128  0.000]   4   0.597  Fe_us_gga_d2.1.8.pseudo
 3    Fe  [  3.686  2.128  0.000]   4   0.597  Fe_us_gga_d2.1.8.pseudo
 4    Fe  [  1.229  0.709  2.006]   3   0.541  Fe_us_gga_d2.1.8.pseudo
 5    Fe  [  3.686  0.709  2.006]   3   0.540  Fe_us_gga_d2.1.8.pseudo
 6    Fe  [  2.457  2.837  2.006]   3   0.540  Fe_us_gga_d2.1.8.pseudo
 7    Fe  [  4.914  2.837  2.006]   3   0.541  Fe_us_gga_d2.1.8.pseudo
 8    Fe  [  4.915  1.419  4.052]   2   0.039  Fe_us_gga_d2.1.8.pseudo
 9    Fe  [  2.458  1.419  4.052]   2   0.039  Fe_us_gga_d2.1.8.pseudo
10    Fe  [  6.144  3.547  4.052]   2   0.039  Fe_us_gga_d2.1.8.pseudo
11    Fe  [  3.686  3.547  4.052]   2   0.039  Fe_us_gga_d2.1.8.pseudo
12    Fe  [  0.000  0.000  5.976]   1   0.045  Fe_us_gga_d2.1.8.pseudo
13    Fe  [  2.457  0.000  5.976]   1   0.045  Fe_us_gga_d2.1.8.pseudo
14    Fe  [  1.229  2.128  5.976]   1   0.045  Fe_us_gga_d2.1.8.pseudo
15    Fe  [  3.686  2.128  5.976]   1   0.045  Fe_us_gga_d2.1.8.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 128.0
Number of bands     = 87
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



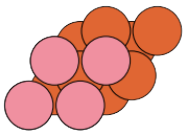
Co overlayer:

```
---------------------------------
Dacapo calculation from Fe-subs/Co-layer/Fe111-sub+Co-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -14344.998101 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9144  0.0000  0.0000] 4.91
a1 [ 2.4572  4.2560  0.0000] 4.91
a2 [ 0.0000  0.0000  18.0252] 18.03
No stress calculated.
Volume = 377.01 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Fe  [  0.000  0.000  0.000]   4   0.441  Fe_us_gga_d2.1.8.pseudo
 1    Fe  [  2.457  0.000  0.000]   4   0.441  Fe_us_gga_d2.1.8.pseudo
 2    Fe  [  1.229  2.128  0.000]   4   0.441  Fe_us_gga_d2.1.8.pseudo
 3    Fe  [  3.686  2.128  0.000]   4   0.441  Fe_us_gga_d2.1.8.pseudo
 4    Fe  [  1.229  0.709  2.006]   3   0.562  Fe_us_gga_d2.1.8.pseudo
 5    Fe  [  3.686  0.709  2.006]   3   0.562  Fe_us_gga_d2.1.8.pseudo
 6    Fe  [  2.457  2.837  2.006]   3   0.562  Fe_us_gga_d2.1.8.pseudo
 7    Fe  [  4.914  2.837  2.006]   3   0.562  Fe_us_gga_d2.1.8.pseudo
 8    Fe  [  4.916  1.420  3.987]   2   0.022  Fe_us_gga_d2.1.8.pseudo
 9    Fe  [  2.459  1.420  3.987]   2   0.023  Fe_us_gga_d2.1.8.pseudo
10    Fe  [  6.145  3.548  3.987]   2   0.022  Fe_us_gga_d2.1.8.pseudo
11    Fe  [  3.688  3.548  3.987]   2   0.023  Fe_us_gga_d2.1.8.pseudo
12    Co  [  0.002  0.001  5.940]   1   0.040  Co_us_gga.pseudo
13    Co  [  2.459  0.001  5.940]   1   0.040  Co_us_gga.pseudo
14    Co  [  1.230  2.129  5.940]   1   0.040  Co_us_gga.pseudo
15    Co  [  3.688  2.129  5.940]   1   0.040  Co_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 132.0
Number of bands     = 89
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Ni overlayer:

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---------------------------------
Dacapo calculation from Fe-subs/Ni-layer/Fe111-sub+Ni-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -15205.102090 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9144  0.0000  0.0000] 4.91
a1 [ 2.4572  4.2560  0.0000] 4.91
a2 [ 0.0000  0.0000  18.0252] 18.03
No stress calculated.
Volume = 377.01 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Fe  [  0.000  0.000  0.000]   4   0.359  Fe_us_gga_d2.1.8.pseudo
 1    Fe  [  2.457  0.000  0.000]   4   0.359  Fe_us_gga_d2.1.8.pseudo
 2    Fe  [  1.229  2.128  0.000]   4   0.359  Fe_us_gga_d2.1.8.pseudo
 3    Fe  [  3.686  2.128  0.000]   4   0.359  Fe_us_gga_d2.1.8.pseudo
 4    Fe  [  1.229  0.709  2.006]   3   0.335  Fe_us_gga_d2.1.8.pseudo
 5    Fe  [  3.686  0.709  2.006]   3   0.335  Fe_us_gga_d2.1.8.pseudo
 6    Fe  [  2.457  2.837  2.006]   3   0.335  Fe_us_gga_d2.1.8.pseudo
 7    Fe  [  4.914  2.837  2.006]   3   0.335  Fe_us_gga_d2.1.8.pseudo
 8    Fe  [  4.915  1.419  3.963]   2   0.037  Fe_us_gga_d2.1.8.pseudo
 9    Fe  [  2.458  1.419  3.963]   2   0.037  Fe_us_gga_d2.1.8.pseudo
10    Fe  [  6.144  3.547  3.963]   2   0.037  Fe_us_gga_d2.1.8.pseudo
11    Fe  [  3.687  3.547  3.963]   2   0.037  Fe_us_gga_d2.1.8.pseudo
12    Ni  [  0.000  0.000  6.021]   1   0.040  Ni_us_gga.pseudo
13    Ni  [  2.457  0.000  6.021]   1   0.040  Ni_us_gga.pseudo
14    Ni  [  1.229  2.128  6.021]   1   0.040  Ni_us_gga.pseudo
15    Ni  [  3.686  2.128  6.021]   1   0.040  Ni_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 136.0
Number of bands     = 92
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```

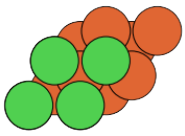

Cu overlayer:

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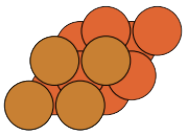
---------------------------------
Dacapo calculation from Fe-subs/Cu-layer/Fe111-sub+Cu-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -16682.372923 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9144  0.0000  0.0000] 4.91
a1 [ 2.4572  4.2560  0.0000] 4.91
a2 [ 0.0000  0.0000  18.0252] 18.03
No stress calculated.
Volume = 377.01 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Fe  [  0.000  0.000  0.000]   4   0.328  Fe_us_gga_d2.1.8.pseudo
 1    Fe  [  2.457  0.000  0.000]   4   0.328  Fe_us_gga_d2.1.8.pseudo
 2    Fe  [  1.229  2.128  0.000]   4   0.328  Fe_us_gga_d2.1.8.pseudo
 3    Fe  [  3.686  2.128  0.000]   4   0.328  Fe_us_gga_d2.1.8.pseudo
 4    Fe  [  1.229  0.709  2.006]   3   0.430  Fe_us_gga_d2.1.8.pseudo
 5    Fe  [  3.686  0.709  2.006]   3   0.430  Fe_us_gga_d2.1.8.pseudo
 6    Fe  [  2.457  2.837  2.006]   3   0.430  Fe_us_gga_d2.1.8.pseudo
 7    Fe  [  4.914  2.837  2.006]   3   0.430  Fe_us_gga_d2.1.8.pseudo
 8    Fe  [  4.915  1.419  3.929]   2   0.002  Fe_us_gga_d2.1.8.pseudo
 9    Fe  [  2.457  1.419  3.929]   2   0.002  Fe_us_gga_d2.1.8.pseudo
10    Fe  [  6.143  3.547  3.929]   2   0.002  Fe_us_gga_d2.1.8.pseudo
11    Fe  [  3.686  3.547  3.929]   2   0.002  Fe_us_gga_d2.1.8.pseudo
12    Cu  [  0.000  0.000  6.086]   1   0.018  Cu_us_gga.pseudo
13    Cu  [  2.457  0.000  6.086]   1   0.018  Cu_us_gga.pseudo
14    Cu  [  1.229  2.128  6.086]   1   0.018  Cu_us_gga.pseudo
15    Cu  [  3.686  2.128  6.086]   1   0.018  Cu_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 140.0
Number of bands     = 95
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Ru overlayer:

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---------------------------------
Dacapo calculation from Fe-subs/Ru-layer/Fe111-sub+Ru-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -12714.080317 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9144  0.0000  0.0000] 4.91
a1 [ 2.4572  4.2560  0.0000] 4.91
a2 [ 0.0000  0.0000  18.0252] 18.03
No stress calculated.
Volume = 377.01 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Fe  [  0.000  0.000  0.000]   4   0.439  Fe_us_gga_d2.1.8.pseudo
 1    Fe  [  2.457  0.000  0.000]   4   0.440  Fe_us_gga_d2.1.8.pseudo
 2    Fe  [  1.229  2.128  0.000]   4   0.440  Fe_us_gga_d2.1.8.pseudo
 3    Fe  [  3.686  2.128  0.000]   4   0.440  Fe_us_gga_d2.1.8.pseudo
 4    Fe  [  1.229  0.709  2.006]   3   0.477  Fe_us_gga_d2.1.8.pseudo
 5    Fe  [  3.686  0.709  2.006]   3   0.477  Fe_us_gga_d2.1.8.pseudo
 6    Fe  [  2.457  2.837  2.006]   3   0.478  Fe_us_gga_d2.1.8.pseudo
 7    Fe  [  4.914  2.837  2.006]   3   0.477  Fe_us_gga_d2.1.8.pseudo
 8    Fe  [  4.919  1.421  3.992]   2   0.044  Fe_us_gga_d2.1.8.pseudo
 9    Fe  [  2.462  1.421  3.992]   2   0.044  Fe_us_gga_d2.1.8.pseudo
10    Fe  [  6.148  3.549  3.992]   2   0.044  Fe_us_gga_d2.1.8.pseudo
11    Fe  [  3.691  3.549  3.992]   2   0.045  Fe_us_gga_d2.1.8.pseudo
12    Ru  [ -0.001 -0.000  6.142]   1   0.039  Ru_us_gga.pseudo
13    Ru  [  2.456 -0.000  6.142]   1   0.039  Ru_us_gga.pseudo
14    Ru  [  1.228  2.128  6.142]   1   0.039  Ru_us_gga.pseudo
15    Ru  [  3.685  2.127  6.142]   1   0.039  Ru_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 128.0
Number of bands     = 87
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```

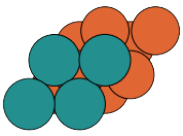

Rh overlayer:

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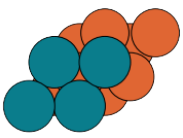
---------------------------------
Dacapo calculation from Fe-subs/Rh-layer/Fe111-sub+Rh-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -13375.030666 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9144  0.0000  0.0000] 4.91
a1 [ 2.4572  4.2560  0.0000] 4.91
a2 [ 0.0000  0.0000  18.0252] 18.03
No stress calculated.
Volume = 377.01 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Fe  [  0.000  0.000  0.000]   4   0.379  Fe_us_gga_d2.1.8.pseudo
 1    Fe  [  2.457  0.000  0.000]   4   0.379  Fe_us_gga_d2.1.8.pseudo
 2    Fe  [  1.229  2.128  0.000]   4   0.379  Fe_us_gga_d2.1.8.pseudo
 3    Fe  [  3.686  2.128  0.000]   4   0.379  Fe_us_gga_d2.1.8.pseudo
 4    Fe  [  1.229  0.709  2.006]   3   0.448  Fe_us_gga_d2.1.8.pseudo
 5    Fe  [  3.686  0.709  2.006]   3   0.448  Fe_us_gga_d2.1.8.pseudo
 6    Fe  [  2.457  2.837  2.006]   3   0.448  Fe_us_gga_d2.1.8.pseudo
 7    Fe  [  4.914  2.837  2.006]   3   0.448  Fe_us_gga_d2.1.8.pseudo
 8    Fe  [  4.917  1.420  3.971]   2   0.043  Fe_us_gga_d2.1.8.pseudo
 9    Fe  [  2.460  1.420  3.971]   2   0.043  Fe_us_gga_d2.1.8.pseudo
10    Fe  [  6.146  3.548  3.971]   2   0.043  Fe_us_gga_d2.1.8.pseudo
11    Fe  [  3.689  3.548  3.971]   2   0.043  Fe_us_gga_d2.1.8.pseudo
12    Rh  [  0.000  0.000  6.113]   1   0.021  Rh_us_gga_fl.pseudo
13    Rh  [  2.457  0.000  6.113]   1   0.021  Rh_us_gga_fl.pseudo
14    Rh  [  1.229  2.128  6.113]   1   0.021  Rh_us_gga_fl.pseudo
15    Rh  [  3.686  2.128  6.113]   1   0.021  Rh_us_gga_fl.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 132.0
Number of bands     = 89
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Pd overlayer:

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--------------------------------
Dacapo calculation from Fe-subs/Pd-layer/Fe111-sub+Pd-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -14175.829795 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9144  0.0000  0.0000] 4.91
a1 [ 2.4572  4.2560  0.0000] 4.91
a2 [ 0.0000  0.0000  18.0252] 18.03
No stress calculated.
Volume = 377.01 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Fe  [  0.000  0.000  0.000]   4   0.257  Fe_us_gga_d2.1.8.pseudo
 1    Fe  [  2.457  0.000  0.000]   4   0.257  Fe_us_gga_d2.1.8.pseudo
 2    Fe  [  1.229  2.128  0.000]   4   0.257  Fe_us_gga_d2.1.8.pseudo
 3    Fe  [  3.686  2.128  0.000]   4   0.257  Fe_us_gga_d2.1.8.pseudo
 4    Fe  [  1.229  0.709  2.006]   3   0.300  Fe_us_gga_d2.1.8.pseudo
 5    Fe  [  3.686  0.709  2.006]   3   0.300  Fe_us_gga_d2.1.8.pseudo
 6    Fe  [  2.457  2.837  2.006]   3   0.300  Fe_us_gga_d2.1.8.pseudo
 7    Fe  [  4.914  2.837  2.006]   3   0.300  Fe_us_gga_d2.1.8.pseudo
 8    Fe  [  4.915  1.419  3.926]   2   0.044  Fe_us_gga_d2.1.8.pseudo
 9    Fe  [  2.457  1.419  3.926]   2   0.044  Fe_us_gga_d2.1.8.pseudo
10    Fe  [  6.143  3.547  3.926]   2   0.044  Fe_us_gga_d2.1.8.pseudo
11    Fe  [  3.686  3.547  3.926]   2   0.044  Fe_us_gga_d2.1.8.pseudo
12    Pd  [  0.005  0.003  6.226]   1   0.033  046-Pd-gpe-n-6projectors-floc.uspp
13    Pd  [  2.462  0.003  6.226]   1   0.032  046-Pd-gpe-n-6projectors-floc.uspp
14    Pd  [  1.233  2.131  6.226]   1   0.032  046-Pd-gpe-n-6projectors-floc.uspp
15    Pd  [  3.691  2.131  6.226]   1   0.033  046-Pd-gpe-n-6projectors-floc.uspp

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 136.0
Number of bands     = 92
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
--------------------------------
```
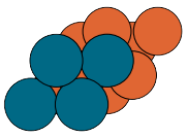
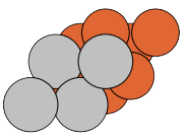



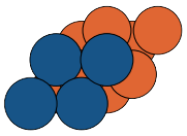
Ag overlayer:

```
---------------------------------
Dacapo calculation from Fe-subs/Ag-layer/Fe111-sub+Ag-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -15153.194149 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9144  0.0000  0.0000] 4.91
a1 [ 2.4572  4.2560  0.0000] 4.91
a2 [ 0.0000  0.0000  18.0252] 18.03
No stress calculated.
Volume = 377.01 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Fe  [  0.000  0.000  0.000]   4   0.317  Fe_us_gga_d2.1.8.pseudo
 1    Fe  [  2.457  0.000  0.000]   4   0.317  Fe_us_gga_d2.1.8.pseudo
 2    Fe  [  1.229  2.128  0.000]   4   0.317  Fe_us_gga_d2.1.8.pseudo
 3    Fe  [  3.686  2.128  0.000]   4   0.317  Fe_us_gga_d2.1.8.pseudo
 4    Fe  [  1.229  0.709  2.006]   3   0.393  Fe_us_gga_d2.1.8.pseudo
 5    Fe  [  3.686  0.709  2.006]   3   0.393  Fe_us_gga_d2.1.8.pseudo
 6    Fe  [  2.457  2.837  2.006]   3   0.393  Fe_us_gga_d2.1.8.pseudo
 7    Fe  [  4.914  2.837  2.006]   3   0.393  Fe_us_gga_d2.1.8.pseudo
 8    Fe  [  4.915  1.419  3.924]   2   0.009  Fe_us_gga_d2.1.8.pseudo
 9    Fe  [  2.458  1.419  3.924]   2   0.009  Fe_us_gga_d2.1.8.pseudo
10    Fe  [  6.144  3.547  3.924]   2   0.009  Fe_us_gga_d2.1.8.pseudo
11    Fe  [  3.687  3.547  3.924]   2   0.009  Fe_us_gga_d2.1.8.pseudo
12    Ag  [  0.001  0.001  6.406]   1   0.006  ag_us.pseudo
13    Ag  [  2.459  0.001  6.406]   1   0.006  ag_us.pseudo
14    Ag  [  1.230  2.129  6.406]   1   0.006  ag_us.pseudo
15    Ag  [  3.687  2.129  6.406]   1   0.006  ag_us.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 140.0
Number of bands     = 95
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



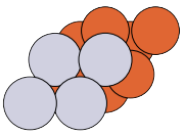
Ir overlayer:

```
---------------------------------
Dacapo calculation from Fe-subs/Ir-layer/Fe111-sub+Ir-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -14173.146988 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9144  0.0000  0.0000] 4.91
a1 [ 2.4572  4.2560  0.0000] 4.91
a2 [ 0.0000  0.0000  18.0252] 18.03
No stress calculated.
Volume = 377.01 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Fe  [  0.000  0.000  0.000]   4   0.371  Fe_us_gga_d2.1.8.pseudo
 1    Fe  [  2.457  0.000  0.000]   4   0.371  Fe_us_gga_d2.1.8.pseudo
 2    Fe  [  1.229  2.128  0.000]   4   0.371  Fe_us_gga_d2.1.8.pseudo
 3    Fe  [  3.686  2.128  0.000]   4   0.371  Fe_us_gga_d2.1.8.pseudo
 4    Fe  [  1.229  0.709  2.006]   3   0.428  Fe_us_gga_d2.1.8.pseudo
 5    Fe  [  3.686  0.709  2.006]   3   0.428  Fe_us_gga_d2.1.8.pseudo
 6    Fe  [  2.457  2.837  2.006]   3   0.428  Fe_us_gga_d2.1.8.pseudo
 7    Fe  [  4.914  2.837  2.006]   3   0.428  Fe_us_gga_d2.1.8.pseudo
 8    Fe  [  4.917  1.420  3.981]   2   0.011  Fe_us_gga_d2.1.8.pseudo
 9    Fe  [  2.460  1.420  3.981]   2   0.011  Fe_us_gga_d2.1.8.pseudo
10    Fe  [  6.145  3.548  3.981]   2   0.011  Fe_us_gga_d2.1.8.pseudo
11    Fe  [  3.688  3.548  3.981]   2   0.011  Fe_us_gga_d2.1.8.pseudo
12    Ir  [  0.000  0.000  6.128]   1   0.003  ir_us_gga_flocal.pseudo
13    Ir  [  2.457  0.000  6.128]   1   0.003  ir_us_gga_flocal.pseudo
14    Ir  [  1.229  2.128  6.128]   1   0.003  ir_us_gga_flocal.pseudo
15    Ir  [  3.686  2.128  6.128]   1   0.003  ir_us_gga_flocal.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 132.0
Number of bands     = 89
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



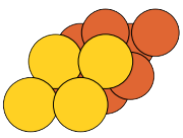
Pt overlayer:

```
---------------------------------
Dacapo calculation from Fe-subs/Pt-layer/Fe111-sub+Pt-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -14825.822225 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9144  0.0000  0.0000] 4.91
a1 [ 2.4572  4.2560  0.0000] 4.91
a2 [ 0.0000  0.0000  18.0252] 18.03
No stress calculated.
Volume = 377.01 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Fe  [  0.000  0.000  0.000]   4   0.233  Fe_us_gga_d2.1.8.pseudo
 1    Fe  [  2.457  0.000  0.000]   4   0.233  Fe_us_gga_d2.1.8.pseudo
 2    Fe  [  1.229  2.128  0.000]   4   0.233  Fe_us_gga_d2.1.8.pseudo
 3    Fe  [  3.686  2.128  0.000]   4   0.233  Fe_us_gga_d2.1.8.pseudo
 4    Fe  [  1.229  0.709  2.006]   3   0.281  Fe_us_gga_d2.1.8.pseudo
 5    Fe  [  3.686  0.709  2.006]   3   0.281  Fe_us_gga_d2.1.8.pseudo
 6    Fe  [  2.457  2.837  2.006]   3   0.281  Fe_us_gga_d2.1.8.pseudo
 7    Fe  [  4.914  2.837  2.006]   3   0.281  Fe_us_gga_d2.1.8.pseudo
 8    Fe  [  4.914  1.419  3.923]   2   0.003  Fe_us_gga_d2.1.8.pseudo
 9    Fe  [  2.457  1.419  3.923]   2   0.003  Fe_us_gga_d2.1.8.pseudo
10    Fe  [  6.143  3.547  3.923]   2   0.003  Fe_us_gga_d2.1.8.pseudo
11    Fe  [  3.686  3.547  3.923]   2   0.003  Fe_us_gga_d2.1.8.pseudo
12    Pt  [  0.002  0.001  6.254]   1   0.010  pt_us_gga.pseudo
13    Pt  [  2.459  0.001  6.254]   1   0.010  pt_us_gga.pseudo
14    Pt  [  1.231  2.129  6.254]   1   0.010  pt_us_gga.pseudo
15    Pt  [  3.688  2.129  6.254]   1   0.010  pt_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 136.0
Number of bands     = 92
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Au overlayer:

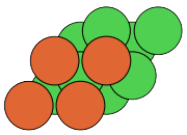
```
---------------------------------
Dacapo calculation from Fe-subs/Au-layer/Fe111-sub+Au-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -15542.130801 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9144  0.0000  0.0000] 4.91
a1 [ 2.4572  4.2560  0.0000] 4.91
a2 [ 0.0000  0.0000  18.0252] 18.03
No stress calculated.
Volume = 377.01 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Fe  [  0.000  0.000  0.000]   4   0.302  Fe_us_gga_d2.1.8.pseudo
 1    Fe  [  2.457  0.000  0.000]   4   0.303  Fe_us_gga_d2.1.8.pseudo
 2    Fe  [  1.229  2.128  0.000]   4   0.303  Fe_us_gga_d2.1.8.pseudo
 3    Fe  [  3.686  2.128  0.000]   4   0.302  Fe_us_gga_d2.1.8.pseudo
 4    Fe  [  1.229  0.709  2.006]   3   0.350  Fe_us_gga_d2.1.8.pseudo
 5    Fe  [  3.686  0.709  2.006]   3   0.350  Fe_us_gga_d2.1.8.pseudo
 6    Fe  [  2.457  2.837  2.006]   3   0.350  Fe_us_gga_d2.1.8.pseudo
 7    Fe  [  4.914  2.837  2.006]   3   0.350  Fe_us_gga_d2.1.8.pseudo
 8    Fe  [  4.912  1.417  3.923]   2   0.015  Fe_us_gga_d2.1.8.pseudo
 9    Fe  [  2.454  1.417  3.923]   2   0.016  Fe_us_gga_d2.1.8.pseudo
10    Fe  [  6.140  3.545  3.923]   2   0.016  Fe_us_gga_d2.1.8.pseudo
11    Fe  [  3.683  3.545  3.923]   2   0.015  Fe_us_gga_d2.1.8.pseudo
12    Au  [  0.004  0.002  6.542]   1   0.012  Au_us_gga.pseudo
13    Au  [  2.461  0.002  6.542]   1   0.013  Au_us_gga.pseudo
14    Au  [  1.233  2.130  6.542]   1   0.012  Au_us_gga.pseudo
15    Au  [  3.690  2.130  6.542]   1   0.012  Au_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 140.0
Number of bands     = 95
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Structures with Ni as the substrate:

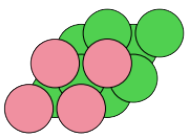
Fe overlayer:

```
--------------------------------
Dacapo calculation from Ni-subs/Fe-layer/Ni111-subs+Fe-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -18996.572545 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9802  0.0000  0.0000] 4.98
a1 [ 2.4901  4.3129  0.0000] 4.98
a2 [ 0.0000  0.0000  18.1326] 18.13
No stress calculated.
Volume = 389.47 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ni  [  0.000  0.000  0.000]   4   0.093  Ni_us_gga.pseudo
 1    Ni  [  2.490  0.000  0.000]   4   0.093  Ni_us_gga.pseudo
 2    Ni  [  1.245  2.156  0.000]   4   0.093  Ni_us_gga.pseudo
 3    Ni  [  3.735  2.156  0.000]   4   0.093  Ni_us_gga.pseudo
 4    Ni  [  1.245  0.719  2.033]   3   0.041  Ni_us_gga.pseudo
 5    Ni  [  3.735  0.719  2.033]   3   0.041  Ni_us_gga.pseudo
 6    Ni  [  2.490  2.875  2.033]   3   0.041  Ni_us_gga.pseudo
 7    Ni  [  4.980  2.875  2.033]   3   0.041  Ni_us_gga.pseudo
 8    Ni  [  4.980  1.437  4.105]   2   0.023  Ni_us_gga.pseudo
 9    Ni  [  2.490  1.437  4.105]   2   0.023  Ni_us_gga.pseudo
10    Ni  [  6.225  3.594  4.105]   2   0.022  Ni_us_gga.pseudo
11    Ni  [  3.735  3.594  4.105]   2   0.023  Ni_us_gga.pseudo
12    Fe  [  0.000  0.000  6.069]   1   0.045  Fe_us_gga_d2.1.8.pseudo
13    Fe  [  2.490  0.000  6.069]   1   0.045  Fe_us_gga_d2.1.8.pseudo
14    Fe  [  1.245  2.157  6.069]   1   0.045  Fe_us_gga_d2.1.8.pseudo
15    Fe  [  3.735  2.157  6.069]   1   0.045  Fe_us_gga_d2.1.8.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 152.0
Number of bands     = 102
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
--------------------------------
```



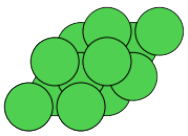
Co overlayer:

```
---------------------------------
Dacapo calculation from Ni-subs/Co-layer/Ni111-subs+Co-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -20033.631085 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9802  0.0000  0.0000] 4.98
a1 [ 2.4901  4.3129  0.0000] 4.98
a2 [ 0.0000  0.0000  18.1326] 18.13
No stress calculated.
Volume = 389.47 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ni  [  0.000  0.000  0.000]   4   0.105  Ni_us_gga.pseudo
 1    Ni  [  2.490  0.000  0.000]   4   0.105  Ni_us_gga.pseudo
 2    Ni  [  1.245  2.156  0.000]   4   0.105  Ni_us_gga.pseudo
 3    Ni  [  3.735  2.156  0.000]   4   0.105  Ni_us_gga.pseudo
 4    Ni  [  1.245  0.719  2.033]   3   0.028  Ni_us_gga.pseudo
 5    Ni  [  3.735  0.719  2.033]   3   0.028  Ni_us_gga.pseudo
 6    Ni  [  2.490  2.875  2.033]   3   0.028  Ni_us_gga.pseudo
 7    Ni  [  4.980  2.875  2.033]   3   0.028  Ni_us_gga.pseudo
 8    Ni  [  4.980  1.438  4.095]   2   0.036  Ni_us_gga.pseudo
 9    Ni  [  2.490  1.438  4.095]   2   0.036  Ni_us_gga.pseudo
10    Ni  [  6.225  3.594  4.095]   2   0.036  Ni_us_gga.pseudo
11    Ni  [  3.735  3.594  4.095]   2   0.036  Ni_us_gga.pseudo
12    Co  [ -0.000 -0.000  6.075]   1   0.035  Co_us_gga.pseudo
13    Co  [  2.490 -0.000  6.075]   1   0.035  Co_us_gga.pseudo
14    Co  [  1.245  2.156  6.075]   1   0.035  Co_us_gga.pseudo
15    Co  [  3.735  2.156  6.075]   1   0.035  Co_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 156.0
Number of bands     = 105
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



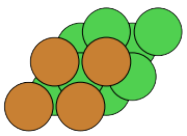
Ni overlayer:

```
---------------------------------
Dacapo calculation from Ni-subs/Ni-layer/Ni111-subs+Ni-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -20894.216183 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9802  0.0000  0.0000] 4.98
a1 [ 2.4901  4.3129  0.0000] 4.98
a2 [ 0.0000  0.0000  18.1326] 18.13
No stress calculated.
Volume = 389.47 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ni  [  0.000  0.000  0.000]   4   0.111  Ni_us_gga.pseudo
 1    Ni  [  2.490  0.000  0.000]   4   0.111  Ni_us_gga.pseudo
 2    Ni  [  1.245  2.156  0.000]   4   0.111  Ni_us_gga.pseudo
 3    Ni  [  3.735  2.156  0.000]   4   0.111  Ni_us_gga.pseudo
 4    Ni  [  1.245  0.719  2.033]   3   0.088  Ni_us_gga.pseudo
 5    Ni  [  3.735  0.719  2.033]   3   0.088  Ni_us_gga.pseudo
 6    Ni  [  2.490  2.875  2.033]   3   0.088  Ni_us_gga.pseudo
 7    Ni  [  4.980  2.875  2.033]   3   0.088  Ni_us_gga.pseudo
 8    Ni  [  4.980  1.438  4.076]   2   0.007  Ni_us_gga.pseudo
 9    Ni  [  2.490  1.438  4.076]   2   0.007  Ni_us_gga.pseudo
10    Ni  [  6.225  3.594  4.076]   2   0.007  Ni_us_gga.pseudo
11    Ni  [  3.735  3.594  4.076]   2   0.006  Ni_us_gga.pseudo
12    Ni  [ -0.000 -0.000  6.092]   1   0.001  Ni_us_gga.pseudo
13    Ni  [  2.490 -0.000  6.092]   1   0.001  Ni_us_gga.pseudo
14    Ni  [  1.245  2.156  6.092]   1   0.001  Ni_us_gga.pseudo
15    Ni  [  3.735  2.156  6.092]   1   0.001  Ni_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 160.0
Number of bands     = 108
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



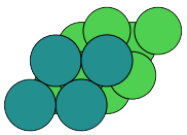
Cu overlayer:

```
---------------------------------
Dacapo calculation from Ni-subs/Cu-layer/Ni111-subs+Cu-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -22372.399656 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9802  0.0000  0.0000] 4.98
a1 [ 2.4901  4.3129  0.0000] 4.98
a2 [ 0.0000  0.0000  18.1326] 18.13
No stress calculated.
Volume = 389.47 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ni  [  0.000  0.000  0.000]   4   0.105  Ni_us_gga.pseudo
 1    Ni  [  2.490  0.000  0.000]   4   0.105  Ni_us_gga.pseudo
 2    Ni  [  1.245  2.156  0.000]   4   0.105  Ni_us_gga.pseudo
 3    Ni  [  3.735  2.156  0.000]   4   0.105  Ni_us_gga.pseudo
 4    Ni  [  1.245  0.719  2.033]   3   0.234  Ni_us_gga.pseudo
 5    Ni  [  3.735  0.719  2.033]   3   0.234  Ni_us_gga.pseudo
 6    Ni  [  2.490  2.875  2.033]   3   0.234  Ni_us_gga.pseudo
 7    Ni  [  4.980  2.875  2.033]   3   0.234  Ni_us_gga.pseudo
 8    Ni  [  4.980  1.438  4.050]   2   0.017  Ni_us_gga.pseudo
 9    Ni  [  2.490  1.438  4.050]   2   0.018  Ni_us_gga.pseudo
10    Ni  [  6.225  3.594  4.050]   2   0.018  Ni_us_gga.pseudo
11    Ni  [  3.735  3.594  4.050]   2   0.018  Ni_us_gga.pseudo
12    Cu  [ -0.000 -0.000  6.118]   1   0.014  Cu_us_gga.pseudo
13    Cu  [  2.490 -0.000  6.118]   1   0.014  Cu_us_gga.pseudo
14    Cu  [  1.245  2.156  6.118]   1   0.014  Cu_us_gga.pseudo
15    Cu  [  3.735  2.156  6.118]   1   0.014  Cu_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 164.0
Number of bands     = 110
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



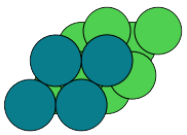
Ru overlayer:

```
---------------------------------
Dacapo calculation from Ni-subs/Ru-layer/Ni111-subs+Ru-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -18404.108955 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9802  0.0000  0.0000] 4.98
a1 [ 2.4901  4.3129  0.0000] 4.98
a2 [ 0.0000  0.0000  18.1326] 18.13
No stress calculated.
Volume = 389.47 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ni  [  0.000  0.000  0.000]   4   0.083  Ni_us_gga.pseudo
 1    Ni  [  2.490  0.000  0.000]   4   0.083  Ni_us_gga.pseudo
 2    Ni  [  1.245  2.156  0.000]   4   0.083  Ni_us_gga.pseudo
 3    Ni  [  3.735  2.156  0.000]   4   0.083  Ni_us_gga.pseudo
 4    Ni  [  1.245  0.719  2.033]   3   0.119  Ni_us_gga.pseudo
 5    Ni  [  3.735  0.719  2.033]   3   0.119  Ni_us_gga.pseudo
 6    Ni  [  2.490  2.875  2.033]   3   0.119  Ni_us_gga.pseudo
 7    Ni  [  4.980  2.875  2.033]   3   0.119  Ni_us_gga.pseudo
 8    Ni  [  4.979  1.437  4.068]   2   0.012  Ni_us_gga.pseudo
 9    Ni  [  2.488  1.437  4.068]   2   0.012  Ni_us_gga.pseudo
10    Ni  [  6.224  3.593  4.068]   2   0.012  Ni_us_gga.pseudo
11    Ni  [  3.734  3.593  4.068]   2   0.012  Ni_us_gga.pseudo
12    Ru  [  0.000  0.000  6.213]   1   0.025  Ru_us_gga.pseudo
13    Ru  [  2.491  0.000  6.213]   1   0.025  Ru_us_gga.pseudo
14    Ru  [  1.246  2.157  6.213]   1   0.025  Ru_us_gga.pseudo
15    Ru  [  3.736  2.157  6.213]   1   0.025  Ru_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 152.0
Number of bands     = 102
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



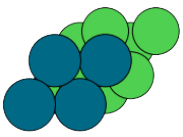
Rh overlayer:

```
--------------------------------
Dacapo calculation from Ni-subs/Rh-layer/Ni111-subs+Rh-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19064.481391 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9802  0.0000  0.0000] 4.98
a1 [ 2.4901  4.3129  0.0000] 4.98
a2 [ 0.0000  0.0000  18.1326] 18.13
No stress calculated.
Volume = 389.47 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ni  [  0.000  0.000  0.000]   4   0.100  Ni_us_gga.pseudo
 1    Ni  [  2.490  0.000  0.000]   4   0.100  Ni_us_gga.pseudo
 2    Ni  [  1.245  2.156  0.000]   4   0.100  Ni_us_gga.pseudo
 3    Ni  [  3.735  2.156  0.000]   4   0.100  Ni_us_gga.pseudo
 4    Ni  [  1.245  0.719  2.033]   3   0.093  Ni_us_gga.pseudo
 5    Ni  [  3.735  0.719  2.033]   3   0.093  Ni_us_gga.pseudo
 6    Ni  [  2.490  2.875  2.033]   3   0.093  Ni_us_gga.pseudo
 7    Ni  [  4.980  2.875  2.033]   3   0.093  Ni_us_gga.pseudo
 8    Ni  [  4.981  1.438  4.075]   2   0.004  Ni_us_gga.pseudo
 9    Ni  [  2.490  1.438  4.075]   2   0.004  Ni_us_gga.pseudo
10    Ni  [  6.226  3.594  4.075]   2   0.004  Ni_us_gga.pseudo
11    Ni  [  3.735  3.594  4.075]   2   0.004  Ni_us_gga.pseudo
12    Rh  [ -0.001 -0.001  6.230]   1   0.005  Rh_us_gga_fl.pseudo
13    Rh  [  2.489 -0.001  6.230]   1   0.005  Rh_us_gga_fl.pseudo
14    Rh  [  1.244  2.156  6.230]   1   0.005  Rh_us_gga_fl.pseudo
15    Rh  [  3.734  2.156  6.230]   1   0.005  Rh_us_gga_fl.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 156.0
Number of bands     = 105
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
--------------------------------
```



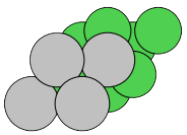
Pd overlayer:

```
---------------------------------
Dacapo calculation from Ni-subs/Pd-layer/Ni111-subs+Pd-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19865.797167 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9802  0.0000  0.0000] 4.98
a1 [ 2.4901  4.3129  0.0000] 4.98
a2 [ 0.0000  0.0000  18.1326] 18.13
No stress calculated.
Volume = 389.47 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ni  [  0.000  0.000  0.000]   4   0.107  Ni_us_gga.pseudo
 1    Ni  [  2.490  0.000  0.000]   4   0.107  Ni_us_gga.pseudo
 2    Ni  [  1.245  2.156  0.000]   4   0.107  Ni_us_gga.pseudo
 3    Ni  [  3.735  2.156  0.000]   4   0.107  Ni_us_gga.pseudo
 4    Ni  [  1.245  0.719  2.033]   3   0.271  Ni_us_gga.pseudo
 5    Ni  [  3.735  0.719  2.033]   3   0.271  Ni_us_gga.pseudo
 6    Ni  [  2.490  2.875  2.033]   3   0.271  Ni_us_gga.pseudo
 7    Ni  [  4.980  2.875  2.033]   3   0.271  Ni_us_gga.pseudo
 8    Ni  [  4.980  1.438  4.032]   2   0.045  Ni_us_gga.pseudo
 9    Ni  [  2.490  1.438  4.032]   2   0.045  Ni_us_gga.pseudo
10    Ni  [  6.225  3.594  4.032]   2   0.045  Ni_us_gga.pseudo
11    Ni  [  3.735  3.594  4.032]   2   0.045  Ni_us_gga.pseudo
12    Pd  [  0.007  0.004  6.280]   1   0.037  046-Pd-gpe-n-6projectors-floc.uspp
13    Pd  [  2.497  0.004  6.280]   1   0.037  046-Pd-gpe-n-6projectors-floc.uspp
14    Pd  [  1.252  2.160  6.280]   1   0.037  046-Pd-gpe-n-6projectors-floc.uspp
15    Pd  [  3.742  2.160  6.280]   1   0.037  046-Pd-gpe-n-6projectors-floc.uspp

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 160.0
Number of bands     = 108
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



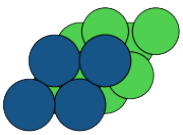
Ag overlayer:

```
---------------------------------
Dacapo calculation from Ni-subs/Ag-layer/Ni111-subs+Ag-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -20843.947566 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9802  0.0000  0.0000] 4.98
a1 [ 2.4901  4.3129  0.0000] 4.98
a2 [ 0.0000  0.0000  18.1326] 18.13
No stress calculated.
Volume = 389.47 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ni  [  0.000  0.000  0.000]   4   0.102  Ni_us_gga.pseudo
 1    Ni  [  2.490  0.000  0.000]   4   0.102  Ni_us_gga.pseudo
 2    Ni  [  1.245  2.156  0.000]   4   0.102  Ni_us_gga.pseudo
 3    Ni  [  3.735  2.156  0.000]   4   0.102  Ni_us_gga.pseudo
 4    Ni  [  1.245  0.719  2.033]   3   0.173  Ni_us_gga.pseudo
 5    Ni  [  3.735  0.719  2.033]   3   0.173  Ni_us_gga.pseudo
 6    Ni  [  2.490  2.875  2.033]   3   0.173  Ni_us_gga.pseudo
 7    Ni  [  4.980  2.875  2.033]   3   0.173  Ni_us_gga.pseudo
 8    Ni  [  4.979  1.437  4.055]   2   0.003  Ni_us_gga.pseudo
 9    Ni  [  2.488  1.437  4.055]   2   0.003  Ni_us_gga.pseudo
10    Ni  [  6.224  3.593  4.055]   2   0.003  Ni_us_gga.pseudo
11    Ni  [  3.734  3.593  4.055]   2   0.002  Ni_us_gga.pseudo
12    Ag  [ -0.002 -0.001  6.436]   1   0.015  ag_us.pseudo
13    Ag  [  2.488 -0.001  6.436]   1   0.015  ag_us.pseudo
14    Ag  [  1.243  2.156  6.436]   1   0.015  ag_us.pseudo
15    Ag  [  3.733  2.156  6.436]   1   0.015  ag_us.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 164.0
Number of bands     = 110
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



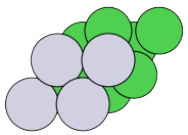
Ir overlayer:

```
---------------------------------
Dacapo calculation from Ni-subs/Ir-layer/Ni111-subs+Ir-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19862.695886 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9802  0.0000  0.0000] 4.98
a1 [ 2.4901  4.3129  0.0000] 4.98
a2 [ 0.0000  0.0000  18.1326] 18.13
No stress calculated.
Volume = 389.47 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ni  [  0.000  0.000  0.000]   4   0.118  Ni_us_gga.pseudo
 1    Ni  [  2.490  0.000  0.000]   4   0.118  Ni_us_gga.pseudo
 2    Ni  [  1.245  2.156  0.000]   4   0.118  Ni_us_gga.pseudo
 3    Ni  [  3.735  2.156  0.000]   4   0.118  Ni_us_gga.pseudo
 4    Ni  [  1.245  0.719  2.033]   3   0.093  Ni_us_gga.pseudo
 5    Ni  [  3.735  0.719  2.033]   3   0.093  Ni_us_gga.pseudo
 6    Ni  [  2.490  2.875  2.033]   3   0.093  Ni_us_gga.pseudo
 7    Ni  [  4.980  2.875  2.033]   3   0.093  Ni_us_gga.pseudo
 8    Ni  [  4.980  1.437  4.083]   2   0.022  Ni_us_gga.pseudo
 9    Ni  [  2.490  1.437  4.083]   2   0.022  Ni_us_gga.pseudo
10    Ni  [  6.225  3.594  4.083]   2   0.022  Ni_us_gga.pseudo
11    Ni  [  3.735  3.594  4.083]   2   0.022  Ni_us_gga.pseudo
12    Ir  [ -0.002 -0.001  6.243]   1   0.024  ir_us_gga_flocal.pseudo
13    Ir  [  2.489 -0.001  6.243]   1   0.024  ir_us_gga_flocal.pseudo
14    Ir  [  1.244  2.156  6.243]   1   0.024  ir_us_gga_flocal.pseudo
15    Ir  [  3.734  2.156  6.243]   1   0.024  ir_us_gga_flocal.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 156.0
Number of bands     = 105
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



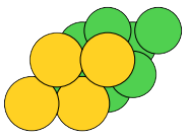
Pt overlayer:

```
---------------------------------
Dacapo calculation from Ni-subs/Pt-layer/Ni111-subs+Pt-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -20516.166824 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9802  0.0000  0.0000] 4.98
a1 [ 2.4901  4.3129  0.0000] 4.98
a2 [ 0.0000  0.0000  18.1326] 18.13
No stress calculated.
Volume = 389.47 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ni  [  0.000  0.000  0.000]   4   0.123  Ni_us_gga.pseudo
 1    Ni  [  2.490  0.000  0.000]   4   0.123  Ni_us_gga.pseudo
 2    Ni  [  1.245  2.156  0.000]   4   0.123  Ni_us_gga.pseudo
 3    Ni  [  3.735  2.156  0.000]   4   0.123  Ni_us_gga.pseudo
 4    Ni  [  1.245  0.719  2.033]   3   0.277  Ni_us_gga.pseudo
 5    Ni  [  3.735  0.719  2.033]   3   0.277  Ni_us_gga.pseudo
 6    Ni  [  2.490  2.875  2.033]   3   0.277  Ni_us_gga.pseudo
 7    Ni  [  4.980  2.875  2.033]   3   0.277  Ni_us_gga.pseudo
 8    Ni  [  4.979  1.437  4.030]   2   0.012  Ni_us_gga.pseudo
 9    Ni  [  2.489  1.437  4.030]   2   0.012  Ni_us_gga.pseudo
10    Ni  [  6.224  3.593  4.030]   2   0.012  Ni_us_gga.pseudo
11    Ni  [  3.734  3.593  4.030]   2   0.012  Ni_us_gga.pseudo
12    Pt  [  0.001  0.000  6.319]   1   0.043  pt_us_gga.pseudo
13    Pt  [  2.491  0.000  6.319]   1   0.043  pt_us_gga.pseudo
14    Pt  [  1.246  2.157  6.319]   1   0.043  pt_us_gga.pseudo
15    Pt  [  3.736  2.157  6.319]   1   0.043  pt_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 160.0
Number of bands     = 108
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Au overlayer:

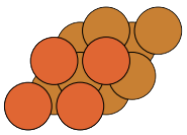
```
---------------------------------
Dacapo calculation from Ni-subs/Au-layer/Ni111-subs+Au-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -21233.236976 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9802  0.0000  0.0000] 4.98
a1 [ 2.4901  4.3129  0.0000] 4.98
a2 [ 0.0000  0.0000  18.1326] 18.13
No stress calculated.
Volume = 389.47 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ni  [  0.000  0.000  0.000]   4   0.122  Ni_us_gga.pseudo
 1    Ni  [  2.490  0.000  0.000]   4   0.122  Ni_us_gga.pseudo
 2    Ni  [  1.245  2.156  0.000]   4   0.122  Ni_us_gga.pseudo
 3    Ni  [  3.735  2.156  0.000]   4   0.122  Ni_us_gga.pseudo
 4    Ni  [  1.245  0.719  2.033]   3   0.181  Ni_us_gga.pseudo
 5    Ni  [  3.735  0.719  2.033]   3   0.181  Ni_us_gga.pseudo
 6    Ni  [  2.490  2.875  2.033]   3   0.181  Ni_us_gga.pseudo
 7    Ni  [  4.980  2.875  2.033]   3   0.182  Ni_us_gga.pseudo
 8    Ni  [  4.980  1.438  4.052]   2   0.027  Ni_us_gga.pseudo
 9    Ni  [  2.490  1.438  4.052]   2   0.027  Ni_us_gga.pseudo
10    Ni  [  6.225  3.594  4.052]   2   0.027  Ni_us_gga.pseudo
11    Ni  [  3.735  3.594  4.052]   2   0.027  Ni_us_gga.pseudo
12    Au  [ -0.002 -0.001  6.563]   1   0.016  Au_us_gga.pseudo
13    Au  [  2.488 -0.001  6.563]   1   0.016  Au_us_gga.pseudo
14    Au  [  1.243  2.155  6.563]   1   0.016  Au_us_gga.pseudo
15    Au  [  3.733  2.155  6.563]   1   0.016  Au_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 164.0
Number of bands     = 110
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Structures with Cu as the substrate:

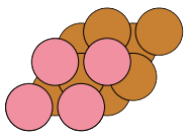
Fe overlayer:

```
--------------------------------
Dacapo calculation from Cu-subs/Fe-layer/Cu111-subs+Fe-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -23427.724373 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.003  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.003  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.003  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.003  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.238  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.238  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.238  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.238  Cu_us_gga.pseudo
 8    Cu  [  5.146  1.485  4.254]   2   0.012  Cu_us_gga.pseudo
 9    Cu  [  2.572  1.485  4.254]   2   0.012  Cu_us_gga.pseudo
10    Cu  [  6.433  3.714  4.254]   2   0.012  Cu_us_gga.pseudo
11    Cu  [  3.859  3.714  4.254]   2   0.012  Cu_us_gga.pseudo
12    Fe  [  0.001  0.001  6.303]   1   0.009  Fe_us_gga_d2.1.8.pseudo
13    Fe  [  2.575  0.001  6.303]   1   0.009  Fe_us_gga_d2.1.8.pseudo
14    Fe  [  1.288  2.230  6.303]   1   0.009  Fe_us_gga_d2.1.8.pseudo
15    Fe  [  3.862  2.230  6.303]   1   0.009  Fe_us_gga_d2.1.8.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 164.0
Number of bands     = 110
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
--------------------------------
```



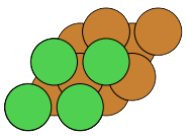
Co overlayer:

```
---------------------------------
Dacapo calculation from Cu-subs/Co-layer/Cu111-subs+Co-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -24465.455678 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.004  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.004  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.004  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.004  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.213  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.213  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.213  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.213  Cu_us_gga.pseudo
 8    Cu  [  5.147  1.486  4.241]   2   0.041  Cu_us_gga.pseudo
 9    Cu  [  2.573  1.486  4.241]   2   0.041  Cu_us_gga.pseudo
10    Cu  [  6.434  3.715  4.241]   2   0.041  Cu_us_gga.pseudo
11    Cu  [  3.860  3.715  4.241]   2   0.041  Cu_us_gga.pseudo
12    Co  [  0.000  0.000  6.268]   1   0.020  Co_us_gga.pseudo
13    Co  [  2.574  0.000  6.268]   1   0.020  Co_us_gga.pseudo
14    Co  [  1.287  2.229  6.268]   1   0.020  Co_us_gga.pseudo
15    Co  [  3.861  2.229  6.268]   1   0.020  Co_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 168.0
Number of bands     = 113
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



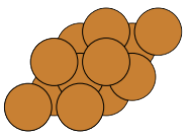
Ni overlayer:

```
---------------------------------
Dacapo calculation from Cu-subs/Ni-layer/Cu111-subs+Ni-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -25326.887351 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.009  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.009  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.009  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.009  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.239  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.239  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.239  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.239  Cu_us_gga.pseudo
 8    Cu  [  5.147  1.486  4.243]   2   0.027  Cu_us_gga.pseudo
 9    Cu  [  2.573  1.486  4.243]   2   0.027  Cu_us_gga.pseudo
10    Cu  [  6.434  3.715  4.243]   2   0.027  Cu_us_gga.pseudo
11    Cu  [  3.860  3.715  4.243]   2   0.027  Cu_us_gga.pseudo
12    Ni  [  0.000  0.000  6.266]   1   0.021  Ni_us_gga.pseudo
13    Ni  [  2.574  0.000  6.266]   1   0.021  Ni_us_gga.pseudo
14    Ni  [  1.287  2.229  6.266]   1   0.021  Ni_us_gga.pseudo
15    Ni  [  3.861  2.229  6.266]   1   0.021  Ni_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 172.0
Number of bands     = 115
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



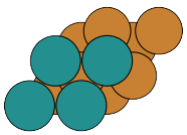
Cu overlayer:

```
---------------------------------
Dacapo calculation from Cu-subs/Cu-layer/Cu111-subs+Cu-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -26805.237724 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.003  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.003  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.003  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.003  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.171  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.171  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.171  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.171  Cu_us_gga.pseudo
 8    Cu  [  5.147  1.486  4.217]   2   0.005  Cu_us_gga.pseudo
 9    Cu  [  2.574  1.486  4.217]   2   0.006  Cu_us_gga.pseudo
10    Cu  [  6.434  3.715  4.217]   2   0.006  Cu_us_gga.pseudo
11    Cu  [  3.861  3.715  4.217]   2   0.006  Cu_us_gga.pseudo
12    Cu  [ -0.000 -0.000  6.290]   1   0.026  Cu_us_gga.pseudo
13    Cu  [  2.573 -0.000  6.290]   1   0.026  Cu_us_gga.pseudo
14    Cu  [  1.287  2.229  6.290]   1   0.026  Cu_us_gga.pseudo
15    Cu  [  3.860  2.229  6.290]   1   0.026  Cu_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 176.0
Number of bands     = 118
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



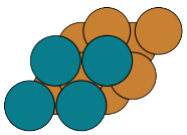
Ru overlayer:

```
---------------------------------
Dacapo calculation from Cu-subs/Ru-layer/Cu111-subs+Ru-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -22837.210288 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.003  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.003  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.003  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.003  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.044  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.044  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.044  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.044  Cu_us_gga.pseudo
 8    Cu  [  5.147  1.486  4.155]   2   0.020  Cu_us_gga.pseudo
 9    Cu  [  2.573  1.486  4.155]   2   0.020  Cu_us_gga.pseudo
10    Cu  [  6.434  3.715  4.155]   2   0.020  Cu_us_gga.pseudo
11    Cu  [  3.860  3.715  4.155]   2   0.020  Cu_us_gga.pseudo
12    Ru  [  0.000  0.000  6.361]   1   0.023  Ru_us_gga.pseudo
13    Ru  [  2.574  0.000  6.361]   1   0.023  Ru_us_gga.pseudo
14    Ru  [  1.287  2.229  6.361]   1   0.023  Ru_us_gga.pseudo
15    Ru  [  3.861  2.229  6.361]   1   0.023  Ru_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 164.0
Number of bands     = 110
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



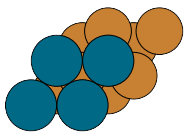
Rh overlayer:

```
---------------------------------
Dacapo calculation from Cu-subs/Rh-layer/Cu111-subs+Rh-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -23497.822496 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.003  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.003  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.003  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.003  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.261  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.261  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.261  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.261  Cu_us_gga.pseudo
 8    Cu  [  5.135  1.479  4.248]   2   0.020  Cu_us_gga.pseudo
 9    Cu  [  2.561  1.479  4.248]   2   0.021  Cu_us_gga.pseudo
10    Cu  [  6.422  3.708  4.248]   2   0.021  Cu_us_gga.pseudo
11    Cu  [  3.848  3.708  4.248]   2   0.021  Cu_us_gga.pseudo
12    Rh  [  0.006  0.004  6.443]   1   0.006  Rh_us_gga_fl.pseudo
13    Rh  [  2.580  0.004  6.443]   1   0.007  Rh_us_gga_fl.pseudo
14    Rh  [  1.293  2.233  6.443]   1   0.007  Rh_us_gga_fl.pseudo
15    Rh  [  3.867  2.233  6.443]   1   0.006  Rh_us_gga_fl.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 168.0
Number of bands     = 113
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



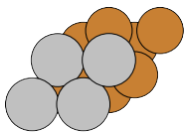
Pd overlayer:

```
---------------------------------
Dacapo calculation from Cu-subs/Pd-layer/Cu111-subs+Pd-overlayer-relaxed-DOS.nc
status = new
version = ifc ser v2-3-3
Energy = -24300.354993 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.021  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.021  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.021  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.021  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.257  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.257  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.257  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.257  Cu_us_gga.pseudo
 8    Cu  [  5.146  1.485  4.235]   2   0.015  Cu_us_gga.pseudo
 9    Cu  [  2.572  1.485  4.235]   2   0.015  Cu_us_gga.pseudo
10    Cu  [  6.433  3.714  4.235]   2   0.015  Cu_us_gga.pseudo
11    Cu  [  3.859  3.714  4.235]   2   0.015  Cu_us_gga.pseudo
12    Pd  [  0.011  0.006  6.451]   1   0.047  046-Pd-gpe-n-6projectors-floc.uspp
13    Pd  [  2.585  0.006  6.451]   1   0.047  046-Pd-gpe-n-6projectors-floc.uspp
14    Pd  [  1.298  2.235  6.451]   1   0.047  046-Pd-gpe-n-6projectors-floc.uspp
15    Pd  [  3.872  2.235  6.451]   1   0.047  046-Pd-gpe-n-6projectors-floc.uspp

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 172.0
Number of bands     = 115
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



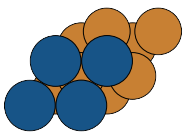
Ag overlayer:

```
---------------------------------
Dacapo calculation from Cu-subs/Ag-layer/Cu111-subs+Ag-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -25278.486588 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.016  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.016  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.016  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.016  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.133  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.133  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.133  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.133  Cu_us_gga.pseudo
 8    Cu  [  5.146  1.485  4.194]   2   0.021  Cu_us_gga.pseudo
 9    Cu  [  2.572  1.485  4.194]   2   0.021  Cu_us_gga.pseudo
10    Cu  [  6.433  3.714  4.194]   2   0.021  Cu_us_gga.pseudo
11    Cu  [  3.859  3.714  4.194]   2   0.021  Cu_us_gga.pseudo
12    Ag  [ -0.002 -0.001  6.589]   1   0.011  ag_us.pseudo
13    Ag  [  2.572 -0.001  6.589]   1   0.011  ag_us.pseudo
14    Ag  [  1.285  2.228  6.589]   1   0.012  ag_us.pseudo
15    Ag  [  3.859  2.228  6.589]   1   0.011  ag_us.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 176.0
Number of bands     = 118
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



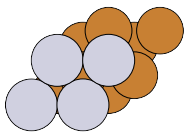
Ir overlayer:

```
---------------------------------
Dacapo calculation from Cu-subs/Ir-layer/Cu111-subs+Ir-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -24296.218233 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.006  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.006  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.006  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.006  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.276  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.276  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.276  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.276  Cu_us_gga.pseudo
 8    Cu  [  5.137  1.480  4.245]   2   0.046  Cu_us_gga.pseudo
 9    Cu  [  2.563  1.480  4.245]   2   0.046  Cu_us_gga.pseudo
10    Cu  [  6.424  3.709  4.245]   2   0.046  Cu_us_gga.pseudo
11    Cu  [  3.850  3.709  4.245]   2   0.046  Cu_us_gga.pseudo
12    Ir  [  0.004  0.002  6.471]   1   0.033  ir_us_gga_flocal.pseudo
13    Ir  [  2.578  0.002  6.471]   1   0.033  ir_us_gga_flocal.pseudo
14    Ir  [  1.291  2.231  6.471]   1   0.033  ir_us_gga_flocal.pseudo
15    Ir  [  3.865  2.231  6.471]   1   0.033  ir_us_gga_flocal.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 168.0
Number of bands     = 113
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



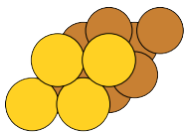
Pt overlayer:

```
---------------------------------
Dacapo calculation from Cu-subs/Pt-layer/Cu111-subs+Pt-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -24951.521746 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.034  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.034  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.034  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.034  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.041  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.041  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.041  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.041  Cu_us_gga.pseudo
 8    Cu  [  5.145  1.484  4.152]   2   0.045  Cu_us_gga.pseudo
 9    Cu  [  2.571  1.484  4.152]   2   0.045  Cu_us_gga.pseudo
10    Cu  [  6.432  3.713  4.152]   2   0.045  Cu_us_gga.pseudo
11    Cu  [  3.858  3.713  4.152]   2   0.045  Cu_us_gga.pseudo
12    Pt  [  0.003  0.002  6.428]   1   0.008  pt_us_gga.pseudo
13    Pt  [  2.577  0.002  6.428]   1   0.008  pt_us_gga.pseudo
14    Pt  [  1.290  2.231  6.428]   1   0.008  pt_us_gga.pseudo
15    Pt  [  3.864  2.231  6.428]   1   0.008  pt_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 172.0
Number of bands     = 115
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Au overlayer:

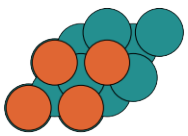
```
---------------------------------
Dacapo calculation from Cu-subs/Au-layer/Cu111-subs+Au-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -25669.007245 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.021  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.021  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.021  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.021  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.049  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.049  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.049  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.049  Cu_us_gga.pseudo
 8    Cu  [  5.148  1.486  4.164]   2   0.013  Cu_us_gga.pseudo
 9    Cu  [  2.575  1.486  4.164]   2   0.013  Cu_us_gga.pseudo
10    Cu  [  6.435  3.715  4.164]   2   0.014  Cu_us_gga.pseudo
11    Cu  [  3.862  3.715  4.164]   2   0.013  Cu_us_gga.pseudo
12    Au  [  0.001  0.001  6.664]   1   0.014  Au_us_gga.pseudo
13    Au  [  2.575  0.001  6.664]   1   0.014  Au_us_gga.pseudo
14    Au  [  1.288  2.230  6.664]   1   0.014  Au_us_gga.pseudo
15    Au  [  3.862  2.230  6.664]   1   0.014  Au_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 176.0
Number of bands     = 118
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Structures with Ru as the substrate:

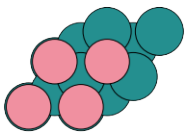
Fe overlayer:

```
---------------------------------
Dacapo calculation from Ru-subs/Fe-layer/Ru111-subs+Fe-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -11530.740527 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.720  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.720  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.720  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.720  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.651  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.651  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.651  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.651  Ru_us_gga.pseudo
 8    Ru  [  5.431  1.569  4.498]   2   0.043  Ru_us_gga.pseudo
 9    Ru  [  2.718  1.569  4.498]   2   0.042  Ru_us_gga.pseudo
10    Ru  [  6.788  3.919  4.498]   2   0.043  Ru_us_gga.pseudo
11    Ru  [  4.075  3.919  4.498]   2   0.043  Ru_us_gga.pseudo
12    Fe  [  0.002  0.001  6.456]   1   0.020  Fe_us_gga_d2.1.8.pseudo
13    Fe  [  2.715  0.001  6.456]   1   0.020  Fe_us_gga_d2.1.8.pseudo
14    Fe  [  1.358  2.351  6.456]   1   0.020  Fe_us_gga_d2.1.8.pseudo
15    Fe  [  4.072  2.351  6.456]   1   0.019  Fe_us_gga_d2.1.8.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 128.0
Number of bands     = 87
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



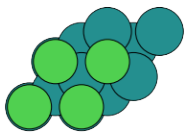
Co overlayer:

```
---------------------------------
Dacapo calculation from Ru-subs/Co-layer/Ru111-subs+Co-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -12567.990224 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.577  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.578  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.578  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.578  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.545  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.545  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.545  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.545  Ru_us_gga.pseudo
 8    Ru  [  5.430  1.568  4.449]   2   0.002  Ru_us_gga.pseudo
 9    Ru  [  2.717  1.568  4.449]   2   0.003  Ru_us_gga.pseudo
10    Ru  [  6.787  3.918  4.449]   2   0.002  Ru_us_gga.pseudo
11    Ru  [  4.073  3.918  4.449]   2   0.002  Ru_us_gga.pseudo
12    Co  [  0.002  0.001  6.438]   1   0.004  Co_us_gga.pseudo
13    Co  [  2.715  0.001  6.438]   1   0.004  Co_us_gga.pseudo
14    Co  [  1.358  2.351  6.438]   1   0.004  Co_us_gga.pseudo
15    Co  [  4.072  2.351  6.438]   1   0.004  Co_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 132.0
Number of bands     = 89
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



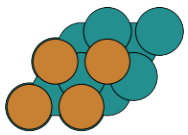
Ni overlayer:

```
---------------------------------
Dacapo calculation from Ru-subs/Ni-layer/Ru111-subs+Ni-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -13428.819822 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.435  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.435  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.435  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.435  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.495  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.495  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.495  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.495  Ru_us_gga.pseudo
 8    Ru  [  5.428  1.568  4.396]   2   0.012  Ru_us_gga.pseudo
 9    Ru  [  2.715  1.568  4.396]   2   0.012  Ru_us_gga.pseudo
10    Ru  [  6.785  3.917  4.396]   2   0.012  Ru_us_gga.pseudo
11    Ru  [  4.072  3.917  4.396]   2   0.012  Ru_us_gga.pseudo
12    Ni  [  0.001  0.000  6.444]   1   0.048  Ni_us_gga.pseudo
13    Ni  [  2.714  0.000  6.444]   1   0.047  Ni_us_gga.pseudo
14    Ni  [  1.357  2.350  6.444]   1   0.047  Ni_us_gga.pseudo
15    Ni  [  4.071  2.350  6.444]   1   0.048  Ni_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 136.0
Number of bands     = 92
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



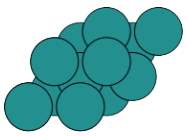
Cu overlayer:

```
---------------------------------
Dacapo calculation from Ru-subs/Cu-layer/Ru111-subs+Cu-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -14907.201208 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.396  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.396  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.396  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.396  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.284  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.284  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.284  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.284  Ru_us_gga.pseudo
 8    Ru  [  5.429  1.568  4.375]   2   0.003  Ru_us_gga.pseudo
 9    Ru  [  2.715  1.568  4.375]   2   0.003  Ru_us_gga.pseudo
10    Ru  [  6.785  3.918  4.375]   2   0.003  Ru_us_gga.pseudo
11    Ru  [  4.072  3.918  4.375]   2   0.003  Ru_us_gga.pseudo
12    Cu  [  0.000  0.000  6.562]   1   0.014  Cu_us_gga.pseudo
13    Cu  [  2.714  0.000  6.562]   1   0.014  Cu_us_gga.pseudo
14    Cu  [  1.357  2.350  6.562]   1   0.014  Cu_us_gga.pseudo
15    Cu  [  4.070  2.350  6.562]   1   0.014  Cu_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 140.0
Number of bands     = 95
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



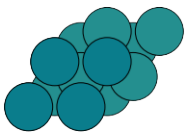
Ru overlayer:

```
---------------------------------
Dacapo calculation from Ru-subs/Ru-layer/Ru111-subs+Ru-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -10940.355552 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.598  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.598  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.598  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.598  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.532  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.532  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.532  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.532  Ru_us_gga.pseudo
 8    Ru  [  5.428  1.567  4.463]   2   0.033  Ru_us_gga.pseudo
 9    Ru  [  2.715  1.567  4.463]   2   0.034  Ru_us_gga.pseudo
10    Ru  [  6.785  3.917  4.463]   2   0.034  Ru_us_gga.pseudo
11    Ru  [  4.072  3.917  4.463]   2   0.034  Ru_us_gga.pseudo
12    Ru  [ -0.000 -0.000  6.614]   1   0.045  Ru_us_gga.pseudo
13    Ru  [  2.713 -0.000  6.614]   1   0.045  Ru_us_gga.pseudo
14    Ru  [  1.356  2.350  6.614]   1   0.045  Ru_us_gga.pseudo
15    Ru  [  4.070  2.350  6.614]   1   0.045  Ru_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 128.0
Number of bands     = 87
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



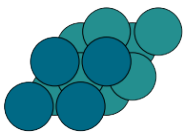
Rh overlayer:

```
--------------------------------
Dacapo calculation from Ru-subs/Rh-layer/Ru111-subs+Rh-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -11600.657558 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.441  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.441  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.441  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.441  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.472  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.472  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.472  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.472  Ru_us_gga.pseudo
 8    Ru  [  5.429  1.568  4.410]   2   0.005  Ru_us_gga.pseudo
 9    Ru  [  2.716  1.568  4.410]   2   0.005  Ru_us_gga.pseudo
10    Ru  [  6.786  3.918  4.410]   2   0.005  Ru_us_gga.pseudo
11    Ru  [  4.073  3.918  4.410]   2   0.005  Ru_us_gga.pseudo
12    Rh  [  0.001  0.000  6.588]   1   0.025  Rh_us_gga_fl.pseudo
13    Rh  [  2.714  0.000  6.588]   1   0.025  Rh_us_gga_fl.pseudo
14    Rh  [  1.357  2.350  6.588]   1   0.025  Rh_us_gga_fl.pseudo
15    Rh  [  4.071  2.350  6.588]   1   0.025  Rh_us_gga_fl.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 132.0
Number of bands     = 89
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
--------------------------------
```



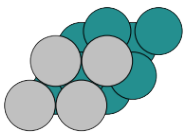
Pd overlayer:

```
---------------------------------
Dacapo calculation from Ru-subs/Pd-layer/Ru111-subs+Pd-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -12402.634431 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.331  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.331  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.331  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.331  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.266  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.266  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.266  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.266  Ru_us_gga.pseudo
 8    Ru  [  5.427  1.567  4.369]   2   0.027  Ru_us_gga.pseudo
 9    Ru  [  2.714  1.567  4.369]   2   0.027  Ru_us_gga.pseudo
10    Ru  [  6.784  3.917  4.369]   2   0.026  Ru_us_gga.pseudo
11    Ru  [  4.071  3.917  4.369]   2   0.027  Ru_us_gga.pseudo
12    Pd  [ -0.000 -0.000  6.682]   1   0.041  046-Pd-gpe-n-6projectors-floc.uspp
13    Pd  [  2.713 -0.000  6.682]   1   0.041  046-Pd-gpe-n-6projectors-floc.uspp
14    Pd  [  1.356  2.350  6.682]   1   0.041  046-Pd-gpe-n-6projectors-floc.uspp
15    Pd  [  4.070  2.350  6.682]   1   0.041  046-Pd-gpe-n-6projectors-floc.uspp

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 136.0
Number of bands     = 92
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



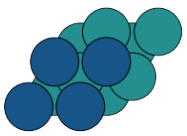
Ag overlayer:

```
---------------------------------
Dacapo calculation from Ru-subs/Ag-layer/Ru111-subs+Ag-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -13381.574045 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.346  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.346  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.346  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.346  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.418  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.418  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.418  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.418  Ru_us_gga.pseudo
 8    Ru  [  5.428  1.567  4.348]   2   0.044  Ru_us_gga.pseudo
 9    Ru  [  2.715  1.568  4.348]   2   0.044  Ru_us_gga.pseudo
10    Ru  [  6.785  3.917  4.348]   2   0.044  Ru_us_gga.pseudo
11    Ru  [  4.072  3.917  4.348]   2   0.044  Ru_us_gga.pseudo
12    Ag  [  0.000  0.000  6.799]   1   0.014  ag_us.pseudo
13    Ag  [  2.714  0.000  6.799]   1   0.014  ag_us.pseudo
14    Ag  [  1.357  2.350  6.799]   1   0.014  ag_us.pseudo
15    Ag  [  4.070  2.350  6.799]   1   0.014  ag_us.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 140.0
Number of bands     = 95
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



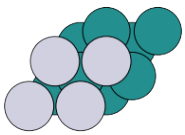
Ir overlayer:

```
---------------------------------
Dacapo calculation from Ru-subs/Ir-layer/Ru111-subs+Ir-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -12399.120361 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.453  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.453  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.453  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.453  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.464  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.464  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.464  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.464  Ru_us_gga.pseudo
 8    Ru  [  5.428  1.568  4.424]   2   0.005  Ru_us_gga.pseudo
 9    Ru  [  2.715  1.568  4.424]   2   0.005  Ru_us_gga.pseudo
10    Ru  [  6.785  3.917  4.424]   2   0.005  Ru_us_gga.pseudo
11    Ru  [  4.072  3.917  4.424]   2   0.005  Ru_us_gga.pseudo
12    Ir  [  0.001  0.001  6.614]   1   0.009  ir_us_gga_flocal.pseudo
13    Ir  [  2.715  0.001  6.614]   1   0.009  ir_us_gga_flocal.pseudo
14    Ir  [  1.358  2.351  6.614]   1   0.009  ir_us_gga_flocal.pseudo
15    Ir  [  4.071  2.351  6.614]   1   0.009  ir_us_gga_flocal.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 132.0
Number of bands     = 89
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



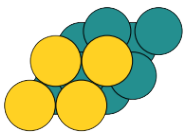
Pt overlayer:

```
---------------------------------
Dacapo calculation from Ru-subs/Pt-layer/Ru111-subs+Pt-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -13054.218072 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.252  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.252  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.252  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.252  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.303  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.303  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.303  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.303  Ru_us_gga.pseudo
 8    Ru  [  5.428  1.567  4.358]   2   0.015  Ru_us_gga.pseudo
 9    Ru  [  2.715  1.567  4.358]   2   0.015  Ru_us_gga.pseudo
10    Ru  [  6.785  3.917  4.358]   2   0.015  Ru_us_gga.pseudo
11    Ru  [  4.071  3.917  4.358]   2   0.015  Ru_us_gga.pseudo
12    Pt  [ -0.000 -0.000  6.705]   1   0.047  pt_us_gga.pseudo
13    Pt  [  2.713 -0.000  6.705]   1   0.047  pt_us_gga.pseudo
14    Pt  [  1.356  2.350  6.705]   1   0.047  pt_us_gga.pseudo
15    Pt  [  4.070  2.350  6.705]   1   0.047  pt_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 136.0
Number of bands     = 92
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Au overlayer:

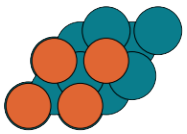
```
---------------------------------
Dacapo calculation from Ru-subs/Au-layer/Ru111-subs+Au-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -13772.572071 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.317  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.317  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.317  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.317  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.318  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.318  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.318  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.318  Ru_us_gga.pseudo
 8    Ru  [  5.428  1.567  4.349]   2   0.006  Ru_us_gga.pseudo
 9    Ru  [  2.714  1.567  4.349]   2   0.006  Ru_us_gga.pseudo
10    Ru  [  6.784  3.917  4.349]   2   0.005  Ru_us_gga.pseudo
11    Ru  [  4.071  3.917  4.349]   2   0.005  Ru_us_gga.pseudo
12    Au  [  0.001  0.001  6.863]   1   0.009  Au_us_gga.pseudo
13    Au  [  2.714  0.001  6.863]   1   0.009  Au_us_gga.pseudo
14    Au  [  1.358  2.350  6.863]   1   0.009  Au_us_gga.pseudo
15    Au  [  4.071  2.350  6.863]   1   0.009  Au_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 140.0
Number of bands     = 95
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Structures with Rh as the substrate:

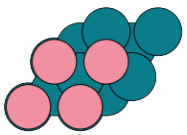
Fe overlayer:

```
--------------------------------
Dacapo calculation from Rh-subs/Fe-layer/Rh111-subs+Fe-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -13508.881306 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh   [  0.000  0.000  0.000]   4   0.289  Rh_us_gga_fl.pseudo
 1    Rh   [  2.704  0.000  0.000]   4   0.289  Rh_us_gga_fl.pseudo
 2    Rh   [  1.352  2.342  0.000]   4   0.289  Rh_us_gga_fl.pseudo
 3    Rh   [  4.056  2.342  0.000]   4   0.289  Rh_us_gga_fl.pseudo
 4    Rh   [  1.352  0.781  2.208]   3   0.299  Rh_us_gga_fl.pseudo
 5    Rh   [  4.056  0.781  2.208]   3   0.299  Rh_us_gga_fl.pseudo
 6    Rh   [  2.704  3.122  2.208]   3   0.299  Rh_us_gga_fl.pseudo
 7    Rh   [  5.408  3.122  2.208]   3   0.299  Rh_us_gga_fl.pseudo
 8    Rh   [  5.408  1.561  4.448]   2   0.001  Rh_us_gga_fl.pseudo
 9    Rh   [  2.704  1.561  4.448]   2   0.001  Rh_us_gga_fl.pseudo
10    Rh   [  6.760  3.903  4.448]   2   0.002  Rh_us_gga_fl.pseudo
11    Rh   [  4.056  3.903  4.448]   2   0.001  Rh_us_gga_fl.pseudo
12    Fe   [  0.001  0.000  6.403]   1   0.001  Fe_us_gga_d2.1.8.pseudo
13    Fe   [  2.705  0.000  6.403]   1   0.001  Fe_us_gga_d2.1.8.pseudo
14    Fe   [  1.353  2.342  6.403]   1   0.001  Fe_us_gga_d2.1.8.pseudo
15    Fe   [  4.057  2.342  6.403]   1   0.001  Fe_us_gga_d2.1.8.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 140.0
Number of bands     = 95
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
--------------------------------
```



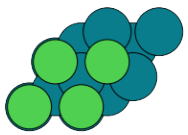
Co overlayer:

```
--------------------------------
Dacapo calculation from Rh-subs/Co-layer/Rh111-subs+Co-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -14546.068251 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.304  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.304  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.304  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.304  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.211  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.211  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.211  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.211  Rh_us_gga_fl.pseudo
 8    Rh  [  5.408  1.561  4.427]   2   0.011  Rh_us_gga_fl.pseudo
 9    Rh  [  2.704  1.561  4.427]   2   0.011  Rh_us_gga_fl.pseudo
10    Rh  [  6.760  3.903  4.427]   2   0.011  Rh_us_gga_fl.pseudo
11    Rh  [  4.056  3.903  4.427]   2   0.011  Rh_us_gga_fl.pseudo
12    Co  [  0.001  0.000  6.411]   1   0.014  Co_us_gga.pseudo
13    Co  [  2.705  0.000  6.411]   1   0.014  Co_us_gga.pseudo
14    Co  [  1.353  2.342  6.411]   1   0.014  Co_us_gga.pseudo
15    Co  [  4.057  2.342  6.411]   1   0.014  Co_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 144.0
Number of bands     = 97
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
--------------------------------
```



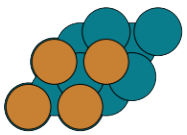
Ni overlayer:

```
---------------------------------
Dacapo calculation from Rh-subs/Ni-layer/Rh111-subs+Ni-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -15406.829227 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.279  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.279  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.279  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.279  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.268  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.268  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.268  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.268  Rh_us_gga_fl.pseudo
 8    Rh  [  5.408  1.561  4.383]   2   0.006  Rh_us_gga_fl.pseudo
 9    Rh  [  2.704  1.561  4.383]   2   0.006  Rh_us_gga_fl.pseudo
10    Rh  [  6.760  3.903  4.383]   2   0.006  Rh_us_gga_fl.pseudo
11    Rh  [  4.056  3.903  4.383]   2   0.006  Rh_us_gga_fl.pseudo
12    Ni  [  0.001  0.000  6.418]   1   0.002  Ni_us_gga.pseudo
13    Ni  [  2.705  0.000  6.418]   1   0.002  Ni_us_gga.pseudo
14    Ni  [  1.353  2.342  6.418]   1   0.001  Ni_us_gga.pseudo
15    Ni  [  4.057  2.342  6.418]   1   0.002  Ni_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 148.0
Number of bands     = 100
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



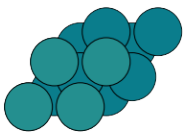
Cu overlayer:

```
---------------------------------
Dacapo calculation from Rh-subs/Cu-layer/Rh111-subs+Cu-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -16885.334938 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.306  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.306  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.306  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.306  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.195  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.195  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.195  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.195  Rh_us_gga_fl.pseudo
 8    Rh  [  5.408  1.561  4.382]   2   0.050  Rh_us_gga_fl.pseudo
 9    Rh  [  2.704  1.561  4.382]   2   0.049  Rh_us_gga_fl.pseudo
10    Rh  [  6.759  3.903  4.382]   2   0.050  Rh_us_gga_fl.pseudo
11    Rh  [  4.056  3.903  4.382]   2   0.050  Rh_us_gga_fl.pseudo
12    Cu  [  0.000  0.000  6.533]   1   0.010  Cu_us_gga.pseudo
13    Cu  [  2.704  0.000  6.533]   1   0.010  Cu_us_gga.pseudo
14    Cu  [  1.352  2.342  6.533]   1   0.010  Cu_us_gga.pseudo
15    Cu  [  4.056  2.342  6.533]   1   0.010  Cu_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 152.0
Number of bands     = 102
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



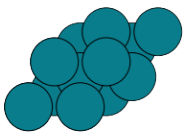
Ru overlayer:

```
---------------------------------
Dacapo calculation from Rh-subs/Ru-layer/Rh111-subs+Ru-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -12918.669013 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.238  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.238  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.238  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.238  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.241  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.241  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.241  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.241  Rh_us_gga_fl.pseudo
 8    Rh  [  5.407  1.561  4.411]   2   0.025  Rh_us_gga_fl.pseudo
 9    Rh  [  2.703  1.561  4.411]   2   0.024  Rh_us_gga_fl.pseudo
10    Rh  [  6.759  3.903  4.411]   2   0.024  Rh_us_gga_fl.pseudo
11    Rh  [  4.055  3.903  4.411]   2   0.025  Rh_us_gga_fl.pseudo
12    Ru  [  0.000  0.000  6.563]   1   0.019  Ru_us_gga.pseudo
13    Ru  [  2.704  0.000  6.563]   1   0.019  Ru_us_gga.pseudo
14    Ru  [  1.352  2.342  6.563]   1   0.019  Ru_us_gga.pseudo
15    Ru  [  4.056  2.342  6.563]   1   0.019  Ru_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 140.0
Number of bands     = 95
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



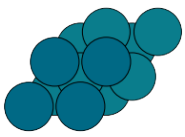
Rh overlayer:

```
---------------------------------
Dacapo calculation from Rh-subs/Rh-layer/Rh111-subs+Rh-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -13578.707552 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.230  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.230  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.230  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.230  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.248  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.248  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.248  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.248  Rh_us_gga_fl.pseudo
 8    Rh  [  5.408  1.561  4.373]   2   0.004  Rh_us_gga_fl.pseudo
 9    Rh  [  2.704  1.561  4.373]   2   0.003  Rh_us_gga_fl.pseudo
10    Rh  [  6.760  3.903  4.373]   2   0.005  Rh_us_gga_fl.pseudo
11    Rh  [  4.056  3.903  4.373]   2   0.004  Rh_us_gga_fl.pseudo
12    Rh  [  0.001  0.001  6.546]   1   0.007  Rh_us_gga_fl.pseudo
13    Rh  [  2.705  0.001  6.546]   1   0.007  Rh_us_gga_fl.pseudo
14    Rh  [  1.353  2.342  6.546]   1   0.007  Rh_us_gga_fl.pseudo
15    Rh  [  4.057  2.342  6.546]   1   0.008  Rh_us_gga_fl.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 144.0
Number of bands     = 97
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



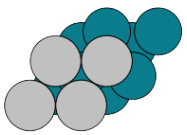
Pd overlayer:

```
---------------------------------
Dacapo calculation from Rh-subs/Pd-layer/Rh111-subs+Pd-overlayer-relaxed.nc
status = finished
version = ifc ser v2-3-3
Energy = -14380.576041 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.289  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.289  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.289  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.289  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.241  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.241  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.241  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.241  Rh_us_gga_fl.pseudo
 8    Rh  [  5.408  1.561  4.349]   2   0.008  Rh_us_gga_fl.pseudo
 9    Rh  [  2.704  1.561  4.349]   2   0.008  Rh_us_gga_fl.pseudo
10    Rh  [  6.760  3.903  4.349]   2   0.008  Rh_us_gga_fl.pseudo
11    Rh  [  4.056  3.903  4.349]   2   0.008  Rh_us_gga_fl.pseudo
12    Pd  [  0.000  0.000  6.656]   1   0.046  046-Pd-gpe-n-6projectors-floc.uspp
13    Pd  [  2.704  0.000  6.656]   1   0.046  046-Pd-gpe-n-6projectors-floc.uspp
14    Pd  [  1.352  2.342  6.656]   1   0.046  046-Pd-gpe-n-6projectors-floc.uspp
15    Pd  [  4.056  2.342  6.656]   1   0.046  046-Pd-gpe-n-6projectors-floc.uspp

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 148.0
Number of bands     = 100
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



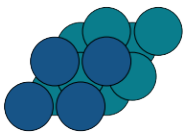
Ag overlayer:

```
---------------------------------
Dacapo calculation from Rh-subs/Ag-layer/Rh111-subs+Ag-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -15359.776916 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.294  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.294  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.294  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.294  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.350  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.350  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.350  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.350  Rh_us_gga_fl.pseudo
 8    Rh  [  5.407  1.561  4.348]   2   0.008  Rh_us_gga_fl.pseudo
 9    Rh  [  2.703  1.561  4.348]   2   0.007  Rh_us_gga_fl.pseudo
10    Rh  [  6.759  3.902  4.348]   2   0.007  Rh_us_gga_fl.pseudo
11    Rh  [  4.055  3.902  4.348]   2   0.007  Rh_us_gga_fl.pseudo
12    Ag  [  0.001  0.000  6.782]   1   0.007  ag_us.pseudo
13    Ag  [  2.705  0.000  6.782]   1   0.007  ag_us.pseudo
14    Ag  [  1.353  2.342  6.782]   1   0.007  ag_us.pseudo
15    Ag  [  4.057  2.342  6.782]   1   0.007  ag_us.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 152.0
Number of bands     = 102
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



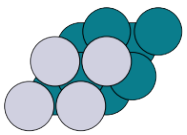
Ir overlayer:

```
---------------------------------
Dacapo calculation from Rh-subs/Ir-layer/Rh111-subs+Ir-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -14377.135193 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.248  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.248  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.248  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.248  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.241  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.241  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.241  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.241  Rh_us_gga_fl.pseudo
 8    Rh  [  5.406  1.560  4.391]   2   0.012  Rh_us_gga_fl.pseudo
 9    Rh  [  2.702  1.560  4.391]   2   0.013  Rh_us_gga_fl.pseudo
10    Rh  [  6.758  3.902  4.391]   2   0.012  Rh_us_gga_fl.pseudo
11    Rh  [  4.054  3.902  4.391]   2   0.012  Rh_us_gga_fl.pseudo
12    Ir  [  0.002  0.001  6.569]   1   0.003  ir_us_gga_flocal.pseudo
13    Ir  [  2.706  0.001  6.569]   1   0.003  ir_us_gga_flocal.pseudo
14    Ir  [  1.354  2.343  6.569]   1   0.003  ir_us_gga_flocal.pseudo
15    Ir  [  4.058  2.343  6.569]   1   0.003  ir_us_gga_flocal.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 144.0
Number of bands     = 97
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



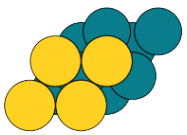
Pt overlayer:

```
---------------------------------
Dacapo calculation from Rh-subs/Pt-layer/Rh111-subs+Pt-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -15032.147600 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.293  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.293  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.293  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.293  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.259  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.259  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.259  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.259  Rh_us_gga_fl.pseudo
 8    Rh  [  5.408  1.561  4.342]   2   0.047  Rh_us_gga_fl.pseudo
 9    Rh  [  2.704  1.561  4.342]   2   0.046  Rh_us_gga_fl.pseudo
10    Rh  [  6.760  3.903  4.342]   2   0.048  Rh_us_gga_fl.pseudo
11    Rh  [  4.056  3.903  4.342]   2   0.046  Rh_us_gga_fl.pseudo
12    Pt  [ -0.000 -0.000  6.681]   1   0.004  pt_us_gga.pseudo
13    Pt  [  2.704 -0.000  6.681]   1   0.004  pt_us_gga.pseudo
14    Pt  [  1.352  2.342  6.681]   1   0.004  pt_us_gga.pseudo
15    Pt  [  4.056  2.342  6.681]   1   0.004  pt_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 148.0
Number of bands     = 100
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Au overlayer:

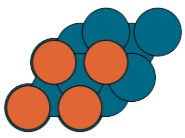
```
---------------------------------
Dacapo calculation from Rh-subs/Au-layer/Rh111-subs+Au-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -15750.667886 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.336  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.336  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.336  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.335  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.356  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.356  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.356  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.356  Rh_us_gga_fl.pseudo
 8    Rh  [  5.406  1.560  4.347]   2   0.034  Rh_us_gga_fl.pseudo
 9    Rh  [  2.702  1.560  4.347]   2   0.034  Rh_us_gga_fl.pseudo
10    Rh  [  6.758  3.902  4.347]   2   0.034  Rh_us_gga_fl.pseudo
11    Rh  [  4.054  3.902  4.347]   2   0.033  Rh_us_gga_fl.pseudo
12    Au  [  0.001  0.000  6.863]   1   0.021  Au_us_gga.pseudo
13    Au  [  2.705  0.000  6.863]   1   0.021  Au_us_gga.pseudo
14    Au  [  1.353  2.342  6.863]   1   0.021  Au_us_gga.pseudo
15    Au  [  4.057  2.342  6.863]   1   0.021  Au_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 152.0
Number of bands     = 102
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Structures with Pd as the substrate:

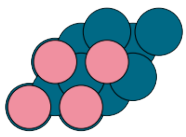
Fe overlayer:

```
---------------------------------
Dacapo calculation from Pd-subs/Fe-layer/Pd111-subs+Fe-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -15910.723421 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.038  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.038  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.038  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.038  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.103  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.103  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.103  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.103  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.572  1.608  4.570]   2   0.013  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.786  1.608  4.570]   2   0.013  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.965  4.021  4.570]   2   0.013  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.179  4.021  4.570]   2   0.013  046-Pd-gpe-n-6projectors-floc.uspp
12    Fe  [  0.002  0.001  6.544]   1   0.014  Fe_us_gga_d2.1.8.pseudo
13    Fe  [  2.788  0.001  6.544]   1   0.014  Fe_us_gga_d2.1.8.pseudo
14    Fe  [  1.395  2.414  6.544]   1   0.014  Fe_us_gga_d2.1.8.pseudo
15    Fe  [  4.181  2.414  6.544]   1   0.014  Fe_us_gga_d2.1.8.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 152.0
Number of bands     = 102
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



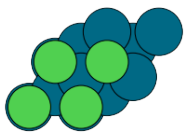
Co overlayer:

```
---------------------------------
Dacapo calculation from Pd-subs/Co-layer/Pd111-subs+Co-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -16948.220847 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.026  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.026  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.026  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.026  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.058  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.058  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.058  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.058  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.572  1.609  4.554]   2   0.023  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.786  1.609  4.554]   2   0.022  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.965  4.021  4.554]   2   0.023  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.179  4.021  4.554]   2   0.023  046-Pd-gpe-n-6projectors-floc.uspp
12    Co  [  0.002  0.001  6.525]   1   0.007  Co_us_gga.pseudo
13    Co  [  2.788  0.001  6.525]   1   0.007  Co_us_gga.pseudo
14    Co  [  1.395  2.414  6.525]   1   0.007  Co_us_gga.pseudo
15    Co  [  4.181  2.414  6.525]   1   0.007  Co_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 156.0
Number of bands     = 105
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



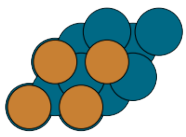
Ni overlayer:

```
--------------------------------
Dacapo calculation from Pd-subs/Ni-layer/Pd111-subs+Ni-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -17809.526961 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.020  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.020  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.020  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.020  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.024  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.024  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.024  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.024  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.575  1.610  4.544]   2   0.025  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.789  1.610  4.544]   2   0.025  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.968  4.023  4.544]   2   0.025  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.182  4.023  4.544]   2   0.025  046-Pd-gpe-n-6projectors-floc.uspp
12    Ni  [  0.003  0.002  6.538]   1   0.006  Ni_us_gga.pseudo
13    Ni  [  2.789  0.002  6.538]   1   0.006  Ni_us_gga.pseudo
14    Ni  [  1.396  2.414  6.538]   1   0.006  Ni_us_gga.pseudo
15    Ni  [  4.182  2.414  6.538]   1   0.006  Ni_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 160.0
Number of bands     = 108
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
--------------------------------
```



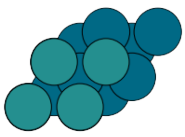
Cu overlayer:

```
---------------------------------
Dacapo calculation from Pd-subs/Cu-layer/Pd111-subs+Cu-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19289.305898 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.018  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.018  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.018  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.018  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.086  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.086  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.086  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.086  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.575  1.610  4.573]   2   0.008  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.789  1.610  4.573]   2   0.008  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.968  4.023  4.573]   2   0.008  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.182  4.023  4.573]   2   0.007  046-Pd-gpe-n-6projectors-floc.uspp
12    Cu  [  0.001  0.000  6.661]   1   0.015  Cu_us_gga.pseudo
13    Cu  [  2.787  0.000  6.661]   1   0.015  Cu_us_gga.pseudo
14    Cu  [  1.394  2.413  6.661]   1   0.015  Cu_us_gga.pseudo
15    Cu  [  4.180  2.413  6.661]   1   0.015  Cu_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 164.0
Number of bands     = 110
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



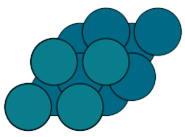
Ru overlayer:

```
---------------------------------
Dacapo calculation from Pd-subs/Ru-layer/Pd111-subs+Ru-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -15320.962618 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.051  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.051  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.051  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.051  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.075  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.076  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.075  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.075  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.574  1.610  4.531]   2   0.004  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.788  1.610  4.531]   2   0.004  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.967  4.023  4.531]   2   0.004  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.181  4.023  4.531]   2   0.004  046-Pd-gpe-n-6projectors-floc.uspp
12    Ru  [ -0.000 -0.000  6.690]   1   0.005  Ru_us_gga.pseudo
13    Ru  [  2.786 -0.000  6.690]   1   0.005  Ru_us_gga.pseudo
14    Ru  [  1.393  2.413  6.690]   1   0.005  Ru_us_gga.pseudo
15    Ru  [  4.179  2.413  6.690]   1   0.005  Ru_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 152.0
Number of bands     = 102
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



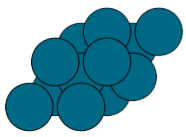
Rh overlayer:

```
---------------------------------
Dacapo calculation from Pd-subs/Rh-layer/Pd111-subs+Rh-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -15981.071498 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.022  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.022  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.022  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.022  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.045  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.045  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.045  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.045  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.575  1.610  4.528]   2   0.031  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.789  1.610  4.528]   2   0.031  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.968  4.023  4.528]   2   0.030  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.182  4.023  4.528]   2   0.031  046-Pd-gpe-n-6projectors-floc.uspp
12    Rh  [ -0.001 -0.001  6.712]   1   0.029  Rh_us_gga_fl.pseudo
13    Rh  [  2.785 -0.001  6.712]   1   0.029  Rh_us_gga_fl.pseudo
14    Rh  [  1.392  2.412  6.712]   1   0.029  Rh_us_gga_fl.pseudo
15    Rh  [  4.178  2.412  6.712]   1   0.029  Rh_us_gga_fl.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 156.0
Number of bands     = 105
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



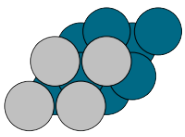
Pd overlayer:

```
---------------------------------
Dacapo calculation from Pd-subs/Pd-layer/Pd111-subs+Pd-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -16783.882889 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.004  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.004  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.004  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.004  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.021  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.021  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.021  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.021  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.574  1.609  4.521]   2   0.027  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.788  1.609  4.521]   2   0.026  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.967  4.022  4.521]   2   0.027  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.181  4.022  4.521]   2   0.026  046-Pd-gpe-n-6projectors-floc.uspp
12    Pd  [  0.002  0.001  6.789]   1   0.011  046-Pd-gpe-n-6projectors-floc.uspp
13    Pd  [  2.788  0.001  6.789]   1   0.011  046-Pd-gpe-n-6projectors-floc.uspp
14    Pd  [  1.395  2.414  6.789]   1   0.011  046-Pd-gpe-n-6projectors-floc.uspp
15    Pd  [  4.181  2.414  6.789]   1   0.011  046-Pd-gpe-n-6projectors-floc.uspp

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 160.0
Number of bands     = 108
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



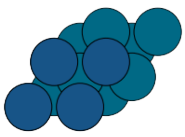
Ag overlayer:

```
---------------------------------
Dacapo calculation from Pd-subs/Ag-layer/Pd111-subs+Ag-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -17764.502848 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.012  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.012  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.012  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.012  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.043  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.043  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.043  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.043  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.574  1.610  4.540]   2   0.026  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.788  1.610  4.540]   2   0.025  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.967  4.023  4.540]   2   0.026  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.181  4.023  4.540]   2   0.026  046-Pd-gpe-n-6projectors-floc.uspp
12    Ag  [  0.001  0.001  6.886]   1   0.014  ag_us.pseudo
13    Ag  [  2.787  0.001  6.886]   1   0.014  ag_us.pseudo
14    Ag  [  1.394  2.413  6.886]   1   0.014  ag_us.pseudo
15    Ag  [  4.180  2.413  6.886]   1   0.014  ag_us.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 164.0
Number of bands     = 110
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



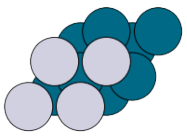
Ir overlayer:

```
---------------------------------
Dacapo calculation from Pd-subs/Ir-layer/Pd111-subs+Ir-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -16779.120803 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.017  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.017  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.017  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.017  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.014  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.014  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.014  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.014  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.571  1.608  4.525]   2   0.046  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.785  1.608  4.525]   2   0.047  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.964  4.021  4.525]   2   0.047  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.178  4.021  4.525]   2   0.047  046-Pd-gpe-n-6projectors-floc.uspp
12    Ir  [  0.001  0.000  6.709]   1   0.023  ir_us_gga_flocal.pseudo
13    Ir  [  2.787  0.000  6.709]   1   0.023  ir_us_gga_flocal.pseudo
14    Ir  [  1.394  2.413  6.709]   1   0.023  ir_us_gga_flocal.pseudo
15    Ir  [  4.180  2.413  6.709]   1   0.023  ir_us_gga_flocal.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 156.0
Number of bands     = 105
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



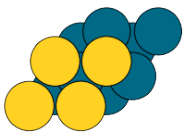
Pt overlayer:

```
---------------------------------
Dacapo calculation from Pd-subs/Pt-layer/Pd111-subs+Pt-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -17435.315694 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.019  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.019  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.019  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.019  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.009  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.009  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.009  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.009  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.572  1.608  4.524]   2   0.003  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.786  1.608  4.524]   2   0.003  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.965  4.021  4.524]   2   0.003  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.179  4.021  4.524]   2   0.003  046-Pd-gpe-n-6projectors-floc.uspp
12    Pt  [  0.000  0.000  6.843]   1   0.013  pt_us_gga.pseudo
13    Pt  [  2.786  0.000  6.843]   1   0.014  pt_us_gga.pseudo
14    Pt  [  1.393  2.413  6.843]   1   0.014  pt_us_gga.pseudo
15    Pt  [  4.179  2.413  6.843]   1   0.014  pt_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 160.0
Number of bands     = 108
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Au overlayer:

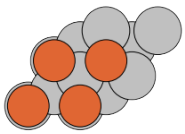
```
---------------------------------
Dacapo calculation from Pd-subs/Au-layer/Pd111-subs+Au-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -18155.337168 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.016  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.016  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.016  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.016  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.020  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.020  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.020  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.020  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.574  1.609  4.542]   2   0.033  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.788  1.609  4.542]   2   0.034  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.967  4.022  4.542]   2   0.033  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.181  4.022  4.542]   2   0.033  046-Pd-gpe-n-6projectors-floc.uspp
12    Au  [  0.001  0.000  6.976]   1   0.024  Au_us_gga.pseudo
13    Au  [  2.787  0.000  6.976]   1   0.024  Au_us_gga.pseudo
14    Au  [  1.394  2.413  6.976]   1   0.024  Au_us_gga.pseudo
15    Au  [  4.180  2.413  6.976]   1   0.024  Au_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 164.0
Number of bands     = 110
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Structures with Ag as the substrate:

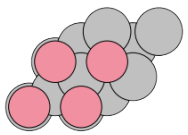
Fe overlayer:

```
---------------------------------
Dacapo calculation from Ag-subs/Fe-layer/Ag111-subs+Fe-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -18846.792165 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.029  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.029  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.029  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.029  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.052  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.052  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.052  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.052  ag_us.pseudo
 8    Ag  [  5.819  1.678  4.756]   2   0.014  ag_us.pseudo
 9    Ag  [  2.906  1.678  4.756]   2   0.014  ag_us.pseudo
10    Ag  [  7.276  4.201  4.756]   2   0.014  ag_us.pseudo
11    Ag  [  4.363  4.201  4.756]   2   0.014  ag_us.pseudo
12    Fe  [  0.001  0.000  6.876]   1   0.010  Fe_us_gga_d2.1.8.pseudo
13    Fe  [  2.914  0.000  6.876]   1   0.010  Fe_us_gga_d2.1.8.pseudo
14    Fe  [  1.457  2.523  6.876]   1   0.010  Fe_us_gga_d2.1.8.pseudo
15    Fe  [  4.371  2.523  6.876]   1   0.010  Fe_us_gga_d2.1.8.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 164.0
Number of bands     = 110
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



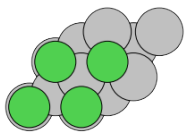
Co overlayer:

```
---------------------------------
Dacapo calculation from Ag-subs/Co-layer/Ag111-subs+Co-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19885.220523 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.020  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.020  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.020  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.020  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.282  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.282  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.282  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.282  ag_us.pseudo
 8    Ag  [  5.825  1.681  4.850]   2   0.031  ag_us.pseudo
 9    Ag  [  2.911  1.681  4.850]   2   0.031  ag_us.pseudo
10    Ag  [  7.281  4.204  4.850]   2   0.031  ag_us.pseudo
11    Ag  [  4.368  4.204  4.850]   2   0.031  ag_us.pseudo
12    Co  [  0.000  0.000  6.953]   1   0.001  Co_us_gga.pseudo
13    Co  [  2.913  0.000  6.953]   1   0.001  Co_us_gga.pseudo
14    Co  [  1.457  2.523  6.953]   1   0.002  Co_us_gga.pseudo
15    Co  [  4.370  2.523  6.953]   1   0.001  Co_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 168.0
Number of bands     = 113
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



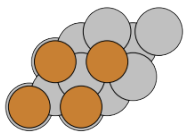
Ni overlayer:

```
---------------------------------
Dacapo calculation from Ag-subs/Ni-layer/Ag111-subs+Ni-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -20747.515775 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.027  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.027  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.027  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.027  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.044  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.044  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.044  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.044  ag_us.pseudo
 8    Ag  [  5.812  1.673  4.749]   2   0.037  ag_us.pseudo
 9    Ag  [  2.898  1.673  4.749]   2   0.037  ag_us.pseudo
10    Ag  [  7.268  4.196  4.749]   2   0.036  ag_us.pseudo
11    Ag  [  4.355  4.196  4.749]   2   0.038  ag_us.pseudo
12    Ni  [ -0.008 -0.004  6.817]   1   0.022  Ni_us_gga.pseudo
13    Ni  [  2.906 -0.004  6.817]   1   0.022  Ni_us_gga.pseudo
14    Ni  [  1.449  2.519  6.817]   1   0.022  Ni_us_gga.pseudo
15    Ni  [  4.362  2.519  6.817]   1   0.022  Ni_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 172.0
Number of bands     = 115
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



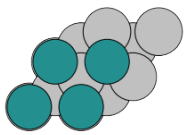
Cu overlayer:

```
---------------------------------
Dacapo calculation from Ag-subs/Cu-layer/Ag111-subs+Cu-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -22227.538250 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.027  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.027  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.027  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.027  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.284  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.284  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.284  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.284  ag_us.pseudo
 8    Ag  [  5.826  1.682  4.844]   2   0.018  ag_us.pseudo
 9    Ag  [  2.913  1.682  4.844]   2   0.018  ag_us.pseudo
10    Ag  [  7.283  4.205  4.844]   2   0.018  ag_us.pseudo
11    Ag  [  4.369  4.205  4.844]   2   0.019  ag_us.pseudo
12    Cu  [  0.000  0.000  6.978]   1   0.008  Cu_us_gga.pseudo
13    Cu  [  2.913  0.000  6.978]   1   0.008  Cu_us_gga.pseudo
14    Cu  [  1.457  2.523  6.978]   1   0.008  Cu_us_gga.pseudo
15    Cu  [  4.370  2.523  6.978]   1   0.008  Cu_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 176.0
Number of bands     = 118
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



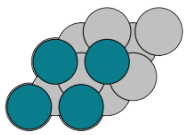
Ru overlayer:

```
---------------------------------
Dacapo calculation from Ag-subs/Ru-layer/Ag111-subs+Ru-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -18257.607047 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.023  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.023  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.023  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.023  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.046  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.046  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.046  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.046  ag_us.pseudo
 8    Ag  [  5.820  1.678  4.725]   2   0.007  ag_us.pseudo
 9    Ag  [  2.907  1.679  4.725]   2   0.007  ag_us.pseudo
10    Ag  [  7.277  4.201  4.725]   2   0.007  ag_us.pseudo
11    Ag  [  4.364  4.201  4.725]   2   0.006  ag_us.pseudo
12    Ru  [  0.001  0.001  6.984]   1   0.010  Ru_us_gga.pseudo
13    Ru  [  2.915  0.001  6.984]   1   0.010  Ru_us_gga.pseudo
14    Ru  [  1.458  2.524  6.984]   1   0.010  Ru_us_gga.pseudo
15    Ru  [  4.371  2.524  6.984]   1   0.010  Ru_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 164.0
Number of bands     = 110
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



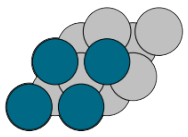
Rh overlayer:

```
---------------------------------
Dacapo calculation from Ag-subs/Rh-layer/Ag111-subs+Rh-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -18919.002068 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.020  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.020  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.020  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.020  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.229  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.229  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.229  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.229  ag_us.pseudo
 8    Ag  [  5.826  1.682  4.815]   2   0.039  ag_us.pseudo
 9    Ag  [  2.913  1.682  4.815]   2   0.039  ag_us.pseudo
10    Ag  [  7.283  4.205  4.815]   2   0.039  ag_us.pseudo
11    Ag  [  4.369  4.205  4.815]   2   0.038  ag_us.pseudo
12    Rh  [  0.000  0.000  7.075]   1   0.037  Rh_us_gga_fl.pseudo
13    Rh  [  2.914  0.000  7.075]   1   0.037  Rh_us_gga_fl.pseudo
14    Rh  [  1.457  2.523  7.075]   1   0.037  Rh_us_gga_fl.pseudo
15    Rh  [  4.370  2.523  7.075]   1   0.037  Rh_us_gga_fl.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 168.0
Number of bands     = 113
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



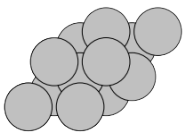
Pd overlayer:

```
---------------------------------
Dacapo calculation from Ag-subs/Pd-layer/Ag111-subs+Pd-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19723.512160 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.026  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.026  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.026  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.026  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.237  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.237  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.237  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.237  ag_us.pseudo
 8    Ag  [  5.826  1.682  4.813]   2   0.047  ag_us.pseudo
 9    Ag  [  2.913  1.682  4.813]   2   0.047  ag_us.pseudo
10    Ag  [  7.283  4.205  4.813]   2   0.047  ag_us.pseudo
11    Ag  [  4.370  4.205  4.813]   2   0.047  ag_us.pseudo
12    Pd  [  0.000  0.000  7.076]   1   0.042  046-Pd-gpe-n-6projectors-floc.uspp
13    Pd  [  2.914  0.000  7.076]   1   0.042  046-Pd-gpe-n-6projectors-floc.uspp
14    Pd  [  1.457  2.523  7.076]   1   0.042  046-Pd-gpe-n-6projectors-floc.uspp
15    Pd  [  4.370  2.523  7.076]   1   0.042  046-Pd-gpe-n-6projectors-floc.uspp

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 172.0
Number of bands     = 115
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



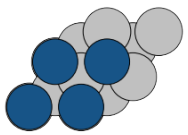
Ag overlayer:

```
---------------------------------
Dacapo calculation from Ag-subs/Ag-layer/Ag111-subs+Ag-overlayer-relaxed-DOS.nc
status = new
version = ifc ser v2-3-3
Energy = -20703.814916 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.025  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.025  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.025  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.025  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.042  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.042  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.042  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.042  ag_us.pseudo
 8    Ag  [  5.826  1.682  4.741]   2   0.021  ag_us.pseudo
 9    Ag  [  2.913  1.682  4.741]   2   0.021  ag_us.pseudo
10    Ag  [  7.283  4.205  4.741]   2   0.021  ag_us.pseudo
11    Ag  [  4.370  4.205  4.741]   2   0.021  ag_us.pseudo
12    Ag  [  0.000  0.000  7.148]   1   0.022  ag_us.pseudo
13    Ag  [  2.913  0.000  7.148]   1   0.022  ag_us.pseudo
14    Ag  [  1.457  2.523  7.148]   1   0.022  ag_us.pseudo
15    Ag  [  4.370  2.523  7.148]   1   0.022  ag_us.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 176.0
Number of bands     = 118
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



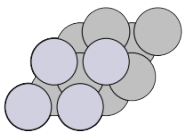
Ir overlayer:

```
---------------------------------
Dacapo calculation from Ag-subs/Ir-layer/Ag111-subs+Ir-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19716.272259 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.021  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.021  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.021  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.021  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.025  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.025  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.025  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.025  ag_us.pseudo
 8    Ag  [  5.820  1.678  4.732]   2   0.004  ag_us.pseudo
 9    Ag  [  2.907  1.678  4.732]   2   0.004  ag_us.pseudo
10    Ag  [  7.277  4.201  4.732]   2   0.004  ag_us.pseudo
11    Ag  [  4.364  4.201  4.732]   2   0.004  ag_us.pseudo
12    Ir  [ -0.001 -0.001  7.002]   1   0.007  ir_us_gga_flocal.pseudo
13    Ir  [  2.912 -0.001  7.002]   1   0.007  ir_us_gga_flocal.pseudo
14    Ir  [  1.456  2.522  7.002]   1   0.007  ir_us_gga_flocal.pseudo
15    Ir  [  4.369  2.522  7.002]   1   0.007  ir_us_gga_flocal.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 168.0
Number of bands     = 113
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



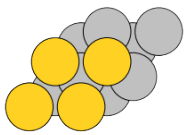
Pt overlayer:

```
---------------------------------
Dacapo calculation from Ag-subs/Pt-layer/Ag111-subs+Pt-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -20374.684333 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.033  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.033  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.033  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.033  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.024  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.024  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.024  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.024  ag_us.pseudo
 8    Ag  [  5.822  1.680  4.725]   2   0.004  ag_us.pseudo
 9    Ag  [  2.909  1.680  4.725]   2   0.003  ag_us.pseudo
10    Ag  [  7.279  4.202  4.725]   2   0.002  ag_us.pseudo
11    Ag  [  4.366  4.202  4.725]   2   0.004  ag_us.pseudo
12    Pt  [  0.002  0.001  7.024]   1   0.011  pt_us_gga.pseudo
13    Pt  [  2.915  0.001  7.024]   1   0.010  pt_us_gga.pseudo
14    Pt  [  1.458  2.524  7.024]   1   0.010  pt_us_gga.pseudo
15    Pt  [  4.372  2.524  7.024]   1   0.011  pt_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 172.0
Number of bands     = 115
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Au overlayer:

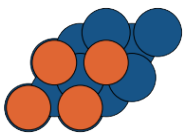
```
---------------------------------
Dacapo calculation from Ag-subs/Au-layer/Ag111-subs+Au-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -21095.045725 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.026  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.026  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.026  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.026  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.032  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.032  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.032  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.032  ag_us.pseudo
 8    Ag  [  5.826  1.682  4.725]   2   0.039  ag_us.pseudo
 9    Ag  [  2.913  1.682  4.725]   2   0.040  ag_us.pseudo
10    Ag  [  7.283  4.205  4.725]   2   0.039  ag_us.pseudo
11    Ag  [  4.370  4.205  4.725]   2   0.039  ag_us.pseudo
12    Au  [  0.000  0.000  7.152]   1   0.014  Au_us_gga.pseudo
13    Au  [  2.914  0.000  7.152]   1   0.014  Au_us_gga.pseudo
14    Au  [  1.457  2.523  7.152]   1   0.014  Au_us_gga.pseudo
15    Au  [  4.370  2.523  7.152]   1   0.014  Au_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 176.0
Number of bands     = 118
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Structures with Ir as the substrate:

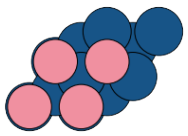
Fe overlayer:

```
--------------------------------
Dacapo calculation from Ir-subs/Fe-layer/Ir111-subs+Fe-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -15904.521444 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.414  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.414  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.414  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.414  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.370  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.370  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.370  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.370  ir_us_gga_flocal.pseudo
 8    Ir  [  5.447  1.572  4.485]   2   0.033  ir_us_gga_flocal.pseudo
 9    Ir  [  2.722  1.572  4.485]   2   0.034  ir_us_gga_flocal.pseudo
10    Ir  [  6.809  3.931  4.485]   2   0.034  ir_us_gga_flocal.pseudo
11    Ir  [  4.085  3.931  4.485]   2   0.033  ir_us_gga_flocal.pseudo
12    Fe  [ -0.000 -0.000  6.460]   1   0.039  Fe_us_gga_d2.1.8.pseudo
13    Fe  [  2.724 -0.000  6.460]   1   0.039  Fe_us_gga_d2.1.8.pseudo
14    Fe  [  1.362  2.359  6.460]   1   0.039  Fe_us_gga_d2.1.8.pseudo
15    Fe  [  4.086  2.359  6.460]   1   0.039  Fe_us_gga_d2.1.8.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 140.0
Number of bands     = 95
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
--------------------------------
```



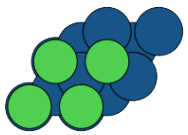
Co overlayer:

```
---------------------------------
Dacapo calculation from Ir-subs/Co-layer/Ir111-subs+Co-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -16941.680990 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.396  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.396  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.396  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.396  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.347  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.347  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.347  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.347  ir_us_gga_flocal.pseudo
 8    Ir  [  5.449  1.573  4.451]   2   0.022  ir_us_gga_flocal.pseudo
 9    Ir  [  2.724  1.573  4.451]   2   0.022  ir_us_gga_flocal.pseudo
10    Ir  [  6.811  3.932  4.451]   2   0.023  ir_us_gga_flocal.pseudo
11    Ir  [  4.086  3.932  4.451]   2   0.022  ir_us_gga_flocal.pseudo
12    Co  [ -0.000 -0.000  6.443]   1   0.040  Co_us_gga.pseudo
13    Co  [  2.724 -0.000  6.443]   1   0.040  Co_us_gga.pseudo
14    Co  [  1.362  2.359  6.443]   1   0.040  Co_us_gga.pseudo
15    Co  [  4.086  2.359  6.443]   1   0.040  Co_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 144.0
Number of bands     = 97
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



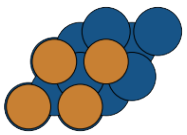
Ni overlayer:

```
---------------------------------
Dacapo calculation from Ir-subs/Ni-layer/Ir111-subs+Ni-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -17802.303557 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.379  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.379  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.379  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.379  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.355  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.355  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.355  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.355  ir_us_gga_flocal.pseudo
 8    Ir  [  5.449  1.573  4.422]   2   0.010  ir_us_gga_flocal.pseudo
 9    Ir  [  2.724  1.573  4.422]   2   0.010  ir_us_gga_flocal.pseudo
10    Ir  [  6.811  3.932  4.422]   2   0.010  ir_us_gga_flocal.pseudo
11    Ir  [  4.087  3.932  4.422]   2   0.010  ir_us_gga_flocal.pseudo
12    Ni  [ -0.000 -0.000  6.452]   1   0.028  Ni_us_gga.pseudo
13    Ni  [  2.724 -0.000  6.452]   1   0.028  Ni_us_gga.pseudo
14    Ni  [  1.362  2.359  6.452]   1   0.028  Ni_us_gga.pseudo
15    Ni  [  4.087  2.359  6.452]   1   0.028  Ni_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 148.0
Number of bands     = 100
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



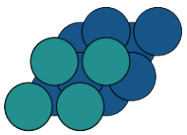
Cu overlayer:

```
---------------------------------
Dacapo calculation from Ir-subs/Cu-layer/Ir111-subs+Cu-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19280.387330 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.411  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.411  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.411  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.411  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.371  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.371  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.371  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.371  ir_us_gga_flocal.pseudo
 8    Ir  [  5.448  1.572  4.405]   2   0.010  ir_us_gga_flocal.pseudo
 9    Ir  [  2.724  1.572  4.405]   2   0.010  ir_us_gga_flocal.pseudo
10    Ir  [  6.810  3.932  4.405]   2   0.010  ir_us_gga_flocal.pseudo
11    Ir  [  4.086  3.932  4.405]   2   0.010  ir_us_gga_flocal.pseudo
12    Cu  [  0.000  0.000  6.549]   1   0.019  Cu_us_gga.pseudo
13    Cu  [  2.725  0.000  6.549]   1   0.019  Cu_us_gga.pseudo
14    Cu  [  1.362  2.360  6.549]   1   0.019  Cu_us_gga.pseudo
15    Cu  [  4.087  2.360  6.549]   1   0.019  Cu_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 152.0
Number of bands     = 102
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



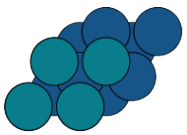
Ru overlayer:

```
---------------------------------
Dacapo calculation from Ir-subs/Ru-layer/Ir111-subs+Ru-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -15314.219925 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.337  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.337  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.337  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.337  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.350  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.350  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.350  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.350  ir_us_gga_flocal.pseudo
 8    Ir  [  5.447  1.572  4.444]   2   0.013  ir_us_gga_flocal.pseudo
 9    Ir  [  2.723  1.572  4.444]   2   0.013  ir_us_gga_flocal.pseudo
10    Ir  [  6.809  3.931  4.444]   2   0.013  ir_us_gga_flocal.pseudo
11    Ir  [  4.085  3.931  4.444]   2   0.013  ir_us_gga_flocal.pseudo
12    Ru  [  0.000  0.000  6.605]   1   0.009  Ru_us_gga.pseudo
13    Ru  [  2.725  0.000  6.605]   1   0.009  Ru_us_gga.pseudo
14    Ru  [  1.362  2.360  6.605]   1   0.009  Ru_us_gga.pseudo
15    Ru  [  4.087  2.360  6.605]   1   0.008  Ru_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 140.0
Number of bands     = 95
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



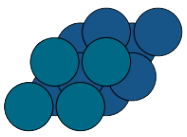
Rh overlayer:

```
---------------------------------
Dacapo calculation from Ir-subs/Rh-layer/Ir111-subs+Rh-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -15974.210880 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.312  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.312  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.312  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.312  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.321  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.321  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.321  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.321  ir_us_gga_flocal.pseudo
 8    Ir  [  5.445  1.571  4.408]   2   0.031  ir_us_gga_flocal.pseudo
 9    Ir  [  2.721  1.571  4.408]   2   0.031  ir_us_gga_flocal.pseudo
10    Ir  [  6.808  3.930  4.408]   2   0.031  ir_us_gga_flocal.pseudo
11    Ir  [  4.083  3.930  4.408]   2   0.031  ir_us_gga_flocal.pseudo
12    Rh  [  0.002  0.001  6.583]   1   0.036  Rh_us_gga_fl.pseudo
13    Rh  [  2.726  0.001  6.583]   1   0.036  Rh_us_gga_fl.pseudo
14    Rh  [  1.364  2.360  6.583]   1   0.036  Rh_us_gga_fl.pseudo
15    Rh  [  4.088  2.360  6.583]   1   0.036  Rh_us_gga_fl.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 144.0
Number of bands     = 97
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



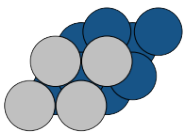
Pd overlayer:

```
---------------------------------
Dacapo calculation from Ir-subs/Pd-layer/Ir111-subs+Pd-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -16775.823458 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.395  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.395  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.395  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.395  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.373  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.373  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.373  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.373  ir_us_gga_flocal.pseudo
 8    Ir  [  5.450  1.573  4.379]   2   0.035  ir_us_gga_flocal.pseudo
 9    Ir  [  2.725  1.573  4.379]   2   0.035  ir_us_gga_flocal.pseudo
10    Ir  [  6.812  3.933  4.379]   2   0.035  ir_us_gga_flocal.pseudo
11    Ir  [  4.087  3.933  4.379]   2   0.035  ir_us_gga_flocal.pseudo
12    Pd  [ -0.001 -0.000  6.673]   1   0.022  046-Pd-gpe-n-6projectors-floc.uspp
13    Pd  [  2.724 -0.000  6.673]   1   0.022  046-Pd-gpe-n-6projectors-floc.uspp
14    Pd  [  1.362  2.359  6.673]   1   0.022  046-Pd-gpe-n-6projectors-floc.uspp
15    Pd  [  4.086  2.359  6.673]   1   0.022  046-Pd-gpe-n-6projectors-floc.uspp

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 148.0
Number of bands     = 100
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



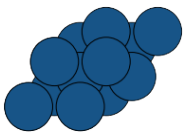
Ag overlayer:

```
---------------------------------
Dacapo calculation from Ir-subs/Ag-layer/Ir111-subs+Ag-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -17754.643612 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.419  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.419  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.419  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.419  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.486  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.486  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.486  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.486  ir_us_gga_flocal.pseudo
 8    Ir  [  5.448  1.572  4.381]   2   0.046  ir_us_gga_flocal.pseudo
 9    Ir  [  2.724  1.572  4.381]   2   0.046  ir_us_gga_flocal.pseudo
10    Ir  [  6.810  3.932  4.381]   2   0.046  ir_us_gga_flocal.pseudo
11    Ir  [  4.086  3.932  4.381]   2   0.046  ir_us_gga_flocal.pseudo
12    Ag  [  0.000  0.000  6.833]   1   0.005  ag_us.pseudo
13    Ag  [  2.725  0.000  6.833]   1   0.005  ag_us.pseudo
14    Ag  [  1.362  2.359  6.833]   1   0.005  ag_us.pseudo
15    Ag  [  4.087  2.359  6.833]   1   0.005  ag_us.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 152.0
Number of bands     = 102
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



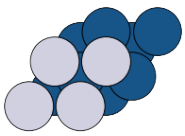
Ir overlayer:

```
---------------------------------
Dacapo calculation from Ir-subs/Ir-layer/Ir111-subs+Ir-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -16772.411581 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.331  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.331  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.331  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.331  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.325  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.325  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.325  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.325  ir_us_gga_flocal.pseudo
 8    Ir  [  5.447  1.572  4.418]   2   0.013  ir_us_gga_flocal.pseudo
 9    Ir  [  2.722  1.572  4.418]   2   0.012  ir_us_gga_flocal.pseudo
10    Ir  [  6.809  3.931  4.418]   2   0.013  ir_us_gga_flocal.pseudo
11    Ir  [  4.084  3.931  4.418]   2   0.013  ir_us_gga_flocal.pseudo
12    Ir  [  0.001  0.001  6.610]   1   0.022  ir_us_gga_flocal.pseudo
13    Ir  [  2.726  0.001  6.610]   1   0.022  ir_us_gga_flocal.pseudo
14    Ir  [  1.363  2.360  6.610]   1   0.022  ir_us_gga_flocal.pseudo
15    Ir  [  4.088  2.360  6.610]   1   0.022  ir_us_gga_flocal.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 144.0
Number of bands     = 97
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



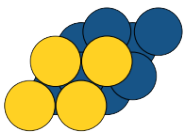
Pt overlayer:

```
---------------------------------
Dacapo calculation from Ir-subs/Pt-layer/Ir111-subs+Pt-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -17427.183316 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.404  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.404  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.404  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.404  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.342  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.342  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.342  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.342  ir_us_gga_flocal.pseudo
 8    Ir  [  5.450  1.573  4.376]   2   0.029  ir_us_gga_flocal.pseudo
 9    Ir  [  2.725  1.573  4.376]   2   0.030  ir_us_gga_flocal.pseudo
10    Ir  [  6.812  3.933  4.376]   2   0.030  ir_us_gga_flocal.pseudo
11    Ir  [  4.087  3.933  4.376]   2   0.030  ir_us_gga_flocal.pseudo
12    Pt  [ -0.001 -0.000  6.718]   1   0.018  pt_us_gga.pseudo
13    Pt  [  2.724 -0.000  6.718]   1   0.018  pt_us_gga.pseudo
14    Pt  [  1.361  2.359  6.718]   1   0.017  pt_us_gga.pseudo
15    Pt  [  4.086  2.359  6.718]   1   0.018  pt_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 148.0
Number of bands     = 100
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Au overlayer:

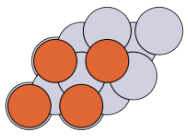
```
---------------------------------
Dacapo calculation from Ir-subs/Au-layer/Ir111-subs+Au-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -18145.410938 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.479  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.479  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.479  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.479  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.474  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.474  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.474  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.474  ir_us_gga_flocal.pseudo
 8    Ir  [  5.448  1.573  4.380]   2   0.014  ir_us_gga_flocal.pseudo
 9    Ir  [  2.724  1.573  4.380]   2   0.013  ir_us_gga_flocal.pseudo
10    Ir  [  6.811  3.932  4.380]   2   0.013  ir_us_gga_flocal.pseudo
11    Ir  [  4.086  3.932  4.380]   2   0.012  ir_us_gga_flocal.pseudo
12    Au  [  0.000  0.000  6.903]   1   0.014  Au_us_gga.pseudo
13    Au  [  2.725  0.000  6.903]   1   0.014  Au_us_gga.pseudo
14    Au  [  1.362  2.360  6.903]   1   0.014  Au_us_gga.pseudo
15    Au  [  4.087  2.360  6.903]   1   0.014  Au_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 152.0
Number of bands     = 102
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Structures with Pt as the substrate:

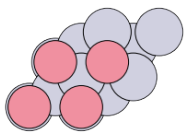
Fe overlayer:

```
---------------------------------
Dacapo calculation from Pt-subs/Fe-layer/Pt111-subs+Fe-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -17864.511503 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt   [  0.000  0.000  0.000]   4   0.320  pt_us_gga.pseudo
 1    Pt   [  2.819  0.000  0.000]   4   0.320  pt_us_gga.pseudo
 2    Pt   [  1.410  2.442  0.000]   4   0.320  pt_us_gga.pseudo
 3    Pt   [  4.229  2.442  0.000]   4   0.320  pt_us_gga.pseudo
 4    Pt   [  1.410  0.814  2.302]   3   0.332  pt_us_gga.pseudo
 5    Pt   [  4.229  0.814  2.302]   3   0.332  pt_us_gga.pseudo
 6    Pt   [  2.819  3.255  2.302]   3   0.332  pt_us_gga.pseudo
 7    Pt   [  5.638  3.255  2.302]   3   0.332  pt_us_gga.pseudo
 8    Pt   [  5.637  1.627  4.655]   2   0.001  pt_us_gga.pseudo
 9    Pt   [  2.817  1.627  4.655]   2   0.001  pt_us_gga.pseudo
10    Pt   [  7.046  4.068  4.655]   2   0.001  pt_us_gga.pseudo
11    Pt   [  4.227  4.068  4.655]   2   0.000  pt_us_gga.pseudo
12    Fe   [ -0.001 -0.001  6.617]   1   0.007  Fe_us_gga_d2.1.8.pseudo
13    Fe   [  2.818 -0.001  6.617]   1   0.007  Fe_us_gga_d2.1.8.pseudo
14    Fe   [  1.409  2.441  6.617]   1   0.007  Fe_us_gga_d2.1.8.pseudo
15    Fe   [  4.228  2.441  6.617]   1   0.007  Fe_us_gga_d2.1.8.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 152.0
Number of bands     = 102
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



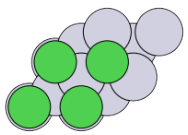
Co overlayer:

```
---------------------------------
Dacapo calculation from Pt-subs/Co-layer/Pt111-subs+Co-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -18901.884513 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.291  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.291  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.291  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.291  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.244  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.244  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.244  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.244  pt_us_gga.pseudo
 8    Pt  [  5.637  1.627  4.634]   2   0.024  pt_us_gga.pseudo
 9    Pt  [  2.818  1.627  4.634]   2   0.024  pt_us_gga.pseudo
10    Pt  [  7.047  4.068  4.634]   2   0.024  pt_us_gga.pseudo
11    Pt  [  4.227  4.068  4.634]   2   0.024  pt_us_gga.pseudo
12    Co  [ -0.001 -0.001  6.584]   1   0.012  Co_us_gga.pseudo
13    Co  [  2.818 -0.001  6.584]   1   0.012  Co_us_gga.pseudo
14    Co  [  1.408  2.441  6.584]   1   0.012  Co_us_gga.pseudo
15    Co  [  4.227  2.441  6.584]   1   0.012  Co_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 156.0
Number of bands     = 105
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



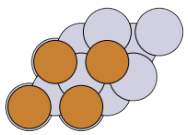
Ni overlayer:

```
---------------------------------
Dacapo calculation from Pt-subs/Ni-layer/Pt111-subs+Ni-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19763.003290 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.267  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.267  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.267  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.267  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.219  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.219  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.219  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.219  pt_us_gga.pseudo
 8    Pt  [  5.637  1.627  4.630]   2   0.022  pt_us_gga.pseudo
 9    Pt  [  2.818  1.627  4.630]   2   0.022  pt_us_gga.pseudo
10    Pt  [  7.047  4.069  4.630]   2   0.022  pt_us_gga.pseudo
11    Pt  [  4.228  4.069  4.630]   2   0.022  pt_us_gga.pseudo
12    Ni  [ -0.002 -0.001  6.609]   1   0.006  Ni_us_gga.pseudo
13    Ni  [  2.817 -0.001  6.609]   1   0.006  Ni_us_gga.pseudo
14    Ni  [  1.407  2.440  6.609]   1   0.006  Ni_us_gga.pseudo
15    Ni  [  4.227  2.440  6.609]   1   0.006  Ni_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 160.0
Number of bands     = 108
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



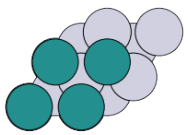
Cu overlayer:

```
---------------------------------
Dacapo calculation from Pt-subs/Cu-layer/Pt111-subs+Cu-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -21242.478515 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.249  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.249  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.249  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.249  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.203  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.203  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.203  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.203  pt_us_gga.pseudo
 8    Pt  [  5.640  1.628  4.649]   2   0.004  pt_us_gga.pseudo
 9    Pt  [  2.821  1.628  4.649]   2   0.005  pt_us_gga.pseudo
10    Pt  [  7.049  4.070  4.649]   2   0.005  pt_us_gga.pseudo
11    Pt  [  4.230  4.070  4.649]   2   0.005  pt_us_gga.pseudo
12    Cu  [ -0.002 -0.001  6.726]   1   0.022  Cu_us_gga.pseudo
13    Cu  [  2.817 -0.001  6.726]   1   0.022  Cu_us_gga.pseudo
14    Cu  [  1.408  2.440  6.726]   1   0.022  Cu_us_gga.pseudo
15    Cu  [  4.227  2.440  6.726]   1   0.022  Cu_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 164.0
Number of bands     = 110
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



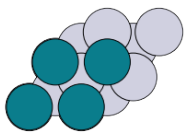
Ru overlayer:

```
---------------------------------
Dacapo calculation from Pt-subs/Ru-layer/Pt111-subs+Ru-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -17274.369776 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.315  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.315  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.315  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.315  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.334  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.334  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.334  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.334  pt_us_gga.pseudo
 8    Pt  [  5.637  1.627  4.620]   2   0.010  pt_us_gga.pseudo
 9    Pt  [  2.818  1.627  4.620]   2   0.010  pt_us_gga.pseudo
10    Pt  [  7.047  4.069  4.620]   2   0.011  pt_us_gga.pseudo
11    Pt  [  4.228  4.069  4.620]   2   0.011  pt_us_gga.pseudo
12    Ru  [ -0.001 -0.000  6.781]   1   0.011  Ru_us_gga.pseudo
13    Ru  [  2.819 -0.000  6.781]   1   0.011  Ru_us_gga.pseudo
14    Ru  [  1.409  2.441  6.781]   1   0.011  Ru_us_gga.pseudo
15    Ru  [  4.228  2.441  6.781]   1   0.011  Ru_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 152.0
Number of bands     = 102
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



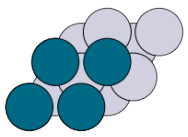
Rh overlayer:

```
---------------------------------
Dacapo calculation from Pt-subs/Rh-layer/Pt111-subs+Rh-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -17934.346514 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.263  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.263  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.263  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.263  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.284  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.284  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.284  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.284  pt_us_gga.pseudo
 8    Pt  [  5.635  1.626  4.616]   2   0.017  pt_us_gga.pseudo
 9    Pt  [  2.816  1.626  4.616]   2   0.016  pt_us_gga.pseudo
10    Pt  [  7.045  4.067  4.616]   2   0.015  pt_us_gga.pseudo
11    Pt  [  4.226  4.067  4.616]   2   0.015  pt_us_gga.pseudo
12    Rh  [  0.000  0.000  6.798]   1   0.014  Rh_us_gga_fl.pseudo
13    Rh  [  2.819  0.000  6.798]   1   0.014  Rh_us_gga_fl.pseudo
14    Rh  [  1.410  2.442  6.798]   1   0.014  Rh_us_gga_fl.pseudo
15    Rh  [  4.229  2.442  6.798]   1   0.014  Rh_us_gga_fl.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 156.0
Number of bands     = 105
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



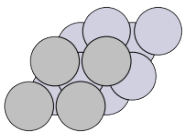
Pd overlayer:

```
---------------------------------
Dacapo calculation from Pt-subs/Pd-layer/Pt111-subs+Pd-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -18736.974863 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.217  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.217  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.217  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.217  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.226  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.226  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.226  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.226  pt_us_gga.pseudo
 8    Pt  [  5.638  1.627  4.620]   2   0.007  pt_us_gga.pseudo
 9    Pt  [  2.819  1.627  4.620]   2   0.007  pt_us_gga.pseudo
10    Pt  [  7.047  4.069  4.620]   2   0.007  pt_us_gga.pseudo
11    Pt  [  4.228  4.069  4.620]   2   0.006  pt_us_gga.pseudo
12    Pd  [  0.000  0.000  6.898]   1   0.017  046-Pd-gpe-n-6projectors-floc.uspp
13    Pd  [  2.819  0.000  6.898]   1   0.017  046-Pd-gpe-n-6projectors-floc.uspp
14    Pd  [  1.410  2.442  6.898]   1   0.017  046-Pd-gpe-n-6projectors-floc.uspp
15    Pd  [  4.229  2.442  6.898]   1   0.017  046-Pd-gpe-n-6projectors-floc.uspp

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 160.0
Number of bands     = 108
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



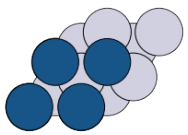
Ag overlayer:

```
---------------------------------
Dacapo calculation from Pt-subs/Ag-layer/Pt111-subs+Ag-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19717.550131 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.234  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.234  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.234  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.234  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.235  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.235  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.235  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.235  pt_us_gga.pseudo
 8    Pt  [  5.638  1.628  4.653]   2   0.027  pt_us_gga.pseudo
 9    Pt  [  2.819  1.628  4.653]   2   0.027  pt_us_gga.pseudo
10    Pt  [  7.048  4.069  4.653]   2   0.028  pt_us_gga.pseudo
11    Pt  [  4.229  4.069  4.653]   2   0.028  pt_us_gga.pseudo
12    Ag  [ -0.003 -0.002  7.037]   1   0.018  ag_us.pseudo
13    Ag  [  2.817 -0.002  7.037]   1   0.018  ag_us.pseudo
14    Ag  [  1.407  2.440  7.037]   1   0.018  ag_us.pseudo
15    Ag  [  4.226  2.440  7.037]   1   0.019  ag_us.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 164.0
Number of bands     = 110
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



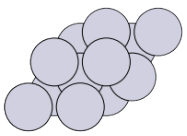
Ir overlayer:

```
---------------------------------
Dacapo calculation from Pt-subs/Ir-layer/Pt111-subs+Ir-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -18732.028311 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.263  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.263  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.263  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.263  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.257  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.257  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.257  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.257  pt_us_gga.pseudo
 8    Pt  [  5.636  1.627  4.609]   2   0.033  pt_us_gga.pseudo
 9    Pt  [  2.817  1.627  4.609]   2   0.033  pt_us_gga.pseudo
10    Pt  [  7.046  4.068  4.609]   2   0.033  pt_us_gga.pseudo
11    Pt  [  4.227  4.068  4.609]   2   0.033  pt_us_gga.pseudo
12    Ir  [ -0.001 -0.001  6.801]   1   0.017  ir_us_gga_flocal.pseudo
13    Ir  [  2.818 -0.001  6.801]   1   0.017  ir_us_gga_flocal.pseudo
14    Ir  [  1.408  2.441  6.801]   1   0.017  ir_us_gga_flocal.pseudo
15    Ir  [  4.228  2.441  6.801]   1   0.017  ir_us_gga_flocal.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 156.0
Number of bands     = 105
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



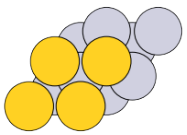
Pt overlayer:

```
---------------------------------
Dacapo calculation from Pt-subs/Pt-layer/Pt111-subs+Pt-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19388.041900 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.200  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.200  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.200  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.200  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.095  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.095  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.095  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.095  pt_us_gga.pseudo
 8    Pt  [  5.638  1.627  4.594]   2   0.040  pt_us_gga.pseudo
 9    Pt  [  2.819  1.627  4.594]   2   0.041  pt_us_gga.pseudo
10    Pt  [  7.048  4.069  4.594]   2   0.041  pt_us_gga.pseudo
11    Pt  [  4.228  4.069  4.594]   2   0.041  pt_us_gga.pseudo
12    Pt  [ -0.000 -0.000  6.918]   1   0.045  pt_us_gga.pseudo
13    Pt  [  2.819 -0.000  6.918]   1   0.045  pt_us_gga.pseudo
14    Pt  [  1.410  2.442  6.918]   1   0.045  pt_us_gga.pseudo
15    Pt  [  4.229  2.442  6.918]   1   0.045  pt_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 160.0
Number of bands     = 108
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Au overlayer:

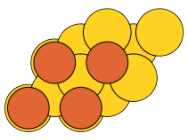
```
---------------------------------
Dacapo calculation from Pt-subs/Au-layer/Pt111-subs+Au-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -20108.070998 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.193  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.193  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.193  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.193  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.201  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.201  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.201  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.201  pt_us_gga.pseudo
 8    Pt  [  5.640  1.628  4.638]   2   0.025  pt_us_gga.pseudo
 9    Pt  [  2.820  1.628  4.638]   2   0.027  pt_us_gga.pseudo
10    Pt  [  7.049  4.070  4.638]   2   0.025  pt_us_gga.pseudo
11    Pt  [  4.230  4.070  4.638]   2   0.026  pt_us_gga.pseudo
12    Au  [ -0.002 -0.001  7.111]   1   0.034  Au_us_gga.pseudo
13    Au  [  2.818 -0.001  7.111]   1   0.034  Au_us_gga.pseudo
14    Au  [  1.408  2.441  7.111]   1   0.034  Au_us_gga.pseudo
15    Au  [  4.227  2.441  7.111]   1   0.034  Au_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 164.0
Number of bands     = 110
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Structures with Au as the substrate:

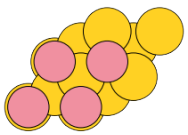
Fe overlayer:

```
--------------------------------
Dacapo calculation from Au-subs/Fe-layer/Au111-subs+Fe-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -20019.256383 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.126  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.126  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.126  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.126  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.157  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.157  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.157  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.157  Au_us_gga.pseudo
 8    Au  [  5.896  1.702  4.845]   2   0.002  Au_us_gga.pseudo
 9    Au  [  2.947  1.702  4.845]   2   0.002  Au_us_gga.pseudo
10    Au  [  7.370  4.255  4.845]   2   0.002  Au_us_gga.pseudo
11    Au  [  4.422  4.255  4.845]   2   0.002  Au_us_gga.pseudo
12    Fe  [  0.000  0.000  6.883]   1   0.005  Fe_us_gga_d2.1.8.pseudo
13    Fe  [  2.949  0.000  6.883]   1   0.005  Fe_us_gga_d2.1.8.pseudo
14    Fe  [  1.475  2.554  6.883]   1   0.005  Fe_us_gga_d2.1.8.pseudo
15    Fe  [  4.423  2.554  6.883]   1   0.005  Fe_us_gga_d2.1.8.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 164.0
Number of bands     = 110
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
--------------------------------
```



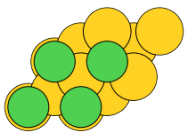
Co overlayer:

```
---------------------------------
Dacapo calculation from Au-subs/Co-layer/Au111-subs+Co-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -21057.574307 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.114  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.114  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.114  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.114  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.138  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.138  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.138  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.138  Au_us_gga.pseudo
 8    Au  [  5.897  1.702  4.836]   2   0.011  Au_us_gga.pseudo
 9    Au  [  2.948  1.702  4.836]   2   0.011  Au_us_gga.pseudo
10    Au  [  7.371  4.256  4.836]   2   0.011  Au_us_gga.pseudo
11    Au  [  4.423  4.256  4.836]   2   0.010  Au_us_gga.pseudo
12    Co  [  0.001  0.000  6.864]   1   0.003  Co_us_gga.pseudo
13    Co  [  2.949  0.000  6.864]   1   0.003  Co_us_gga.pseudo
14    Co  [  1.475  2.554  6.864]   1   0.004  Co_us_gga.pseudo
15    Co  [  4.424  2.554  6.864]   1   0.003  Co_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 168.0
Number of bands     = 113
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



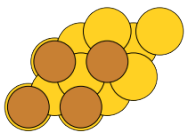
Ni overlayer:

```
---------------------------------
Dacapo calculation from Au-subs/Ni-layer/Au111-subs+Ni-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -21919.659574 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.111  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.111  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.111  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.111  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.134  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.134  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.134  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.134  Au_us_gga.pseudo
 8    Au  [  5.897  1.702  4.834]   2   0.006  Au_us_gga.pseudo
 9    Au  [  2.948  1.702  4.834]   2   0.006  Au_us_gga.pseudo
10    Au  [  7.371  4.256  4.834]   2   0.006  Au_us_gga.pseudo
11    Au  [  4.422  4.256  4.834]   2   0.006  Au_us_gga.pseudo
12    Ni  [ -0.000 -0.000  6.860]   1   0.002  Ni_us_gga.pseudo
13    Ni  [  2.949 -0.000  6.860]   1   0.002  Ni_us_gga.pseudo
14    Ni  [  1.474  2.554  6.860]   1   0.002  Ni_us_gga.pseudo
15    Ni  [  4.423  2.554  6.860]   1   0.002  Ni_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 172.0
Number of bands     = 115
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



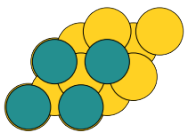
Cu overlayer:

```
---------------------------------
Dacapo calculation from Au-subs/Cu-layer/Au111-subs+Cu-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -23399.743592 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.116  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.117  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.117  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.117  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.276  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.276  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.276  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.276  Au_us_gga.pseudo
 8    Au  [  5.898  1.703  4.888]   2   0.003  Au_us_gga.pseudo
 9    Au  [  2.950  1.703  4.888]   2   0.003  Au_us_gga.pseudo
10    Au  [  7.373  4.257  4.888]   2   0.003  Au_us_gga.pseudo
11    Au  [  4.424  4.257  4.888]   2   0.005  Au_us_gga.pseudo
12    Cu  [  0.000  0.000  6.997]   1   0.037  Cu_us_gga.pseudo
13    Cu  [  2.949  0.000  6.997]   1   0.037  Cu_us_gga.pseudo
14    Cu  [  1.475  2.554  6.997]   1   0.037  Cu_us_gga.pseudo
15    Cu  [  4.423  2.554  6.997]   1   0.037  Cu_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 176.0
Number of bands     = 118
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



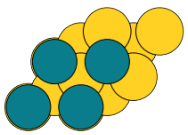
Ru overlayer:

```
--------------------------------
Dacapo calculation from Au-subs/Ru-layer/Au111-subs+Ru-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19429.504933 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.099  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.099  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.099  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.099  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.096  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.096  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.096  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.096  Au_us_gga.pseudo
 8    Au  [  5.895  1.701  4.797]   2   0.012  Au_us_gga.pseudo
 9    Au  [  2.946  1.701  4.797]   2   0.012  Au_us_gga.pseudo
10    Au  [  7.369  4.254  4.797]   2   0.012  Au_us_gga.pseudo
11    Au  [  4.420  4.254  4.797]   2   0.012  Au_us_gga.pseudo
12    Ru  [  0.002  0.001  7.015]   1   0.003  Ru_us_gga.pseudo
13    Ru  [  2.951  0.001  7.015]   1   0.003  Ru_us_gga.pseudo
14    Ru  [  1.477  2.555  7.015]   1   0.003  Ru_us_gga.pseudo
15    Ru  [  4.425  2.555  7.015]   1   0.003  Ru_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 164.0
Number of bands     = 110
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
--------------------------------
```



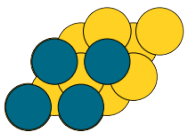
Rh overlayer:

```
---------------------------------
Dacapo calculation from Au-subs/Rh-layer/Au111-subs+Rh-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -20090.768396 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.090  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.090  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.090  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.089  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.091  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.091  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.091  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.091  Au_us_gga.pseudo
 8    Au  [  5.896  1.702  4.809]   2   0.003  Au_us_gga.pseudo
 9    Au  [  2.947  1.702  4.809]   2   0.002  Au_us_gga.pseudo
10    Au  [  7.370  4.255  4.809]   2   0.002  Au_us_gga.pseudo
11    Au  [  4.422  4.255  4.809]   2   0.002  Au_us_gga.pseudo
12    Rh  [  0.002  0.001  7.035]   1   0.002  Rh_us_gga_fl.pseudo
13    Rh  [  2.950  0.001  7.035]   1   0.002  Rh_us_gga_fl.pseudo
14    Rh  [  1.476  2.555  7.035]   1   0.002  Rh_us_gga_fl.pseudo
15    Rh  [  4.425  2.555  7.035]   1   0.002  Rh_us_gga_fl.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 168.0
Number of bands     = 113
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



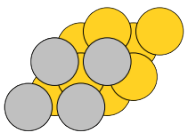
Pd overlayer:

```
---------------------------------
Dacapo calculation from Au-subs/Pd-layer/Au111-subs+Pd-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -20895.197225 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.101  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.101  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.101  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.101  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.076  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.076  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.076  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.076  Au_us_gga.pseudo
 8    Au  [  5.899  1.703  4.805]   2   0.009  Au_us_gga.pseudo
 9    Au  [  2.950  1.703  4.805]   2   0.008  Au_us_gga.pseudo
10    Au  [  7.373  4.257  4.805]   2   0.009  Au_us_gga.pseudo
11    Au  [  4.424  4.257  4.805]   2   0.008  Au_us_gga.pseudo
12    Pd  [  0.002  0.001  7.056]   1   0.011  046-Pd-gpe-n-6projectors-floc.uspp
13    Pd  [  2.951  0.001  7.056]   1   0.011  046-Pd-gpe-n-6projectors-floc.uspp
14    Pd  [  1.476  2.555  7.056]   1   0.011  046-Pd-gpe-n-6projectors-floc.uspp
15    Pd  [  4.425  2.555  7.056]   1   0.011  046-Pd-gpe-n-6projectors-floc.uspp

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 172.0
Number of bands     = 115
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



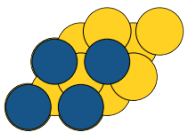
Ag overlayer:

```
---------------------------------
Dacapo calculation from Au-subs/Ag-layer/Au111-subs+Ag-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -21875.820170 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.104  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.104  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.104  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.104  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.107  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.107  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.107  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.107  Au_us_gga.pseudo
 8    Au  [  5.898  1.703  4.832]   2   0.026  Au_us_gga.pseudo
 9    Au  [  2.949  1.703  4.832]   2   0.026  Au_us_gga.pseudo
10    Au  [  7.372  4.256  4.832]   2   0.026  Au_us_gga.pseudo
11    Au  [  4.423  4.256  4.832]   2   0.026  Au_us_gga.pseudo
12    Ag  [  0.000  0.000  7.202]   1   0.005  ag_us.pseudo
13    Ag  [  2.949  0.000  7.202]   1   0.005  ag_us.pseudo
14    Ag  [  1.474  2.554  7.202]   1   0.005  ag_us.pseudo
15    Ag  [  4.423  2.554  7.202]   1   0.005  ag_us.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 176.0
Number of bands     = 118
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



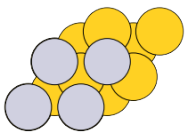
Ir overlayer:

```
---------------------------------
Dacapo calculation from Au-subs/Ir-layer/Au111-subs+Ir-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -20887.532184 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.088  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.088  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.088  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.088  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.133  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.133  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.133  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.133  Au_us_gga.pseudo
 8    Au  [  5.896  1.702  4.810]   2   0.043  Au_us_gga.pseudo
 9    Au  [  2.947  1.702  4.810]   2   0.043  Au_us_gga.pseudo
10    Au  [  7.370  4.255  4.810]   2   0.043  Au_us_gga.pseudo
11    Au  [  4.422  4.255  4.810]   2   0.043  Au_us_gga.pseudo
12    Ir  [ -0.001 -0.000  7.052]   1   0.016  ir_us_gga_flocal.pseudo
13    Ir  [  2.948 -0.000  7.052]   1   0.017  ir_us_gga_flocal.pseudo
14    Ir  [  1.474  2.553  7.052]   1   0.016  ir_us_gga_flocal.pseudo
15    Ir  [  4.422  2.553  7.052]   1   0.017  ir_us_gga_flocal.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 168.0
Number of bands     = 113
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



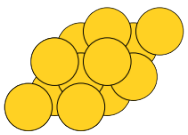
Pt overlayer:

```
---------------------------------
Dacapo calculation from Au-subs/Pt-layer/Au111-subs+Pt-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -21545.813448 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.098  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.098  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.098  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.098  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.067  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.067  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.067  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.067  Au_us_gga.pseudo
 8    Au  [  5.895  1.701  4.790]   2   0.008  Au_us_gga.pseudo
 9    Au  [  2.946  1.701  4.790]   2   0.008  Au_us_gga.pseudo
10    Au  [  7.369  4.255  4.790]   2   0.009  Au_us_gga.pseudo
11    Au  [  4.421  4.255  4.790]   2   0.008  Au_us_gga.pseudo
12    Pt  [  0.000  0.000  7.102]   1   0.007  pt_us_gga.pseudo
13    Pt  [  2.949  0.000  7.102]   1   0.007  pt_us_gga.pseudo
14    Pt  [  1.475  2.554  7.102]   1   0.007  pt_us_gga.pseudo
15    Pt  [  4.423  2.554  7.102]   1   0.006  pt_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 172.0
Number of bands     = 115
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Au overlayer:

```
---------------------------------
Dacapo calculation from Au-subs/Au-layer/Au111-subs+Au-overlayer-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -22266.561178 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.096  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.096  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.096  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.096  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.065  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.065  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.065  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.065  Au_us_gga.pseudo
 8    Au  [  5.898  1.703  4.802]   2   0.015  Au_us_gga.pseudo
 9    Au  [  2.949  1.703  4.802]   2   0.014  Au_us_gga.pseudo
10    Au  [  7.372  4.256  4.802]   2   0.014  Au_us_gga.pseudo
11    Au  [  4.423  4.256  4.802]   2   0.015  Au_us_gga.pseudo
12    Au  [  0.001  0.000  7.235]   1   0.022  Au_us_gga.pseudo
13    Au  [  2.949  0.000  7.235]   1   0.022  Au_us_gga.pseudo
14    Au  [  1.475  2.554  7.235]   1   0.022  Au_us_gga.pseudo
15    Au  [  4.424  2.554  7.235]   1   0.022  Au_us_gga.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 176.0
Number of bands     = 118
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```

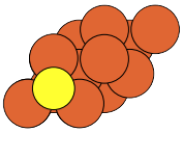


S POISONED SURFACE STRUCTURES

Structures with Fe as the substrate:

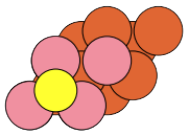
Fe overlayer:

```
---------------------------------
Dacapo calculation from Fe-subs+S/Fe-layer/Fe111-sub+Fe-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -13632.192211 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9144  0.0000  0.0000] 4.91
a1 [ 2.4572  4.2560  0.0000] 4.91
a2 [ 0.0000  0.0000  18.0252] 18.03
No stress calculated.
Volume = 377.01 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Fe  [  0.000  0.000  0.000]   4   0.618  Fe_us_gga_d2.1.8.pseudo
 1    Fe  [  2.457  0.000  0.000]   4   0.617  Fe_us_gga_d2.1.8.pseudo
 2    Fe  [  1.229  2.128  0.000]   4   0.617  Fe_us_gga_d2.1.8.pseudo
 3    Fe  [  3.686  2.128  0.000]   4   0.409  Fe_us_gga_d2.1.8.pseudo
 4    Fe  [  1.229  0.709  2.006]   3   0.624  Fe_us_gga_d2.1.8.pseudo
 5    Fe  [  3.686  0.709  2.006]   3   0.595  Fe_us_gga_d2.1.8.pseudo
 6    Fe  [  2.457  2.837  2.006]   3   0.595  Fe_us_gga_d2.1.8.pseudo
 7    Fe  [  4.914  2.837  2.006]   3   0.590  Fe_us_gga_d2.1.8.pseudo
 8    Fe  [  4.913  1.424  4.060]   2   0.032  Fe_us_gga_d2.1.8.pseudo
 9    Fe  [  2.465  1.423  4.059]   2   0.034  Fe_us_gga_d2.1.8.pseudo
10    Fe  [  6.146  3.548  3.932]   2   0.039  Fe_us_gga_d2.1.8.pseudo
11    Fe  [  3.689  3.543  4.060]   2   0.032  Fe_us_gga_d2.1.8.pseudo
12    Fe  [ -0.029 -0.017  6.001]   1   0.038  Fe_us_gga_d2.1.8.pseudo
13    Fe  [  2.489 -0.015  6.001]   1   0.036  Fe_us_gga_d2.1.8.pseudo
14    Fe  [  1.231  2.164  6.001]   1   0.036  Fe_us_gga_d2.1.8.pseudo
15    Fe  [  3.688  2.129  5.958]   1   0.007  Fe_us_gga_d2.1.8.pseudo
16     S  [  1.229  0.710  7.635]   0   0.046  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 134.0
Number of bands     = 91
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



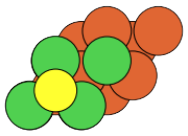
Co overlayer:

```
---------------------------------
Dacapo calculation from Fe-subs+S/Co-layer/Fe111-sub+Co-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -14668.980642 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9144  0.0000  0.0000] 4.91
a1 [ 2.4572  4.2560  0.0000] 4.91
a2 [ 0.0000  0.0000  18.0252] 18.03
No stress calculated.
Volume = 377.01 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Fe  [  0.000  0.000  0.000]   4   0.512  Fe_us_gga_d2.1.8.pseudo
 1    Fe  [  2.457  0.000  0.000]   4   0.509  Fe_us_gga_d2.1.8.pseudo
 2    Fe  [  1.229  2.128  0.000]   4   0.509  Fe_us_gga_d2.1.8.pseudo
 3    Fe  [  3.686  2.128  0.000]   4   0.472  Fe_us_gga_d2.1.8.pseudo
 4    Fe  [  1.229  0.709  2.006]   3   0.504  Fe_us_gga_d2.1.8.pseudo
 5    Fe  [  3.686  0.709  2.006]   3   0.467  Fe_us_gga_d2.1.8.pseudo
 6    Fe  [  2.457  2.837  2.006]   3   0.467  Fe_us_gga_d2.1.8.pseudo
 7    Fe  [  4.914  2.837  2.006]   3   0.460  Fe_us_gga_d2.1.8.pseudo
 8    Fe  [  4.915  1.419  4.017]   2   0.016  Fe_us_gga_d2.1.8.pseudo
 9    Fe  [  2.457  1.419  4.018]   2   0.017  Fe_us_gga_d2.1.8.pseudo
10    Fe  [  6.144  3.547  3.950]   2   0.001  Fe_us_gga_d2.1.8.pseudo
11    Fe  [  3.686  3.547  4.017]   2   0.016  Fe_us_gga_d2.1.8.pseudo
12    Co  [ -0.014 -0.008  6.021]   1   0.042  Co_us_gga.pseudo
13    Co  [  2.474 -0.009  6.020]   1   0.038  Co_us_gga.pseudo
14    Co  [  1.230  2.147  6.020]   1   0.038  Co_us_gga.pseudo
15    Co  [  3.687  2.129  5.963]   1   0.032  Co_us_gga.pseudo
16     S  [  1.231  0.711  7.635]   0   0.045  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 138.0
Number of bands     = 93
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



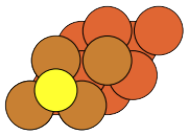
Ni overlayer:

```
---------------------------------
Dacapo calculation from Fe-subs+S/Ni-layer/Fe111-sub+Ni-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -15528.645034 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9144  0.0000  0.0000] 4.91
a1 [ 2.4572  4.2560  0.0000] 4.91
a2 [ 0.0000  0.0000  18.0252] 18.03
No stress calculated.
Volume = 377.01 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Fe  [  0.000  0.000  0.000]   4   0.406  Fe_us_gga_d2.1.8.pseudo
 1    Fe  [  2.457  0.000  0.000]   4   0.405  Fe_us_gga_d2.1.8.pseudo
 2    Fe  [  1.229  2.128  0.000]   4   0.405  Fe_us_gga_d2.1.8.pseudo
 3    Fe  [  3.686  2.128  0.000]   4   0.484  Fe_us_gga_d2.1.8.pseudo
 4    Fe  [  1.229  0.709  2.006]   3   0.380  Fe_us_gga_d2.1.8.pseudo
 5    Fe  [  3.686  0.709  2.006]   3   0.448  Fe_us_gga_d2.1.8.pseudo
 6    Fe  [  2.457  2.837  2.006]   3   0.448  Fe_us_gga_d2.1.8.pseudo
 7    Fe  [  4.914  2.837  2.006]   3   0.440  Fe_us_gga_d2.1.8.pseudo
 8    Fe  [  4.916  1.418  3.970]   2   0.011  Fe_us_gga_d2.1.8.pseudo
 9    Fe  [  2.458  1.419  3.970]   2   0.012  Fe_us_gga_d2.1.8.pseudo
10    Fe  [  6.142  3.546  3.962]   2   0.010  Fe_us_gga_d2.1.8.pseudo
11    Fe  [  3.686  3.548  3.970]   2   0.011  Fe_us_gga_d2.1.8.pseudo
12    Ni  [ -0.018 -0.010  6.040]   1   0.049  Ni_us_gga.pseudo
13    Ni  [  2.476 -0.010  6.039]   1   0.047  Ni_us_gga.pseudo
14    Ni  [  1.230  2.149  6.039]   1   0.047  Ni_us_gga.pseudo
15    Ni  [  3.687  2.129  6.012]   1   0.027  Ni_us_gga.pseudo
16     S  [  1.229  0.710  7.645]   0   0.013  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 142.0
Number of bands     = 96
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



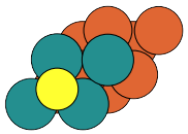
Cu overlayer:

```
---------------------------------
Dacapo calculation from Fe-subs+S/Cu-layer/Fe111-sub+Cu-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -17004.997530 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9144  0.0000  0.0000] 4.91
a1 [ 2.4572  4.2560  0.0000] 4.91
a2 [ 0.0000  0.0000  18.0252] 18.03
No stress calculated.
Volume = 377.01 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Fe  [  0.000  0.000  0.000]   4   0.363  Fe_us_gga_d2.1.8.pseudo
 1    Fe  [  2.457  0.000  0.000]   4   0.363  Fe_us_gga_d2.1.8.pseudo
 2    Fe  [  1.229  2.128  0.000]   4   0.363  Fe_us_gga_d2.1.8.pseudo
 3    Fe  [  3.686  2.128  0.000]   4   0.488  Fe_us_gga_d2.1.8.pseudo
 4    Fe  [  1.229  0.709  2.006]   3   0.588  Fe_us_gga_d2.1.8.pseudo
 5    Fe  [  3.686  0.709  2.006]   3   0.530  Fe_us_gga_d2.1.8.pseudo
 6    Fe  [  2.457  2.837  2.006]   3   0.530  Fe_us_gga_d2.1.8.pseudo
 7    Fe  [  4.914  2.837  2.006]   3   0.539  Fe_us_gga_d2.1.8.pseudo
 8    Fe  [  4.913  1.423  3.918]   2   0.005  Fe_us_gga_d2.1.8.pseudo
 9    Fe  [  2.465  1.423  3.918]   2   0.006  Fe_us_gga_d2.1.8.pseudo
10    Fe  [  6.146  3.548  3.989]   2   0.020  Fe_us_gga_d2.1.8.pseudo
11    Fe  [  3.689  3.543  3.918]   2   0.005  Fe_us_gga_d2.1.8.pseudo
12    Cu  [ -0.015 -0.008  6.094]   1   0.015  Cu_us_gga.pseudo
13    Cu  [  2.474 -0.008  6.094]   1   0.014  Cu_us_gga.pseudo
14    Cu  [  1.230  2.147  6.094]   1   0.014  Cu_us_gga.pseudo
15    Cu  [  3.687  2.129  6.074]   1   0.003  Cu_us_gga.pseudo
16     S  [  1.228  0.709  7.825]   0   0.010  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 146.0
Number of bands     = 98
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



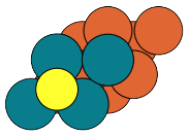
Ru overlayer:

```
---------------------------------
Dacapo calculation from Fe-subs+S/Ru-layer/Fe111-sub+Ru-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -13037.762716 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9144  0.0000  0.0000] 4.91
a1 [ 2.4572  4.2560  0.0000] 4.91
a2 [ 0.0000  0.0000  18.0252] 18.03
No stress calculated.
Volume = 377.01 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Fe  [  0.000  0.000  0.000]   4   0.468  Fe_us_gga_d2.1.8.pseudo
 1    Fe  [  2.457  0.000  0.000]   4   0.466  Fe_us_gga_d2.1.8.pseudo
 2    Fe  [  1.229  2.128  0.000]   4   0.466  Fe_us_gga_d2.1.8.pseudo
 3    Fe  [  3.686  2.128  0.000]   4   0.412  Fe_us_gga_d2.1.8.pseudo
 4    Fe  [  1.229  0.709  2.006]   3   0.044  Fe_us_gga_d2.1.8.pseudo
 5    Fe  [  3.686  0.709  2.006]   3   0.722  Fe_us_gga_d2.1.8.pseudo
 6    Fe  [  2.457  2.837  2.006]   3   0.722  Fe_us_gga_d2.1.8.pseudo
 7    Fe  [  4.914  2.837  2.006]   3   0.704  Fe_us_gga_d2.1.8.pseudo
 8    Fe  [  4.930  1.413  3.995]   2   0.023  Fe_us_gga_d2.1.8.pseudo
 9    Fe  [  2.450  1.415  3.997]   2   0.027  Fe_us_gga_d2.1.8.pseudo
10    Fe  [  6.148  3.549  3.931]   2   0.004  Fe_us_gga_d2.1.8.pseudo
11    Fe  [  3.689  3.563  3.995]   2   0.023  Fe_us_gga_d2.1.8.pseudo
12    Ru  [ -0.018 -0.011  6.096]   1   0.004  Ru_us_gga.pseudo
13    Ru  [  2.478 -0.011  6.096]   1   0.003  Ru_us_gga.pseudo
14    Ru  [  1.229  2.152  6.096]   1   0.003  Ru_us_gga.pseudo
15    Ru  [  3.686  2.128  7.017]   1   0.016  Ru_us_gga.pseudo
16     S  [  1.232  0.712  8.034]   0   0.045  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 134.0
Number of bands     = 91
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



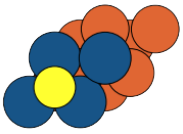
Rh overlayer:

```
---------------------------------
Dacapo calculation from Fe-subs+S/Rh-layer/Fe111-sub+Rh-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -13697.947720 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9144  0.0000  0.0000] 4.91
a1 [ 2.4572  4.2560  0.0000] 4.91
a2 [ 0.0000  0.0000  18.0252] 18.03
No stress calculated.
Volume = 377.01 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Fe  [  0.000  0.000  0.000]   4   0.439  Fe_us_gga_d2.1.8.pseudo
 1    Fe  [  2.457  0.000  0.000]   4   0.425  Fe_us_gga_d2.1.8.pseudo
 2    Fe  [  1.229  2.128  0.000]   4   0.425  Fe_us_gga_d2.1.8.pseudo
 3    Fe  [  3.686  2.128  0.000]   4   0.403  Fe_us_gga_d2.1.8.pseudo
 4    Fe  [  1.229  0.709  2.006]   3   0.041  Fe_us_gga_d2.1.8.pseudo
 5    Fe  [  3.686  0.709  2.006]   3   0.655  Fe_us_gga_d2.1.8.pseudo
 6    Fe  [  2.457  2.837  2.006]   3   0.655  Fe_us_gga_d2.1.8.pseudo
 7    Fe  [  4.914  2.837  2.006]   3   0.657  Fe_us_gga_d2.1.8.pseudo
 8    Fe  [  4.924  1.425  3.984]   2   0.027  Fe_us_gga_d2.1.8.pseudo
 9    Fe  [  2.467  1.424  3.986]   2   0.027  Fe_us_gga_d2.1.8.pseudo
10    Fe  [  6.147  3.549  3.923]   2   0.046  Fe_us_gga_d2.1.8.pseudo
11    Fe  [  3.696  3.552  3.984]   2   0.027  Fe_us_gga_d2.1.8.pseudo
12    Rh  [ -0.012 -0.007  6.086]   1   0.047  Rh_us_gga_fl.pseudo
13    Rh  [  2.481 -0.007  6.094]   1   0.044  Rh_us_gga_fl.pseudo
14    Rh  [  1.234  2.152  6.094]   1   0.044  Rh_us_gga_fl.pseudo
15    Rh  [  3.692  2.132  6.634]   1   0.008  Rh_us_gga_fl.pseudo
16     S  [  1.228  0.709  7.918]   0   0.008  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 138.0
Number of bands     = 93
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Ir overlayer:

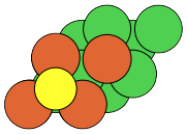
```
---------------------------------
Dacapo calculation from Fe-subs+S/Ir-layer/Fe111-sub+Ir-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -14495.399148 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9144  0.0000  0.0000] 4.91
a1 [ 2.4572  4.2560  0.0000] 4.91
a2 [ 0.0000  0.0000  18.0252] 18.03
No stress calculated.
Volume = 377.01 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Fe  [  0.000  0.000  0.000]   4   0.437  Fe_us_gga_d2.1.8.pseudo
 1    Fe  [  2.457  0.000  0.000]   4   0.427  Fe_us_gga_d2.1.8.pseudo
 2    Fe  [  1.229  2.128  0.000]   4   0.427  Fe_us_gga_d2.1.8.pseudo
 3    Fe  [  3.686  2.128  0.000]   4   0.505  Fe_us_gga_d2.1.8.pseudo
 4    Fe  [  1.229  0.709  2.006]   3   0.095  Fe_us_gga_d2.1.8.pseudo
 5    Fe  [  3.686  0.709  2.006]   3   0.684  Fe_us_gga_d2.1.8.pseudo
 6    Fe  [  2.457  2.837  2.006]   3   0.684  Fe_us_gga_d2.1.8.pseudo
 7    Fe  [  4.914  2.837  2.006]   3   0.678  Fe_us_gga_d2.1.8.pseudo
 8    Fe  [  4.927  1.419  3.983]   2   0.019  Fe_us_gga_d2.1.8.pseudo
 9    Fe  [  2.458  1.419  3.984]   2   0.018  Fe_us_gga_d2.1.8.pseudo
10    Fe  [  6.144  3.547  3.966]   2   0.028  Fe_us_gga_d2.1.8.pseudo
11    Fe  [  3.692  3.558  3.983]   2   0.019  Fe_us_gga_d2.1.8.pseudo
12    Ir  [ -0.014 -0.008  6.110]   1   0.010  ir_us_gga_flocal.pseudo
13    Ir  [  2.476 -0.008  6.111]   1   0.032  ir_us_gga_flocal.pseudo
14    Ir  [  1.231  2.148  6.111]   1   0.032  ir_us_gga_flocal.pseudo
15    Ir  [  3.689  2.130  6.610]   1   0.025  ir_us_gga_flocal.pseudo
16     S  [  1.226  0.708  7.997]   0   0.029  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 138.0
Number of bands     = 93
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Structures with Ni as the substrate:

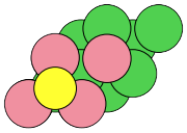
Fe overlayer:

```
---------------------------------
Dacapo calculation from Ni-subs+S/Fe-layer/Ni111-subs+Fe-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19320.914461 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9802  0.0000  0.0000] 4.98
a1 [ 2.4901  4.3129  0.0000] 4.98
a2 [ 0.0000  0.0000  18.1326] 18.13
No stress calculated.
Volume = 389.47 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ni  [  0.000  0.000  0.000]   4   0.091  Ni_us_gga.pseudo
 1    Ni  [  2.490  0.000  0.000]   4   0.089  Ni_us_gga.pseudo
 2    Ni  [  1.245  2.156  0.000]   4   0.089  Ni_us_gga.pseudo
 3    Ni  [  3.735  2.156  0.000]   4   0.111  Ni_us_gga.pseudo
 4    Ni  [  1.245  0.719  2.033]   3   0.039  Ni_us_gga.pseudo
 5    Ni  [  3.735  0.719  2.033]   3   0.172  Ni_us_gga.pseudo
 6    Ni  [  2.490  2.875  2.033]   3   0.172  Ni_us_gga.pseudo
 7    Ni  [  4.980  2.875  2.033]   3   0.173  Ni_us_gga.pseudo
 8    Ni  [  4.982  1.436  4.103]   2   0.029  Ni_us_gga.pseudo
 9    Ni  [  2.487  1.436  4.103]   2   0.031  Ni_us_gga.pseudo
10    Ni  [  6.224  3.594  4.037]   2   0.001  Ni_us_gga.pseudo
11    Ni  [  3.734  3.597  4.103]   2   0.030  Ni_us_gga.pseudo
12    Fe  [ -0.061 -0.035  6.110]   1   0.026  Fe_us_gga_d2.1.8.pseudo
13    Fe  [  2.549 -0.033  6.111]   1   0.027  Fe_us_gga_d2.1.8.pseudo
14    Fe  [  1.246  2.224  6.111]   1   0.027  Fe_us_gga_d2.1.8.pseudo
15    Fe  [  3.735  2.156  6.013]   1   0.030  Fe_us_gga_d2.1.8.pseudo
16     S  [  1.243  0.718  7.683]   0   0.029  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 158.0
Number of bands     = 106
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



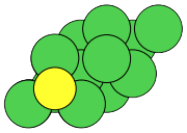
Co overlayer:

```
---------------------------------
Dacapo calculation from Ni-subs+S/Co-layer/Ni111-subs+Co-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -20357.880971 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9802  0.0000  0.0000] 4.98
a1 [ 2.4901  4.3129  0.0000] 4.98
a2 [ 0.0000  0.0000  18.1326] 18.13
No stress calculated.
Volume = 389.47 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ni  [  0.000  0.000  0.000]   4   0.098  Ni_us_gga.pseudo
 1    Ni  [  2.490  0.000  0.000]   4   0.097  Ni_us_gga.pseudo
 2    Ni  [  1.245  2.156  0.000]   4   0.097  Ni_us_gga.pseudo
 3    Ni  [  3.735  2.156  0.000]   4   0.111  Ni_us_gga.pseudo
 4    Ni  [  1.245  0.719  2.033]   3   0.071  Ni_us_gga.pseudo
 5    Ni  [  3.735  0.719  2.033]   3   0.160  Ni_us_gga.pseudo
 6    Ni  [  2.490  2.875  2.033]   3   0.160  Ni_us_gga.pseudo
 7    Ni  [  4.980  2.875  2.033]   3   0.161  Ni_us_gga.pseudo
 8    Ni  [  4.983  1.436  4.079]   2   0.015  Ni_us_gga.pseudo
 9    Ni  [  2.487  1.436  4.080]   2   0.015  Ni_us_gga.pseudo
10    Ni  [  6.225  3.594  4.059]   2   0.005  Ni_us_gga.pseudo
11    Ni  [  3.735  3.598  4.079]   2   0.015  Ni_us_gga.pseudo
12    Co  [ -0.036 -0.021  6.107]   1   0.024  Co_us_gga.pseudo
13    Co  [  2.526 -0.022  6.107]   1   0.024  Co_us_gga.pseudo
14    Co  [  1.244  2.198  6.107]   1   0.024  Co_us_gga.pseudo
15    Co  [  3.735  2.157  6.013]   1   0.048  Co_us_gga.pseudo
16     S  [  1.246  0.719  7.645]   0   0.028  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 162.0
Number of bands     = 109
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



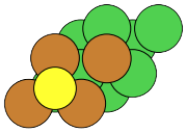
Ni overlayer:

```
---------------------------------
Dacapo calculation from Ni-subs+S/Ni-layer/Ni111-subs+Ni-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -21217.945087 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9802  0.0000  0.0000] 4.98
a1 [ 2.4901  4.3129  0.0000] 4.98
a2 [ 0.0000  0.0000  18.1326] 18.13
No stress calculated.
Volume = 389.47 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ni  [  0.000  0.000  0.000]   4   0.108  Ni_us_gga.pseudo
 1    Ni  [  2.490  0.000  0.000]   4   0.106  Ni_us_gga.pseudo
 2    Ni  [  1.245  2.156  0.000]   4   0.106  Ni_us_gga.pseudo
 3    Ni  [  3.735  2.156  0.000]   4   0.098  Ni_us_gga.pseudo
 4    Ni  [  1.245  0.719  2.033]   3   0.092  Ni_us_gga.pseudo
 5    Ni  [  3.735  0.719  2.033]   3   0.141  Ni_us_gga.pseudo
 6    Ni  [  2.490  2.875  2.033]   3   0.141  Ni_us_gga.pseudo
 7    Ni  [  4.980  2.875  2.033]   3   0.141  Ni_us_gga.pseudo
 8    Ni  [  4.979  1.439  4.068]   2   0.004  Ni_us_gga.pseudo
 9    Ni  [  2.492  1.439  4.068]   2   0.004  Ni_us_gga.pseudo
10    Ni  [  6.226  3.594  4.078]   2   0.003  Ni_us_gga.pseudo
11    Ni  [  3.735  3.592  4.068]   2   0.004  Ni_us_gga.pseudo
12    Ni  [ -0.033 -0.019  6.111]   1   0.009  Ni_us_gga.pseudo
13    Ni  [  2.522 -0.019  6.111]   1   0.008  Ni_us_gga.pseudo
14    Ni  [  1.245  2.193  6.111]   1   0.008  Ni_us_gga.pseudo
15    Ni  [  3.734  2.156  6.079]   1   0.009  Ni_us_gga.pseudo
16     S  [  1.245  0.719  7.649]   0   0.023  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 166.0
Number of bands     = 111
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



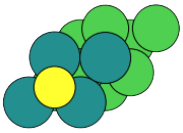
Cu overlayer:

```
---------------------------------
Dacapo calculation from Ni-subs+S/Cu-layer/Ni111-subs+Cu-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -22694.962275 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9802  0.0000  0.0000] 4.98
a1 [ 2.4901  4.3129  0.0000] 4.98
a2 [ 0.0000  0.0000  18.1326] 18.13
No stress calculated.
Volume = 389.47 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ni  [  0.000  0.000  0.000]   4   0.100  Ni_us_gga.pseudo
 1    Ni  [  2.490  0.000  0.000]   4   0.096  Ni_us_gga.pseudo
 2    Ni  [  1.245  2.156  0.000]   4   0.096  Ni_us_gga.pseudo
 3    Ni  [  3.735  2.156  0.000]   4   0.017  Ni_us_gga.pseudo
 4    Ni  [  1.245  0.719  2.033]   3   0.306  Ni_us_gga.pseudo
 5    Ni  [  3.735  0.719  2.033]   3   0.254  Ni_us_gga.pseudo
 6    Ni  [  2.490  2.875  2.033]   3   0.254  Ni_us_gga.pseudo
 7    Ni  [  4.980  2.875  2.033]   3   0.255  Ni_us_gga.pseudo
 8    Ni  [  4.981  1.438  4.023]   2   0.008  Ni_us_gga.pseudo
 9    Ni  [  2.490  1.438  4.023]   2   0.008  Ni_us_gga.pseudo
10    Ni  [  6.226  3.594  4.092]   2   0.001  Ni_us_gga.pseudo
11    Ni  [  3.735  3.595  4.023]   2   0.008  Ni_us_gga.pseudo
12    Cu  [ -0.019 -0.011  6.134]   1   0.045  Cu_us_gga.pseudo
13    Cu  [  2.508 -0.011  6.134]   1   0.044  Cu_us_gga.pseudo
14    Cu  [  1.245  2.178  6.134]   1   0.044  Cu_us_gga.pseudo
15    Cu  [  3.734  2.156  6.101]   1   0.029  Cu_us_gga.pseudo
16     S  [  1.246  0.719  7.836]   0   0.016  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 170.0
Number of bands     = 114
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



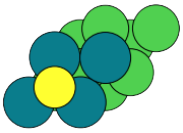
Ru overlayer:

```
---------------------------------
Dacapo calculation from Ni-subs+S/Ru-layer/Ni111-subs+Ru-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -18727.602732 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9802  0.0000  0.0000] 4.98
a1 [ 2.4901  4.3129  0.0000] 4.98
a2 [ 0.0000  0.0000  18.1326] 18.13
No stress calculated.
Volume = 389.47 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ni  [  0.000  0.000  0.000]   4   0.104  Ni_us_gga.pseudo
 1    Ni  [  2.490  0.000  0.000]   4   0.103  Ni_us_gga.pseudo
 2    Ni  [  1.245  2.156  0.000]   4   0.103  Ni_us_gga.pseudo
 3    Ni  [  3.735  2.156  0.000]   4   0.109  Ni_us_gga.pseudo
 4    Ni  [  1.245  0.719  2.033]   3   0.140  Ni_us_gga.pseudo
 5    Ni  [  3.735  0.719  2.033]   3   0.197  Ni_us_gga.pseudo
 6    Ni  [  2.490  2.875  2.033]   3   0.197  Ni_us_gga.pseudo
 7    Ni  [  4.980  2.875  2.033]   3   0.201  Ni_us_gga.pseudo
 8    Ni  [  4.970  1.443  4.087]   2   0.042  Ni_us_gga.pseudo
 9    Ni  [  2.501  1.444  4.089]   2   0.040  Ni_us_gga.pseudo
10    Ni  [  6.225  3.594  4.004]   2   0.012  Ni_us_gga.pseudo
11    Ni  [  3.735  3.583  4.087]   2   0.042  Ni_us_gga.pseudo
12    Ru  [ -0.028 -0.016  6.178]   1   0.020  Ru_us_gga.pseudo
13    Ru  [  2.516 -0.016  6.182]   1   0.019  Ru_us_gga.pseudo
14    Ru  [  1.244  2.187  6.182]   1   0.019  Ru_us_gga.pseudo
15    Ru  [  3.734  2.156  7.017]   1   0.029  Ru_us_gga.pseudo
16     S  [  1.242  0.717  8.063]   0   0.003  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 158.0
Number of bands     = 106
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Rh overlayer:

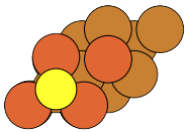
```
---------------------------------
Dacapo calculation from Ni-subs+S/Rh-layer/Ni111-subs+Rh-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19387.596772 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 4.9802  0.0000  0.0000] 4.98
a1 [ 2.4901  4.3129  0.0000] 4.98
a2 [ 0.0000  0.0000  18.1326] 18.13
No stress calculated.
Volume = 389.47 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ni  [  0.000  0.000  0.000]   4   0.102  Ni_us_gga.pseudo
 1    Ni  [  2.490  0.000  0.000]   4   0.102  Ni_us_gga.pseudo
 2    Ni  [  1.245  2.156  0.000]   4   0.102  Ni_us_gga.pseudo
 3    Ni  [  3.735  2.156  0.000]   4   0.113  Ni_us_gga.pseudo
 4    Ni  [  1.245  0.719  2.033]   3   0.098  Ni_us_gga.pseudo
 5    Ni  [  3.735  0.719  2.033]   3   0.206  Ni_us_gga.pseudo
 6    Ni  [  2.490  2.875  2.033]   3   0.206  Ni_us_gga.pseudo
 7    Ni  [  4.980  2.875  2.033]   3   0.207  Ni_us_gga.pseudo
 8    Ni  [  4.967  1.446  4.084]   2   0.022  Ni_us_gga.pseudo
 9    Ni  [  2.505  1.446  4.086]   2   0.017  Ni_us_gga.pseudo
10    Ni  [  6.226  3.595  4.010]   2   0.002  Ni_us_gga.pseudo
11    Ni  [  3.736  3.578  4.084]   2   0.022  Ni_us_gga.pseudo
12    Rh  [ -0.029 -0.017  6.190]   1   0.033  Rh_us_gga_fl.pseudo
13    Rh  [  2.517 -0.018  6.192]   1   0.023  Rh_us_gga_fl.pseudo
14    Rh  [  1.243  2.188  6.192]   1   0.023  Rh_us_gga_fl.pseudo
15    Rh  [  3.734  2.156  6.754]   1   0.008  Rh_us_gga_fl.pseudo
16     S  [  1.243  0.718  7.952]   0   0.017  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 162.0
Number of bands     = 109
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Structures with Cu as the substrate:

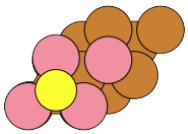
Fe overlayer:

```
--------------------------------
Dacapo calculation from Cu-subs+S/Fe-layer/Cu111-sub+Fe-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -23752.619947 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.017  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.020  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.020  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.002  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.260  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.166  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.166  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.160  Cu_us_gga.pseudo
 8    Cu  [  5.150  1.483  4.255]   2   0.020  Cu_us_gga.pseudo
 9    Cu  [  2.567  1.482  4.257]   2   0.019  Cu_us_gga.pseudo
10    Cu  [  6.433  3.714  4.148]   2   0.013  Cu_us_gga.pseudo
11    Cu  [  3.859  3.718  4.255]   2   0.020  Cu_us_gga.pseudo
12    Fe  [ -0.093 -0.054  6.318]   1   0.035  Fe_us_gga_d2.1.8.pseudo
13    Fe  [  2.669 -0.057  6.321]   1   0.034  Fe_us_gga_d2.1.8.pseudo
14    Fe  [  1.285  2.340  6.321]   1   0.034  Fe_us_gga_d2.1.8.pseudo
15    Fe  [  3.863  2.230  6.264]   1   0.035  Fe_us_gga_d2.1.8.pseudo
16     S  [  1.287  0.743  7.788]   0   0.034  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 170.0
Number of bands     = 114
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
--------------------------------
```



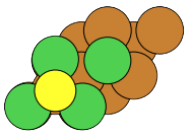
Co overlayer:

```
---------------------------------
Dacapo calculation from Cu-subs+S/Co-layer/Cu111-sub+Co-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -24790.116522 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.020  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.021  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.021  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.023  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.250  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.150  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.150  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.146  Cu_us_gga.pseudo
 8    Cu  [  5.147  1.485  4.247]   2   0.018  Cu_us_gga.pseudo
 9    Cu  [  2.572  1.485  4.248]   2   0.017  Cu_us_gga.pseudo
10    Cu  [  6.434  3.715  4.140]   2   0.022  Cu_us_gga.pseudo
11    Cu  [  3.860  3.715  4.247]   2   0.018  Cu_us_gga.pseudo
12    Co  [ -0.085 -0.049  6.273]   1   0.028  Co_us_gga.pseudo
13    Co  [  2.658 -0.049  6.274]   1   0.027  Co_us_gga.pseudo
14    Co  [  1.286  2.326  6.274]   1   0.027  Co_us_gga.pseudo
15    Co  [  3.863  2.230  6.260]   1   0.021  Co_us_gga.pseudo
16     S  [  1.286  0.743  7.691]   0   0.049  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 174.0
Number of bands     = 117
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



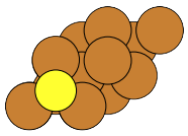
Ni overlayer:

```
---------------------------------
Dacapo calculation from Cu-subs+S/Ni-layer/Cu111-sub+Ni-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -25650.675242 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.013  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.015  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.015  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.057  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.264  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.159  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.159  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.157  Cu_us_gga.pseudo
 8    Cu  [  5.145  1.487  4.239]   2   0.014  Cu_us_gga.pseudo
 9    Cu  [  2.576  1.487  4.239]   2   0.013  Cu_us_gga.pseudo
10    Cu  [  6.434  3.715  4.163]   2   0.026  Cu_us_gga.pseudo
11    Cu  [  3.860  3.712  4.239]   2   0.014  Cu_us_gga.pseudo
12    Ni  [ -0.060 -0.035  6.266]   1   0.015  Ni_us_gga.pseudo
13    Ni  [  2.633 -0.034  6.265]   1   0.015  Ni_us_gga.pseudo
14    Ni  [  1.287  2.298  6.265]   1   0.015  Ni_us_gga.pseudo
15    Ni  [  3.861  2.229  6.267]   1   0.016  Ni_us_gga.pseudo
16     S  [  1.288  0.743  7.719]   0   0.018  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 178.0
Number of bands     = 119
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



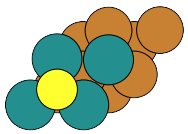
Cu overlayer:

```
---------------------------------
Dacapo calculation from Cu-subs+S/Cu-layer/Cu111-sub+Cu-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -27127.939950 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.047  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.046  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.046  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.031  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.063  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.100  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.100  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.096  Cu_us_gga.pseudo
 8    Cu  [  5.143  1.485  4.173]   2   0.017  Cu_us_gga.pseudo
 9    Cu  [  2.573  1.486  4.172]   2   0.021  Cu_us_gga.pseudo
10    Cu  [  6.433  3.714  4.254]   2   0.037  Cu_us_gga.pseudo
11    Cu  [  3.858  3.712  4.173]   2   0.017  Cu_us_gga.pseudo
12    Cu  [ -0.030 -0.017  6.309]   1   0.036  Cu_us_gga.pseudo
13    Cu  [  2.602 -0.017  6.309]   1   0.037  Cu_us_gga.pseudo
14    Cu  [  1.286  2.262  6.309]   1   0.037  Cu_us_gga.pseudo
15    Cu  [  3.858  2.228  6.245]   1   0.014  Cu_us_gga.pseudo
16     S  [  1.288  0.743  7.949]   0   0.031  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 182.0
Number of bands     = 122
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



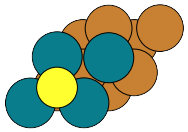
Ru overlayer:

```
---------------------------------
Dacapo calculation from Cu-subs+S/Ru-layer/Cu111-sub+Ru-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -23160.811058 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.013  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.013  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.013  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.056  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.352  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.283  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.283  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.277  Cu_us_gga.pseudo
 8    Cu  [  5.129  1.496  4.255]   2   0.026  Cu_us_gga.pseudo
 9    Cu  [  2.582  1.491  4.256]   2   0.045  Cu_us_gga.pseudo
10    Cu  [  6.434  3.715  4.116]   2   0.010  Cu_us_gga.pseudo
11    Cu  [  3.860  3.693  4.255]   2   0.026  Cu_us_gga.pseudo
12    Ru  [ -0.044 -0.025  6.381]   1   0.025  Ru_us_gga.pseudo
13    Ru  [  2.618 -0.027  6.389]   1   0.036  Ru_us_gga.pseudo
14    Ru  [  1.285  2.281  6.389]   1   0.036  Ru_us_gga.pseudo
15    Ru  [  3.858  2.227  6.951]   1   0.008  Ru_us_gga.pseudo
16     S  [  1.285  0.742  8.147]   0   0.024  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 170.0
Number of bands     = 114
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



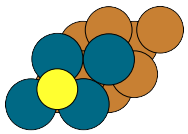
Rh overlayer:

```
---------------------------------
Dacapo calculation from Cu-subs+S/Rh-layer/Cu111-sub+Rh-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -23821.308429 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.023  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.024  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.024  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.052  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.340  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.206  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.206  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.202  Cu_us_gga.pseudo
 8    Cu  [  5.131  1.497  4.258]   2   0.041  Cu_us_gga.pseudo
 9    Cu  [  2.593  1.497  4.258]   2   0.048  Cu_us_gga.pseudo
10    Cu  [  6.434  3.715  4.135]   2   0.009  Cu_us_gga.pseudo
11    Cu  [  3.862  3.695  4.258]   2   0.041  Cu_us_gga.pseudo
12    Rh  [ -0.046 -0.026  6.403]   1   0.015  Rh_us_gga_fl.pseudo
13    Rh  [  2.624 -0.024  6.412]   1   0.017  Rh_us_gga_fl.pseudo
14    Rh  [  1.292  2.285  6.412]   1   0.017  Rh_us_gga_fl.pseudo
15    Rh  [  3.868  2.233  6.651]   1   0.005  Rh_us_gga_fl.pseudo
16     S  [  1.283  0.741  8.061]   0   0.009  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 174.0
Number of bands     = 117
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



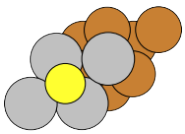
Pd overlayer:

```
---------------------------------
Dacapo calculation from Cu-subs+S/Pd-layer/Cu111-sub+Pd-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -24622.383877 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.018  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.015  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.015  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.064  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.325  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.195  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.195  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.198  Cu_us_gga.pseudo
 8    Cu  [  5.138  1.491  4.246]   2   0.022  Cu_us_gga.pseudo
 9    Cu  [  2.585  1.492  4.244]   2   0.019  Cu_us_gga.pseudo
10    Cu  [  6.434  3.715  4.159]   2   0.041  Cu_us_gga.pseudo
11    Cu  [  3.860  3.704  4.246]   2   0.022  Cu_us_gga.pseudo
12    Pd  [ -0.021 -0.012  6.441]   1   0.020  046-Pd-gpe-n-6projectors-floc.uspp
13    Pd  [  2.604 -0.009  6.438]   1   0.042  046-Pd-gpe-n-6projectors-floc.uspp
14    Pd  [  1.294  2.260  6.438]   1   0.042  046-Pd-gpe-n-6projectors-floc.uspp
15    Pd  [  3.869  2.234  6.560]   1   0.022  046-Pd-gpe-n-6projectors-floc.uspp
16     S  [  1.291  0.746  8.189]   0   0.008  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 178.0
Number of bands     = 119
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



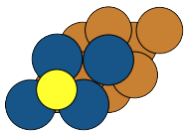
Ag overlayer:

```
---------------------------------
Dacapo calculation from Cu-subs+S/Ag-layer/Cu111-sub+Ag-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -25600.974954 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.026  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.010  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.010  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.023  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.196  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.184  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.184  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.254  Cu_us_gga.pseudo
 8    Cu  [  5.092  1.453  4.245]   2   0.029  Cu_us_gga.pseudo
 9    Cu  [  2.546  1.470  4.141]   2   0.002  Cu_us_gga.pseudo
10    Cu  [  6.413  3.703  4.251]   2   0.021  Cu_us_gga.pseudo
11    Cu  [  3.804  3.683  4.245]   2   0.030  Cu_us_gga.pseudo
12    Ag  [ -0.079 -0.046  7.090]   1   0.018  ag_us.pseudo
13    Ag  [  2.516 -0.037  6.418]   1   0.044  ag_us.pseudo
14    Ag  [  1.226  2.197  6.418]   1   0.044  ag_us.pseudo
15    Ag  [  3.852  2.224  8.090]   1   0.042  ag_us.pseudo
16     S  [  1.672  0.966  8.661]   0   0.040  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 182.0
Number of bands     = 122
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



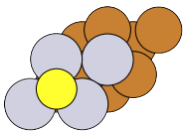
Ir overlayer:

```
---------------------------------
Dacapo calculation from Cu-subs+S/Ir-layer/Cu111-sub+Ir-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -24619.256364 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.020  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.021  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.021  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.028  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.218  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.266  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.266  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.260  Cu_us_gga.pseudo
 8    Cu  [  5.170  1.474  4.229]   2   0.035  Cu_us_gga.pseudo
 9    Cu  [  2.549  1.472  4.234]   2   0.036  Cu_us_gga.pseudo
10    Cu  [  6.435  3.715  4.262]   2   0.039  Cu_us_gga.pseudo
11    Cu  [  3.861  3.740  4.229]   2   0.035  Cu_us_gga.pseudo
12    Ir  [ -0.045 -0.026  6.571]   1   0.019  ir_us_gga_flocal.pseudo
13    Ir  [  2.615 -0.025  6.615]   1   0.037  ir_us_gga_flocal.pseudo
14    Ir  [  1.286  2.278  6.615]   1   0.036  ir_us_gga_flocal.pseudo
15    Ir  [  3.862  2.230  6.284]   1   0.035  ir_us_gga_flocal.pseudo
16     S  [  1.264  0.730  8.276]   0   0.028  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 174.0
Number of bands     = 117
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



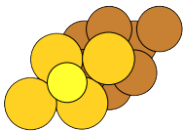
Pt overlayer:

```
---------------------------------
Dacapo calculation from Cu-subs+S/Pt-layer/Cu111-sub+Pt-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -25272.962832 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.053  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.046  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.046  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.038  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.260  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.276  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.276  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.287  Cu_us_gga.pseudo
 8    Cu  [  5.146  1.470  4.224]   2   0.015  Cu_us_gga.pseudo
 9    Cu  [  2.547  1.470  4.219]   2   0.006  Cu_us_gga.pseudo
10    Cu  [  6.422  3.708  4.262]   2   0.013  Cu_us_gga.pseudo
11    Cu  [  3.846  3.722  4.224]   2   0.015  Cu_us_gga.pseudo
12    Pt  [ -0.032 -0.019  6.600]   1   0.029  pt_us_gga.pseudo
13    Pt  [  2.580 -0.017  6.586]   1   0.015  pt_us_gga.pseudo
14    Pt  [  1.276  2.243  6.586]   1   0.015  pt_us_gga.pseudo
15    Pt  [  3.848  2.222  6.408]   1   0.036  pt_us_gga.pseudo
16     S  [  1.287  0.743  8.421]   0   0.016  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 178.0
Number of bands     = 119
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Au overlayer:

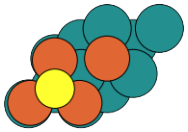
```
---------------------------------
Dacapo calculation from Cu-subs+S/Au-layer/Cu111-sub+Au-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -25991.261285 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.1477  0.0000  0.0000] 5.15
a1 [ 2.5739  4.4581  0.0000] 5.15
a2 [ 0.0000  0.0000  18.4062] 18.41
No stress calculated.
Volume = 422.40 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Cu  [  0.000  0.000  0.000]   4   0.057  Cu_us_gga.pseudo
 1    Cu  [  2.574  0.000  0.000]   4   0.017  Cu_us_gga.pseudo
 2    Cu  [  1.287  2.229  0.000]   4   0.017  Cu_us_gga.pseudo
 3    Cu  [  3.861  2.229  0.000]   4   0.042  Cu_us_gga.pseudo
 4    Cu  [  1.287  0.743  2.102]   3   0.109  Cu_us_gga.pseudo
 5    Cu  [  3.861  0.743  2.102]   3   0.289  Cu_us_gga.pseudo
 6    Cu  [  2.574  2.972  2.102]   3   0.289  Cu_us_gga.pseudo
 7    Cu  [  5.148  2.972  2.102]   3   0.100  Cu_us_gga.pseudo
 8    Cu  [  5.136  1.476  4.180]   2   0.047  Cu_us_gga.pseudo
 9    Cu  [  2.595  1.498  4.238]   2   0.038  Cu_us_gga.pseudo
10    Cu  [  6.434  3.715  4.269]   2   0.031  Cu_us_gga.pseudo
11    Cu  [  3.846  3.710  4.180]   2   0.047  Cu_us_gga.pseudo
12    Au  [ -0.186 -0.107  7.608]   1   0.033  Au_us_gga.pseudo
13    Au  [  2.446 -0.077  6.444]   1   0.043  Au_us_gga.pseudo
14    Au  [  1.156  2.157  6.443]   1   0.043  Au_us_gga.pseudo
15    Au  [  3.817  2.204  8.289]   1   0.016  Au_us_gga.pseudo
16     S  [  1.692  0.977  8.866]   0   0.027  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 182.0
Number of bands     = 122
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Structures with Ru as the substrate:

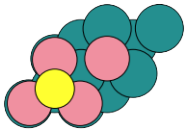
Fe overlayer:

```
---------------------------------
Dacapo calculation from Ru-subs+S/Fe-layer/Ru111-subs+Fe-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -11855.504750 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.722  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.717  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.717  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.680  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.836  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.638  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.638  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.640  Ru_us_gga.pseudo
 8    Ru  [  5.425  1.575  4.485]   2   0.013  Ru_us_gga.pseudo
 9    Ru  [  2.725  1.574  4.485]   2   0.009  Ru_us_gga.pseudo
10    Ru  [  6.789  3.919  4.468]   2   0.008  Ru_us_gga.pseudo
11    Ru  [  4.076  3.911  4.485]   2   0.013  Ru_us_gga.pseudo
12    Fe  [  0.084  0.048  6.478]   1   0.022  Fe_us_gga_d2.1.8.pseudo
13    Fe  [  2.638  0.048  6.478]   1   0.013  Fe_us_gga_d2.1.8.pseudo
14    Fe  [  1.360  2.261  6.478]   1   0.013  Fe_us_gga_d2.1.8.pseudo
15    Fe  [  4.072  2.351  6.442]   1   0.038  Fe_us_gga_d2.1.8.pseudo
16     S  [  1.362  0.786  8.096]   0   0.002  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 134.0
Number of bands     = 91
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



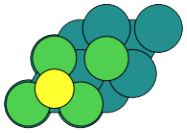
Co overlayer:

```
---------------------------------
Dacapo calculation from Ru-subs+S/Co-layer/Ru111-subs+Co-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -12892.565205 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.590  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.576  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.576  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.620  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.735  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.620  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.621  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.619  Ru_us_gga.pseudo
 8    Ru  [  5.421  1.574  4.439]   2   0.009  Ru_us_gga.pseudo
 9    Ru  [  2.725  1.573  4.440]   2   0.011  Ru_us_gga.pseudo
10    Ru  [  6.787  3.918  4.419]   2   0.033  Ru_us_gga.pseudo
11    Ru  [  4.074  3.908  4.439]   2   0.009  Ru_us_gga.pseudo
12    Co  [  0.052  0.030  6.455]   1   0.047  Co_us_gga.pseudo
13    Co  [  2.666  0.026  6.456]   1   0.049  Co_us_gga.pseudo
14    Co  [  1.356  2.296  6.456]   1   0.049  Co_us_gga.pseudo
15    Co  [  4.073  2.351  6.431]   1   0.008  Co_us_gga.pseudo
16     S  [  1.360  0.785  8.005]   0   0.013  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 138.0
Number of bands     = 93
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



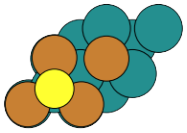
Ni overlayer:

```
---------------------------------
Dacapo calculation from Ru-subs+S/Ni-layer/Ru111-subs+Ni-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -13752.961967 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.470  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.463  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.463  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.631  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.593  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.504  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.504  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.494  Ru_us_gga.pseudo
 8    Ru  [  5.432  1.567  4.398]   2   0.005  Ru_us_gga.pseudo
 9    Ru  [  2.713  1.567  4.400]   2   0.004  Ru_us_gga.pseudo
10    Ru  [  6.786  3.918  4.399]   2   0.015  Ru_us_gga.pseudo
11    Ru  [  4.073  3.921  4.398]   2   0.005  Ru_us_gga.pseudo
12    Ni  [ -0.020 -0.012  6.501]   1   0.028  Ni_us_gga.pseudo
13    Ni  [  2.737 -0.011  6.502]   1   0.029  Ni_us_gga.pseudo
14    Ni  [  1.359  2.376  6.502]   1   0.029  Ni_us_gga.pseudo
15    Ni  [  4.072  2.351  6.447]   1   0.003  Ni_us_gga.pseudo
16     S  [  1.358  0.784  7.952]   0   0.024  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 142.0
Number of bands     = 96
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



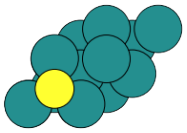
Cu overlayer:

```
---------------------------------
Dacapo calculation from Ru-subs+S/Cu-layer/Ru111-subs+Cu-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -15230.413601 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.414  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.406  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.406  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.637  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.633  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.402  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.402  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.411  Ru_us_gga.pseudo
 8    Ru  [  5.429  1.567  4.357]   2   0.032  Ru_us_gga.pseudo
 9    Ru  [  2.715  1.567  4.357]   2   0.034  Ru_us_gga.pseudo
10    Ru  [  6.785  3.917  4.438]   2   0.016  Ru_us_gga.pseudo
11    Ru  [  4.072  3.918  4.357]   2   0.032  Ru_us_gga.pseudo
12    Cu  [ -0.041 -0.024  6.591]   1   0.041  Cu_us_gga.pseudo
13    Cu  [  2.756 -0.024  6.591]   1   0.044  Cu_us_gga.pseudo
14    Cu  [  1.358  2.399  6.591]   1   0.044  Cu_us_gga.pseudo
15    Cu  [  4.071  2.350  6.497]   1   0.027  Cu_us_gga.pseudo
16     S  [  1.357  0.783  8.133]   0   0.024  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 146.0
Number of bands     = 98
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



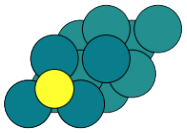
Ru overlayer:

```
---------------------------------
Dacapo calculation from Ru-subs+S/Ru-layer/Ru111-subs+Ru-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -11264.484133 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.658  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.642  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.642  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.428  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.646  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.613  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.612  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.600  Ru_us_gga.pseudo
 8    Ru  [  5.428  1.573  4.480]   2   0.027  Ru_us_gga.pseudo
 9    Ru  [  2.723  1.572  4.481]   2   0.031  Ru_us_gga.pseudo
10    Ru  [  6.788  3.919  4.354]   2   0.001  Ru_us_gga.pseudo
11    Ru  [  4.077  3.914  4.480]   2   0.027  Ru_us_gga.pseudo
12    Ru  [ -0.020 -0.012  6.644]   1   0.008  Ru_us_gga.pseudo
13    Ru  [  2.741 -0.011  6.646]   1   0.007  Ru_us_gga.pseudo
14    Ru  [  1.361  2.380  6.646]   1   0.008  Ru_us_gga.pseudo
15    Ru  [  4.072  2.351  6.605]   1   0.005  Ru_us_gga.pseudo
16     S  [  1.359  0.785  8.368]   0   0.024  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 134.0
Number of bands     = 91
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



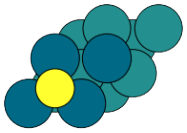
Rh overlayer:

```
---------------------------------
Dacapo calculation from Ru-subs+S/Rh-layer/Ru111-subs+Rh-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -11924.533005 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.506  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.492  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.492  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.509  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.489  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.506  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.507  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.495  Ru_us_gga.pseudo
 8    Ru  [  5.427  1.571  4.427]   2   0.027  Ru_us_gga.pseudo
 9    Ru  [  2.716  1.568  4.430]   2   0.028  Ru_us_gga.pseudo
10    Ru  [  6.787  3.918  4.362]   2   0.003  Ru_us_gga.pseudo
11    Ru  [  4.074  3.915  4.427]   2   0.026  Ru_us_gga.pseudo
12    Rh  [ -0.012 -0.007  6.645]   1   0.007  Rh_us_gga_fl.pseudo
13    Rh  [  2.734 -0.010  6.646]   1   0.008  Rh_us_gga_fl.pseudo
14    Rh  [  1.358  2.373  6.646]   1   0.008  Rh_us_gga_fl.pseudo
15    Rh  [  4.072  2.351  6.606]   1   0.016  Rh_us_gga_fl.pseudo
16     S  [  1.361  0.786  8.292]   0   0.047  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 138.0
Number of bands     = 93
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



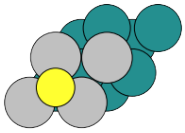
Pd overlayer:

```
---------------------------------
Dacapo calculation from Ru-subs+S/Pd-layer/Ru111-subs+Pd-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -12725.480978 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.377  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.358  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.358  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.564  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.298  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.493  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.493  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.487  Ru_us_gga.pseudo
 8    Ru  [  5.430  1.568  4.369]   2   0.006  Ru_us_gga.pseudo
 9    Ru  [  2.716  1.568  4.371]   2   0.005  Ru_us_gga.pseudo
10    Ru  [  6.787  3.918  4.382]   2   0.044  Ru_us_gga.pseudo
11    Ru  [  4.073  3.918  4.369]   2   0.006  Ru_us_gga.pseudo
12    Pd  [ -0.014 -0.008  6.686]   1   0.035  046-Pd-gpe-n-6projectors-floc.uspp
13    Pd  [  2.730 -0.008  6.685]   1   0.037  046-Pd-gpe-n-6projectors-floc.uspp
14    Pd  [  1.358  2.368  6.685]   1   0.037  046-Pd-gpe-n-6projectors-floc.uspp
15    Pd  [  4.072  2.351  6.678]   1   0.029  046-Pd-gpe-n-6projectors-floc.uspp
16     S  [  1.358  0.784  8.359]   0   0.036  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 142.0
Number of bands     = 96
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



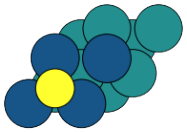
Ag overlayer:

```
---------------------------------
Dacapo calculation from Ru-subs+S/Ag-layer/Ru111-subs+Ag-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -13703.539754 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.403  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.391  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.391  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.575  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.567  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.444  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.444  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.459  Ru_us_gga.pseudo
 8    Ru  [  5.429  1.570  4.344]   2   0.013  Ru_us_gga.pseudo
 9    Ru  [  2.722  1.572  4.345]   2   0.010  Ru_us_gga.pseudo
10    Ru  [  6.786  3.918  4.418]   2   0.015  Ru_us_gga.pseudo
11    Ru  [  4.074  3.917  4.344]   2   0.013  Ru_us_gga.pseudo
12    Ag  [ -0.008 -0.004  6.799]   1   0.035  ag_us.pseudo
13    Ag  [  2.743 -0.002  6.805]   1   0.019  ag_us.pseudo
14    Ag  [  1.370  2.377  6.805]   1   0.019  ag_us.pseudo
15    Ag  [  4.084  2.358  6.793]   1   0.025  ag_us.pseudo
16     S  [  1.360  0.785  8.670]   0   0.027  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 146.0
Number of bands     = 98
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



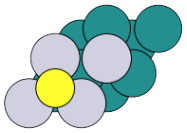
Ir overlayer:

```
---------------------------------
Dacapo calculation from Ru-subs+S/Ir-layer/Ru111-subs+Ir-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -12722.790094 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.519  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.502  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.502  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.557  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.527  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.533  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.533  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.507  Ru_us_gga.pseudo
 8    Ru  [  5.428  1.571  4.435]   2   0.009  Ru_us_gga.pseudo
 9    Ru  [  2.715  1.567  4.436]   2   0.013  Ru_us_gga.pseudo
10    Ru  [  6.787  3.918  4.379]   2   0.043  Ru_us_gga.pseudo
11    Ru  [  4.074  3.915  4.435]   2   0.009  Ru_us_gga.pseudo
12    Ir  [ -0.023 -0.014  6.665]   1   0.022  ir_us_gga_flocal.pseudo
13    Ir  [  2.744 -0.016  6.665]   1   0.016  ir_us_gga_flocal.pseudo
14    Ir  [  1.358  2.385  6.665]   1   0.016  ir_us_gga_flocal.pseudo
15    Ir  [  4.071  2.351  6.605]   1   0.012  ir_us_gga_flocal.pseudo
16     S  [  1.360  0.785  8.346]   0   0.025  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 138.0
Number of bands     = 93
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



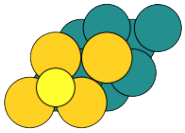
Pt overlayer:

```
---------------------------------
Dacapo calculation from Ru-subs+S/Pt-layer/Ru111-subs+Pt-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -13376.742705 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.332  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.311  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.311  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.638  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.292  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.416  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.416  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.416  Ru_us_gga.pseudo
 8    Ru  [  5.432  1.566  4.362]   2   0.004  Ru_us_gga.pseudo
 9    Ru  [  2.713  1.566  4.362]   2   0.003  Ru_us_gga.pseudo
10    Ru  [  6.785  3.917  4.423]   2   0.027  Ru_us_gga.pseudo
11    Ru  [  4.072  3.921  4.362]   2   0.004  Ru_us_gga.pseudo
12    Pt  [ -0.018 -0.010  6.749]   1   0.026  pt_us_gga.pseudo
13    Pt  [  2.732 -0.010  6.749]   1   0.027  pt_us_gga.pseudo
14    Pt  [  1.358  2.371  6.749]   1   0.027  pt_us_gga.pseudo
15    Pt  [  4.072  2.351  6.687]   1   0.022  pt_us_gga.pseudo
16     S  [  1.357  0.784  8.490]   0   0.008  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 142.0
Number of bands     = 96
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Au overlayer:

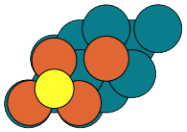
```
---------------------------------
Dacapo calculation from Ru-subs+S/Au-layer/Ru111-subs+Au-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -14093.893833 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4266  0.0000  0.0000] 5.43
a1 [ 2.7133  4.6996  0.0000] 5.43
a2 [ 0.0000  0.0000  18.8616] 18.86
No stress calculated.
Volume = 481.03 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ru  [  0.000  0.000  0.000]   4   0.341  Ru_us_gga.pseudo
 1    Ru  [  2.713  0.000  0.000]   4   0.327  Ru_us_gga.pseudo
 2    Ru  [  1.357  2.350  0.000]   4   0.327  Ru_us_gga.pseudo
 3    Ru  [  4.070  2.350  0.000]   4   0.657  Ru_us_gga.pseudo
 4    Ru  [  1.357  0.783  2.215]   3   0.597  Ru_us_gga.pseudo
 5    Ru  [  4.070  0.783  2.215]   3   0.379  Ru_us_gga.pseudo
 6    Ru  [  2.713  3.133  2.215]   3   0.379  Ru_us_gga.pseudo
 7    Ru  [  5.427  3.133  2.215]   3   0.374  Ru_us_gga.pseudo
 8    Ru  [  5.432  1.560  4.334]   2   0.027  Ru_us_gga.pseudo
 9    Ru  [  2.707  1.563  4.334]   2   0.017  Ru_us_gga.pseudo
10    Ru  [  6.776  3.912  4.473]   2   0.040  Ru_us_gga.pseudo
11    Ru  [  4.067  3.924  4.334]   2   0.027  Ru_us_gga.pseudo
12    Au  [ -0.016 -0.009  6.882]   1   0.028  Au_us_gga.pseudo
13    Au  [  2.729 -0.009  6.886]   1   0.031  Au_us_gga.pseudo
14    Au  [  1.357  2.368  6.886]   1   0.031  Au_us_gga.pseudo
15    Au  [  4.070  2.350  6.716]   1   0.020  Au_us_gga.pseudo
16     S  [  1.357  0.783  8.782]   0   0.022  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 146.0
Number of bands     = 98
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Structures with Rh as the substrate:

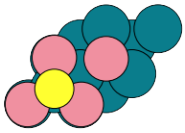
Fe overlayer:

```
---------------------------------
Dacapo calculation from Rh-subs+S/Fe-layer/Rh111-subs+Fe-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -13833.562917 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.287  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.297  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.297  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.393  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.402  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.308  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.308  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.314  Rh_us_gga_fl.pseudo
 8    Rh  [  5.402  1.562  4.439]   2   0.010  Rh_us_gga_fl.pseudo
 9    Rh  [  2.707  1.563  4.441]   2   0.011  Rh_us_gga_fl.pseudo
10    Rh  [  6.760  3.903  4.472]   2   0.002  Rh_us_gga_fl.pseudo
11    Rh  [  4.054  3.897  4.439]   2   0.010  Rh_us_gga_fl.pseudo
12    Fe  [  0.075  0.043  6.433]   1   0.027  Fe_us_gga_d2.1.8.pseudo
13    Fe  [  2.627  0.037  6.434]   1   0.029  Fe_us_gga_d2.1.8.pseudo
14    Fe  [  1.346  2.257  6.434]   1   0.029  Fe_us_gga_d2.1.8.pseudo
15    Fe  [  4.064  2.347  6.392]   1   0.038  Fe_us_gga_d2.1.8.pseudo
16     S  [  1.352  0.781  8.046]   0   0.030  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 146.0
Number of bands     = 98
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



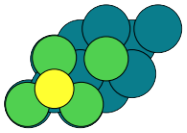
Co overlayer:

```
---------------------------------
Dacapo calculation from Rh-subs+S/Co-layer/Rh111-subs+Co-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -14870.528823 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.296  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.300  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.300  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.341  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.275  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.330  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.330  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.327  Rh_us_gga_fl.pseudo
 8    Rh  [  5.402  1.563  4.414]   2   0.020  Rh_us_gga_fl.pseudo
 9    Rh  [  2.707  1.563  4.414]   2   0.022  Rh_us_gga_fl.pseudo
10    Rh  [  6.758  3.902  4.394]   2   0.034  Rh_us_gga_fl.pseudo
11    Rh  [  4.055  3.896  4.414]   2   0.021  Rh_us_gga_fl.pseudo
12    Co  [ -0.052 -0.030  6.451]   1   0.022  Co_us_gga.pseudo
13    Co  [  2.757 -0.031  6.452]   1   0.024  Co_us_gga.pseudo
14    Co  [  1.352  2.403  6.452]   1   0.025  Co_us_gga.pseudo
15    Co  [  4.056  2.342  6.403]   1   0.009  Co_us_gga.pseudo
16     S  [  1.352  0.781  7.879]   0   0.016  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 150.0
Number of bands     = 101
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



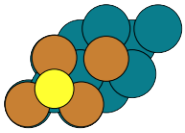
Ni overlayer:

```
---------------------------------
Dacapo calculation from Rh-subs+S/Ni-layer/Rh111-subs+Ni-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -15730.957729 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.302  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.309  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.309  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.277  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.304  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.341  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.341  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.333  Rh_us_gga_fl.pseudo
 8    Rh  [  5.405  1.561  4.377]   2   0.013  Rh_us_gga_fl.pseudo
 9    Rh  [  2.705  1.562  4.376]   2   0.014  Rh_us_gga_fl.pseudo
10    Rh  [  6.757  3.901  4.405]   2   0.025  Rh_us_gga_fl.pseudo
11    Rh  [  4.054  3.900  4.377]   2   0.013  Rh_us_gga_fl.pseudo
12    Ni  [ -0.052 -0.030  6.470]   1   0.020  Ni_us_gga.pseudo
13    Ni  [  2.756 -0.029  6.471]   1   0.020  Ni_us_gga.pseudo
14    Ni  [  1.353  2.401  6.471]   1   0.020  Ni_us_gga.pseudo
15    Ni  [  4.058  2.343  6.408]   1   0.044  Ni_us_gga.pseudo
16     S  [  1.351  0.780  7.871]   0   0.012  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 154.0
Number of bands     = 104
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



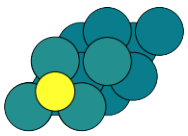
Cu overlayer:

```
---------------------------------
Dacapo calculation from Rh-subs+S/Cu-layer/Rh111-subs+Cu-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -17208.369202 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.324  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.332  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.332  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.224  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.384  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.314  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.314  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.304  Rh_us_gga_fl.pseudo
 8    Rh  [  5.411  1.558  4.353]   2   0.036  Rh_us_gga_fl.pseudo
 9    Rh  [  2.701  1.559  4.353]   2   0.033  Rh_us_gga_fl.pseudo
10    Rh  [  6.759  3.902  4.443]   2   0.009  Rh_us_gga_fl.pseudo
11    Rh  [  4.055  3.907  4.353]   2   0.034  Rh_us_gga_fl.pseudo
12    Cu  [ -0.050 -0.029  6.575]   1   0.041  Cu_us_gga.pseudo
13    Cu  [  2.754 -0.028  6.575]   1   0.041  Cu_us_gga.pseudo
14    Cu  [  1.352  2.399  6.575]   1   0.041  Cu_us_gga.pseudo
15    Cu  [  4.057  2.342  6.450]   1   0.040  Cu_us_gga.pseudo
16     S  [  1.351  0.780  8.105]   0   0.014  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 158.0
Number of bands     = 106
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



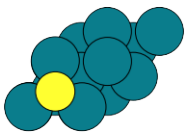
Ru overlayer:

```
---------------------------------
Dacapo calculation from Rh-subs+S/Ru-layer/Rh111-subs+Ru-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -13242.613680 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.249  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.261  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.261  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.353  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.212  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.358  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.358  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.351  Rh_us_gga_fl.pseudo
 8    Rh  [  5.404  1.562  4.426]   2   0.007  Rh_us_gga_fl.pseudo
 9    Rh  [  2.703  1.561  4.425]   2   0.006  Rh_us_gga_fl.pseudo
10    Rh  [  6.760  3.903  4.356]   2   0.011  Rh_us_gga_fl.pseudo
11    Rh  [  4.054  3.899  4.426]   2   0.007  Rh_us_gga_fl.pseudo
12    Ru  [ -0.030 -0.017  6.599]   1   0.011  Ru_us_gga.pseudo
13    Ru  [  2.732 -0.016  6.600]   1   0.011  Ru_us_gga.pseudo
14    Ru  [  1.352  2.374  6.600]   1   0.011  Ru_us_gga.pseudo
15    Ru  [  4.054  2.341  6.552]   1   0.024  Ru_us_gga.pseudo
16     S  [  1.351  0.780  8.318]   0   0.045  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 146.0
Number of bands     = 98
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



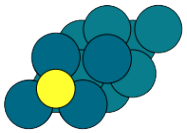
Rh overlayer:

```
---------------------------------
Dacapo calculation from Rh-subs+S/Rh-layer/Rh111-subs+Rh-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -13902.474460 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.272  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.274  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.274  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.313  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.147  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.348  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.348  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.340  Rh_us_gga_fl.pseudo
 8    Rh  [  5.405  1.561  4.379]   2   0.047  Rh_us_gga_fl.pseudo
 9    Rh  [  2.705  1.562  4.379]   2   0.047  Rh_us_gga_fl.pseudo
10    Rh  [  6.758  3.902  4.377]   2   0.013  Rh_us_gga_fl.pseudo
11    Rh  [  4.055  3.900  4.379]   2   0.047  Rh_us_gga_fl.pseudo
12    Rh  [ -0.031 -0.018  6.620]   1   0.030  Rh_us_gga_fl.pseudo
13    Rh  [  2.736 -0.018  6.621]   1   0.027  Rh_us_gga_fl.pseudo
14    Rh  [  1.352  2.378  6.621]   1   0.027  Rh_us_gga_fl.pseudo
15    Rh  [  4.058  2.343  6.558]   1   0.016  Rh_us_gga_fl.pseudo
16     S  [  1.352  0.781  8.250]   0   0.029  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 150.0
Number of bands     = 101
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



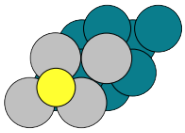
Pd overlayer:

```
---------------------------------
Dacapo calculation from Rh-subs+S/Pd-layer/Rh111-subs+Pd-overlayer+S-relaxed.nc
status = running
version = ifc ser v2-3-3
Energy = -14702.872468 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.277  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.290  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.290  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.196  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.428  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.699  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.699  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.689  Rh_us_gga_fl.pseudo
 8    Rh  [  5.394  1.568  4.296]   2   0.075  Rh_us_gga_fl.pseudo
 9    Rh  [  2.716  1.568  4.295]   2   0.081  Rh_us_gga_fl.pseudo
10    Rh  [  6.759  3.902  4.297]   2   0.285  Rh_us_gga_fl.pseudo
11    Rh  [  4.055  3.887  4.296]   2   0.075  Rh_us_gga_fl.pseudo
12    Pd  [ -0.074 -0.043  6.540]   1   0.559  046-Pd-gpe-n-6projectors-floc.uspp
13    Pd  [  2.778 -0.043  6.540]   1   0.555  046-Pd-gpe-n-6projectors-floc.uspp
14    Pd  [  1.352  2.427  6.540]   1   0.555  046-Pd-gpe-n-6projectors-floc.uspp
15    Pd  [  4.056  2.342  6.667]   1   0.127  046-Pd-gpe-n-6projectors-floc.uspp
16     S  [  1.352  0.781  7.983]   0   3.325  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 154.0
Number of bands     = 104
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



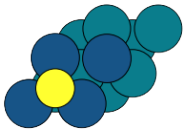
Ag overlayer:

```
---------------------------------
Dacapo calculation from Rh-subs+S/Ag-layer/Rh111-subs+Ag-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -15681.532167 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.295  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.307  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.307  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.232  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.472  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.371  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.371  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.334  Rh_us_gga_fl.pseudo
 8    Rh  [  5.400  1.555  4.332]   2   0.015  Rh_us_gga_fl.pseudo
 9    Rh  [  2.698  1.558  4.328]   2   0.029  Rh_us_gga_fl.pseudo
10    Rh  [  6.751  3.898  4.411]   2   0.008  Rh_us_gga_fl.pseudo
11    Rh  [  4.047  3.899  4.332]   2   0.015  Rh_us_gga_fl.pseudo
12    Ag  [ -0.054 -0.031  6.800]   1   0.049  ag_us.pseudo
13    Ag  [  2.681 -0.036  6.773]   1   0.035  ag_us.pseudo
14    Ag  [  1.309  2.340  6.773]   1   0.035  ag_us.pseudo
15    Ag  [  4.014  2.317  6.763]   1   0.038  ag_us.pseudo
16     S  [  1.340  0.774  8.645]   0   0.041  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 158.0
Number of bands     = 106
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



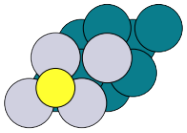
Ir overlayer:

```
---------------------------------
Dacapo calculation from Rh-subs+S/Ir-layer/Rh111-subs+Ir-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -14700.668535 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.272  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.271  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.271  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.304  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.178  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.353  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.353  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.334  Rh_us_gga_fl.pseudo
 8    Rh  [  5.407  1.559  4.390]   2   0.022  Rh_us_gga_fl.pseudo
 9    Rh  [  2.702  1.560  4.390]   2   0.026  Rh_us_gga_fl.pseudo
10    Rh  [  6.756  3.901  4.390]   2   0.021  Rh_us_gga_fl.pseudo
11    Rh  [  4.054  3.903  4.390]   2   0.024  Rh_us_gga_fl.pseudo
12    Ir  [ -0.039 -0.023  6.641]   1   0.016  ir_us_gga_flocal.pseudo
13    Ir  [  2.745 -0.022  6.641]   1   0.016  ir_us_gga_flocal.pseudo
14    Ir  [  1.354  2.388  6.641]   1   0.016  ir_us_gga_flocal.pseudo
15    Ir  [  4.059  2.343  6.546]   1   0.010  ir_us_gga_flocal.pseudo
16     S  [  1.352  0.781  8.302]   0   0.030  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 150.0
Number of bands     = 101
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



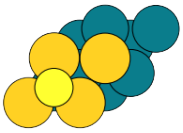
Pt overlayer:

```
---------------------------------
Dacapo calculation from Rh-subs+S/Pt-layer/Rh111-subs+Pt-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -15354.640754 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.323  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.332  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.332  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.223  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.279  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.382  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.382  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.365  Rh_us_gga_fl.pseudo
 8    Rh  [  5.409  1.559  4.335]   2   0.006  Rh_us_gga_fl.pseudo
 9    Rh  [  2.702  1.560  4.334]   2   0.007  Rh_us_gga_fl.pseudo
10    Rh  [  6.757  3.901  4.430]   2   0.030  Rh_us_gga_fl.pseudo
11    Rh  [  4.055  3.905  4.335]   2   0.007  Rh_us_gga_fl.pseudo
12    Pt  [ -0.026 -0.015  6.742]   1   0.042  pt_us_gga.pseudo
13    Pt  [  2.730 -0.015  6.743]   1   0.040  pt_us_gga.pseudo
14    Pt  [  1.352  2.372  6.743]   1   0.040  pt_us_gga.pseudo
15    Pt  [  4.056  2.342  6.625]   1   0.001  pt_us_gga.pseudo
16     S  [  1.350  0.780  8.454]   0   0.044  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 154.0
Number of bands     = 104
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Au overlayer:

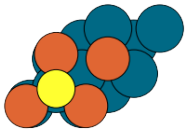
```
---------------------------------
Dacapo calculation from Rh-subs+S/Au-layer/Rh111-subs+Au-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -16071.785983 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4080  0.0000  0.0000] 5.41
a1 [ 2.7040  4.6834  0.0000] 5.41
a2 [ 0.0000  0.0000  18.8312] 18.83
No stress calculated.
Volume = 476.95 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Rh  [  0.000  0.000  0.000]   4   0.308  Rh_us_gga_fl.pseudo
 1    Rh  [  2.704  0.000  0.000]   4   0.311  Rh_us_gga_fl.pseudo
 2    Rh  [  1.352  2.342  0.000]   4   0.313  Rh_us_gga_fl.pseudo
 3    Rh  [  4.056  2.342  0.000]   4   0.278  Rh_us_gga_fl.pseudo
 4    Rh  [  1.352  0.781  2.208]   3   0.545  Rh_us_gga_fl.pseudo
 5    Rh  [  4.056  0.781  2.208]   3   0.333  Rh_us_gga_fl.pseudo
 6    Rh  [  2.704  3.122  2.208]   3   0.325  Rh_us_gga_fl.pseudo
 7    Rh  [  5.408  3.122  2.208]   3   0.312  Rh_us_gga_fl.pseudo
 8    Rh  [  5.420  1.552  4.323]   2   0.013  Rh_us_gga_fl.pseudo
 9    Rh  [  2.687  1.550  4.323]   2   0.028  Rh_us_gga_fl.pseudo
10    Rh  [  6.754  3.902  4.475]   2   0.005  Rh_us_gga_fl.pseudo
11    Rh  [  4.055  3.918  4.326]   2   0.013  Rh_us_gga_fl.pseudo
12    Au  [ -0.027 -0.020  6.909]   1   0.036  Au_us_gga.pseudo
13    Au  [  2.717 -0.022  6.956]   1   0.034  Au_us_gga.pseudo
14    Au  [  1.343  2.354  6.912]   1   0.033  Au_us_gga.pseudo
15    Au  [  4.047  2.332  6.629]   1   0.028  Au_us_gga.pseudo
16     S  [  1.324  0.781  8.809]   0   0.013  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 158.0
Number of bands     = 106
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Structures with Pd as the substrate:

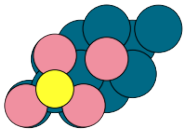
Fe overlayer:

```
---------------------------------
Dacapo calculation from Pd-subs+S/Fe-layer/Pd111-subs+Fe-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -16235.857611 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.039  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.041  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.041  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.042  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.267  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.141  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.141  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.137  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.578  1.611  4.609]   2   0.027  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.790  1.611  4.604]   2   0.035  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.970  4.024  4.475]   2   0.028  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.184  4.025  4.609]   2   0.026  046-Pd-gpe-n-6projectors-floc.uspp
12    Fe  [ -0.205 -0.119  6.618]   1   0.046  Fe_us_gga_d2.1.8.pseudo
13    Fe  [  3.002 -0.114  6.617]   1   0.049  Fe_us_gga_d2.1.8.pseudo
14    Fe  [  1.402  2.657  6.617]   1   0.049  Fe_us_gga_d2.1.8.pseudo
15    Fe  [  4.174  2.410  6.563]   1   0.008  Fe_us_gga_d2.1.8.pseudo
16     S  [  1.397  0.806  7.804]   0   0.012  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 158.0
Number of bands     = 106
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



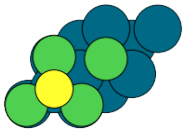
Co overlayer:

```
---------------------------------
Dacapo calculation from Pd-subs+S/Co-layer/Pd111-subs+Co-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -17273.191441 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.026  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.027  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.027  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.035  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.209  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.097  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.097  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.106  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.579  1.606  4.589]   2   0.012  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.784  1.607  4.585]   2   0.015  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.964  4.021  4.521]   2   0.006  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.180  4.029  4.589]   2   0.012  046-Pd-gpe-n-6projectors-floc.uspp
12    Co  [ -0.156 -0.090  6.648]   1   0.021  Co_us_gga.pseudo
13    Co  [  2.945 -0.085  6.648]   1   0.024  Co_us_gga.pseudo
14    Co  [  1.398  2.593  6.648]   1   0.024  Co_us_gga.pseudo
15    Co  [  4.178  2.412  6.539]   1   0.020  Co_us_gga.pseudo
16     S  [  1.393  0.804  7.835]   0   0.022  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 162.0
Number of bands     = 109
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



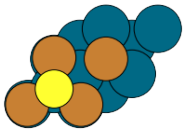
Ni overlayer:

```
---------------------------------
Dacapo calculation from Pd-subs+S/Ni-layer/Pd111-subs+Ni-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -18134.027624 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.020  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.020  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.020  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.037  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.104  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.067  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.067  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.069  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.578  1.608  4.560]   2   0.015  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.787  1.609  4.558]   2   0.010  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.966  4.022  4.558]   2   0.015  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.182  4.027  4.560]   2   0.015  046-Pd-gpe-n-6projectors-floc.uspp
12    Ni  [ -0.094 -0.055  6.648]   1   0.013  Ni_us_gga.pseudo
13    Ni  [  2.881 -0.051  6.647]   1   0.009  Ni_us_gga.pseudo
14    Ni  [  1.397  2.521  6.647]   1   0.009  Ni_us_gga.pseudo
15    Ni  [  4.179  2.413  6.547]   1   0.033  Ni_us_gga.pseudo
16     S  [  1.392  0.804  7.909]   0   0.023  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 166.0
Number of bands     = 111
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



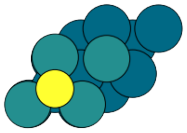
Cu overlayer:

```
---------------------------------
Dacapo calculation from Pd-subs+S/Cu-layer/Pd111-subs+Cu-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19612.327936 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.028  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.024  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.024  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.093  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.003  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.101  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.101  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.102  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.576  1.610  4.547]   2   0.029  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.788  1.610  4.547]   2   0.022  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.969  4.024  4.599]   2   0.044  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.183  4.024  4.547]   2   0.029  046-Pd-gpe-n-6projectors-floc.uspp
12    Cu  [ -0.054 -0.031  6.686]   1   0.027  Cu_us_gga.pseudo
13    Cu  [  2.842 -0.031  6.686]   1   0.027  Cu_us_gga.pseudo
14    Cu  [  1.394  2.477  6.686]   1   0.027  Cu_us_gga.pseudo
15    Cu  [  4.180  2.413  6.613]   1   0.029  Cu_us_gga.pseudo
16     S  [  1.393  0.804  8.158]   0   0.043  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 170.0
Number of bands     = 114
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



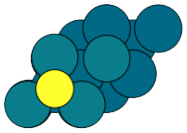
Ru overlayer:

```
---------------------------------
Dacapo calculation from Pd-subs+S/Ru-layer/Pd111-subs+Ru-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -15645.288449 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.040  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.042  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.042  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.038  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.169  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.088  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.088  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.092  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.576  1.608  4.549]   2   0.011  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.784  1.608  4.543]   2   0.011  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.964  4.021  4.486]   2   0.006  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.181  4.025  4.549]   2   0.011  046-Pd-gpe-n-6projectors-floc.uspp
12    Ru  [ -0.071 -0.041  6.765]   1   0.025  Ru_us_gga.pseudo
13    Ru  [  2.861 -0.029  6.762]   1   0.024  Ru_us_gga.pseudo
14    Ru  [  1.405  2.492  6.762]   1   0.024  Ru_us_gga.pseudo
15    Ru  [  4.172  2.409  6.659]   1   0.034  Ru_us_gga.pseudo
16     S  [  1.391  0.803  8.373]   0   0.022  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 158.0
Number of bands     = 106
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



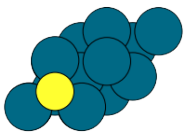
Rh overlayer:

```
---------------------------------
Dacapo calculation from Pd-subs+S/Rh-layer/Pd111-subs+Rh-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -16305.457945 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.021  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.018  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.018  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.041  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.111  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.031  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.031  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.033  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.580  1.604  4.532]   2   0.042  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.781  1.606  4.536]   2   0.042  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.964  4.021  4.537]   2   0.010  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.179  4.030  4.532]   2   0.042  046-Pd-gpe-n-6projectors-floc.uspp
12    Rh  [ -0.063 -0.037  6.808]   1   0.032  Rh_us_gga_fl.pseudo
13    Rh  [  2.851 -0.040  6.811]   1   0.029  Rh_us_gga_fl.pseudo
14    Rh  [  1.391  2.489  6.811]   1   0.029  Rh_us_gga_fl.pseudo
15    Rh  [  4.186  2.417  6.668]   1   0.027  Rh_us_gga_fl.pseudo
16     S  [  1.394  0.805  8.301]   0   0.002  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 162.0
Number of bands     = 109
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



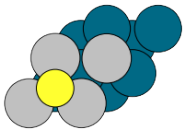
Pd overlayer:

```
---------------------------------
Dacapo calculation from Pd-subs+S/Pd-layer/Pd111-subs+Pd-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -17107.162008 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.002  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.005  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.005  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.025  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.000  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.077  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.077  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.067  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.576  1.605  4.522]   2   0.044  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.784  1.607  4.522]   2   0.042  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.962  4.019  4.572]   2   0.018  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.178  4.026  4.522]   2   0.045  046-Pd-gpe-n-6projectors-floc.uspp
12    Pd  [ -0.044 -0.025  6.845]   1   0.033  046-Pd-gpe-n-6projectors-floc.uspp
13    Pd  [  2.834 -0.023  6.844]   1   0.029  046-Pd-gpe-n-6projectors-floc.uspp
14    Pd  [  1.397  2.465  6.844]   1   0.029  046-Pd-gpe-n-6projectors-floc.uspp
15    Pd  [  4.183  2.415  6.769]   1   0.047  046-Pd-gpe-n-6projectors-floc.uspp
16     S  [  1.393  0.804  8.374]   0   0.004  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 166.0
Number of bands     = 111
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



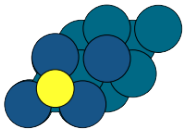
Ag overlayer:

```
---------------------------------
Dacapo calculation from Pd-subs+S/Ag-layer/Pd111-subs+Ag-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -18086.291941 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.019  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.012  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.012  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.094  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.028  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.158  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.158  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.165  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.600  1.620  4.541]   2   0.030  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.806  1.620  4.541]   2   0.020  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.991  4.037  4.629]   2   0.036  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.203  4.039  4.541]   2   0.031  046-Pd-gpe-n-6projectors-floc.uspp
12    Ag  [ -0.017 -0.010  6.970]   1   0.047  ag_us.pseudo
13    Ag  [  2.826 -0.006  6.971]   1   0.026  ag_us.pseudo
14    Ag  [  1.408  2.450  6.971]   1   0.026  ag_us.pseudo
15    Ag  [  4.195  2.422  6.874]   1   0.046  ag_us.pseudo
16     S  [  1.397  0.806  8.772]   0   0.025  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 170.0
Number of bands     = 114
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



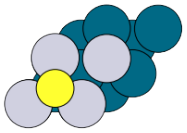
Ir overlayer:

```
---------------------------------
Dacapo calculation from Pd-subs+S/Ir-layer/Pd111-subs+Ir-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -17103.435657 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.019  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.016  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.016  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.048  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.131  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.019  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.019  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.021  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.584  1.602  4.539]   2   0.037  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.778  1.604  4.542]   2   0.038  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.965  4.021  4.535]   2   0.042  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.179  4.035  4.539]   2   0.038  046-Pd-gpe-n-6projectors-floc.uspp
12    Ir  [ -0.082 -0.047  6.839]   1   0.037  ir_us_gga_flocal.pseudo
13    Ir  [  2.867 -0.049  6.839]   1   0.031  ir_us_gga_flocal.pseudo
14    Ir  [  1.391  2.508  6.839]   1   0.031  ir_us_gga_flocal.pseudo
15    Ir  [  4.185  2.416  6.650]   1   0.019  ir_us_gga_flocal.pseudo
16     S  [  1.394  0.805  8.352]   0   0.022  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 162.0
Number of bands     = 109
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



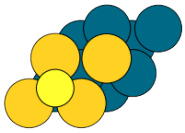
Pt overlayer:

```
---------------------------------
Dacapo calculation from Pd-subs+S/Pt-layer/Pd111-subs+Pt-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -17758.389901 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.016  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.015  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.015  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.044  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.003  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.113  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.113  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.108  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.581  1.605  4.515]   2   0.022  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.782  1.606  4.514]   2   0.023  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  6.966  4.022  4.596]   2   0.024  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.181  4.030  4.515]   2   0.022  046-Pd-gpe-n-6projectors-floc.uspp
12    Pt  [ -0.044 -0.026  6.910]   1   0.032  pt_us_gga.pseudo
13    Pt  [  2.834 -0.024  6.908]   1   0.034  pt_us_gga.pseudo
14    Pt  [  1.396  2.466  6.908]   1   0.034  pt_us_gga.pseudo
15    Pt  [  4.181  2.414  6.773]   1   0.021  pt_us_gga.pseudo
16     S  [  1.394  0.805  8.488]   0   0.019  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 166.0
Number of bands     = 111
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Au overlayer:

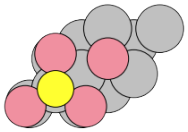
```
---------------------------------
Dacapo calculation from Pd-subs+S/Au-layer/Pd111-subs+Au-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -18476.628010 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.5720  0.0000  0.0000] 5.57
a1 [ 2.7860  4.8255  0.0000] 5.57
a2 [ 0.0000  0.0000  19.0990] 19.10
No stress calculated.
Volume = 513.53 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pd  [  0.000  0.000  0.000]   4   0.026  046-Pd-gpe-n-6projectors-floc.uspp
 1    Pd  [  2.786  0.000  0.000]   4   0.019  046-Pd-gpe-n-6projectors-floc.uspp
 2    Pd  [  1.393  2.413  0.000]   4   0.019  046-Pd-gpe-n-6projectors-floc.uspp
 3    Pd  [  4.179  2.413  0.000]   4   0.093  046-Pd-gpe-n-6projectors-floc.uspp
 4    Pd  [  1.393  0.804  2.275]   3   0.128  046-Pd-gpe-n-6projectors-floc.uspp
 5    Pd  [  4.179  0.804  2.275]   3   0.169  046-Pd-gpe-n-6projectors-floc.uspp
 6    Pd  [  2.786  3.217  2.275]   3   0.169  046-Pd-gpe-n-6projectors-floc.uspp
 7    Pd  [  5.572  3.217  2.275]   3   0.185  046-Pd-gpe-n-6projectors-floc.uspp
 8    Pd  [  5.621  1.627  4.518]   2   0.015  046-Pd-gpe-n-6projectors-floc.uspp
 9    Pd  [  2.817  1.626  4.514]   2   0.019  046-Pd-gpe-n-6projectors-floc.uspp
10    Pd  [  7.009  4.046  4.649]   2   0.035  046-Pd-gpe-n-6projectors-floc.uspp
11    Pd  [  4.220  4.054  4.518]   2   0.014  046-Pd-gpe-n-6projectors-floc.uspp
12    Au  [ -0.010 -0.006  7.016]   1   0.022  Au_us_gga.pseudo
13    Au  [  2.827 -0.004  7.011]   1   0.036  Au_us_gga.pseudo
14    Au  [  1.410  2.451  7.011]   1   0.036  Au_us_gga.pseudo
15    Au  [  4.196  2.423  6.829]   1   0.017  Au_us_gga.pseudo
16     S  [  1.405  0.811  8.822]   0   0.013  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 170.0
Number of bands     = 114
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Structures with Ag as the substrate:

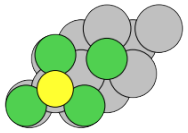
Co overlayer:

```
---------------------------------
Dacapo calculation from Ag-subs+S/Co-layer/Ag111-subs+Co-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -20210.876822 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.033  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.035  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.035  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.013  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.320  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.185  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.185  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.180  ag_us.pseudo
 8    Ag  [  5.821  1.680  4.863]   2   0.005  ag_us.pseudo
 9    Ag  [  2.909  1.680  4.868]   2   0.007  ag_us.pseudo
10    Ag  [  7.279  4.203  4.708]   2   0.041  ag_us.pseudo
11    Ag  [  4.365  4.202  4.863]   2   0.004  ag_us.pseudo
12    Co  [ -0.236 -0.136  6.971]   1   0.034  Co_us_gga.pseudo
13    Co  [  3.146 -0.138  6.973]   1   0.034  Co_us_gga.pseudo
14    Co  [  1.453  2.794  6.973]   1   0.034  Co_us_gga.pseudo
15    Co  [  4.377  2.527  6.949]   1   0.046  Co_us_gga.pseudo
16     S  [  1.454  0.840  7.922]   0   0.042  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 174.0
Number of bands     = 117
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



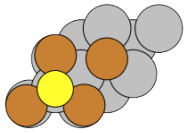
Ni overlayer:

```
---------------------------------
Dacapo calculation from Ag-subs+S/Ni-layer/Ag111-subs+Ni-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -21072.282882 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.035  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.039  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.039  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.038  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.318  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.198  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.198  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.199  ag_us.pseudo
 8    Ag  [  5.822  1.685  4.858]   2   0.004  ag_us.pseudo
 9    Ag  [  2.912  1.681  4.853]   2   0.006  ag_us.pseudo
10    Ag  [  7.283  4.205  4.723]   2   0.016  ag_us.pseudo
11    Ag  [  4.370  4.199  4.858]   2   0.004  ag_us.pseudo
12    Ni  [ -0.182 -0.105  6.952]   1   0.009  Ni_us_gga.pseudo
13    Ni  [  3.102 -0.099  6.953]   1   0.008  Ni_us_gga.pseudo
14    Ni  [  1.466  2.736  6.953]   1   0.008  Ni_us_gga.pseudo
15    Ni  [  4.357  2.515  6.937]   1   0.031  Ni_us_gga.pseudo
16     S  [  1.457  0.841  7.969]   0   0.032  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 178.0
Number of bands     = 119
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



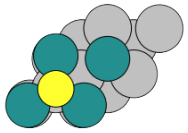
Cu overlayer:

```
---------------------------------
Dacapo calculation from Ag-subs+S/Cu-layer/Ag111-subs+Cu-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -22550.958369 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.072  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.071  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.071  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.017  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.154  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.068  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.068  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.079  ag_us.pseudo
 8    Ag  [  5.830  1.680  4.768]   2   0.023  ag_us.pseudo
 9    Ag  [  2.908  1.679  4.749]   2   0.012  ag_us.pseudo
10    Ag  [  7.284  4.205  4.746]   2   0.016  ag_us.pseudo
11    Ag  [  4.370  4.209  4.768]   2   0.023  ag_us.pseudo
12    Cu  [ -0.158 -0.091  6.979]   1   0.003  Cu_us_gga.pseudo
13    Cu  [  3.085 -0.076  6.977]   1   0.017  Cu_us_gga.pseudo
14    Cu  [  1.476  2.709  6.977]   1   0.017  Cu_us_gga.pseudo
15    Cu  [  4.356  2.515  6.830]   1   0.038  Cu_us_gga.pseudo
16     S  [  1.459  0.842  8.188]   0   0.036  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 182.0
Number of bands     = 122
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



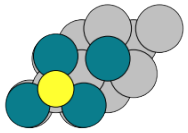
Ru overlayer:

```
---------------------------------
Dacapo calculation from Ag-subs+S/Ru-layer/Ag111-subs+Ru-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -18582.809399 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.027  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.029  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.029  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.011  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.121  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.102  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.102  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.101  ag_us.pseudo
 8    Ag  [  5.835  1.673  4.755]   2   0.047  ag_us.pseudo
 9    Ag  [  2.890  1.669  4.759]   2   0.044  ag_us.pseudo
10    Ag  [  7.280  4.203  4.674]   2   0.045  ag_us.pseudo
11    Ag  [  4.366  4.217  4.755]   2   0.047  ag_us.pseudo
12    Ru  [ -0.122 -0.071  7.045]   1   0.023  Ru_us_gga.pseudo
13    Ru  [  3.044 -0.077  7.051]   1   0.029  Ru_us_gga.pseudo
14    Ru  [  1.455  2.675  7.051]   1   0.029  Ru_us_gga.pseudo
15    Ru  [  4.364  2.519  6.962]   1   0.031  Ru_us_gga.pseudo
16     S  [  1.459  0.842  8.468]   0   0.035  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 170.0
Number of bands     = 114
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



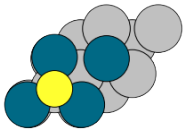
Rh overlayer:

```
---------------------------------
Dacapo calculation from Ag-subs+S/Rh-layer/Ag111-subs+Rh-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19244.000236 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.030  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.031  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.031  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.031  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.182  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.110  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.110  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.106  ag_us.pseudo
 8    Ag  [  5.826  1.681  4.793]   2   0.009  ag_us.pseudo
 9    Ag  [  2.910  1.680  4.802]   2   0.030  ag_us.pseudo
10    Ag  [  7.282  4.204  4.707]   2   0.024  ag_us.pseudo
11    Ag  [  4.368  4.205  4.793]   2   0.010  ag_us.pseudo
12    Rh  [ -0.121 -0.070  7.080]   1   0.037  Rh_us_gga_fl.pseudo
13    Rh  [  3.034 -0.075  7.084]   1   0.034  Rh_us_gga_fl.pseudo
14    Rh  [  1.452  2.665  7.084]   1   0.033  Rh_us_gga_fl.pseudo
15    Rh  [  4.380  2.529  7.043]   1   0.025  Rh_us_gga_fl.pseudo
16     S  [  1.458  0.842  8.388]   0   0.029  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 174.0
Number of bands     = 117
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



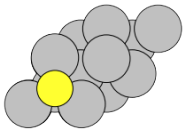
Pd overlayer:

```
---------------------------------
Dacapo calculation from Ag-subs+S/Pd-layer/Ag111-subs+Pd-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -20046.699580 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.040  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.040  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.040  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.076  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.094  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.046  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.046  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.041  ag_us.pseudo
 8    Ag  [  5.825  1.684  4.750]   2   0.031  ag_us.pseudo
 9    Ag  [  2.917  1.684  4.753]   2   0.036  ag_us.pseudo
10    Ag  [  7.285  4.206  4.716]   2   0.041  ag_us.pseudo
11    Ag  [  4.371  4.202  4.750]   2   0.030  ag_us.pseudo
12    Pd  [ -0.078 -0.045  7.036]   1   0.029  046-Pd-gpe-n-6projectors-floc.uspp
13    Pd  [  2.991 -0.043  7.036]   1   0.025  046-Pd-gpe-n-6projectors-floc.uspp
14    Pd  [  1.458  2.612  7.036]   1   0.025  046-Pd-gpe-n-6projectors-floc.uspp
15    Pd  [  4.379  2.528  7.022]   1   0.047  046-Pd-gpe-n-6projectors-floc.uspp
16     S  [  1.456  0.840  8.452]   0   0.039  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 178.0
Number of bands     = 119
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



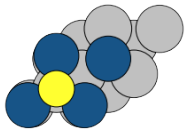
Ag overlayer:

```
---------------------------------
Dacapo calculation from Ag-subs+S/Ag-layer/Ag111-subs+Ag-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -21025.852832 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.058  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.056  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.056  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.012  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.025  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.099  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.099  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.092  ag_us.pseudo
 8    Ag  [  5.827  1.677  4.726]   2   0.014  ag_us.pseudo
 9    Ag  [  2.904  1.677  4.727]   2   0.012  ag_us.pseudo
10    Ag  [  7.280  4.203  4.835]   2   0.039  ag_us.pseudo
11    Ag  [  4.366  4.208  4.726]   2   0.014  ag_us.pseudo
12    Ag  [ -0.053 -0.031  7.165]   1   0.029  ag_us.pseudo
13    Ag  [  2.962 -0.032  7.164]   1   0.032  ag_us.pseudo
14    Ag  [  1.453  2.581  7.164]   1   0.032  ag_us.pseudo
15    Ag  [  4.362  2.519  7.034]   1   0.009  ag_us.pseudo
16     S  [  1.456  0.841  8.870]   0   0.024  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 182.0
Number of bands     = 122
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



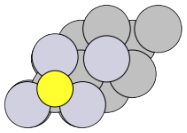
Ir overlayer:

```
---------------------------------
Dacapo calculation from Ag-subs+S/Ir-layer/Ag111-subs+Ir-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -20041.440303 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.029  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.031  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.031  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.031  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.150  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.096  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.096  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.090  ag_us.pseudo
 8    Ag  [  5.836  1.675  4.777]   2   0.010  ag_us.pseudo
 9    Ag  [  2.901  1.675  4.788]   2   0.032  ag_us.pseudo
10    Ag  [  7.283  4.205  4.692]   2   0.005  ag_us.pseudo
11    Ag  [  4.368  4.216  4.777]   2   0.010  ag_us.pseudo
12    Ir  [ -0.151 -0.087  7.095]   1   0.032  ir_us_gga_flocal.pseudo
13    Ir  [  3.059 -0.090  7.096]   1   0.031  ir_us_gga_flocal.pseudo
14    Ir  [  1.451  2.694  7.096]   1   0.031  ir_us_gga_flocal.pseudo
15    Ir  [  4.383  2.530  7.016]   1   0.025  ir_us_gga_flocal.pseudo
16     S  [  1.457  0.841  8.427]   0   0.040  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 174.0
Number of bands     = 117
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



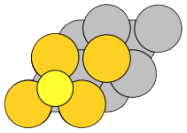
Pt overlayer:

```
---------------------------------
Dacapo calculation from Ag-subs+S/Pt-layer/Ag111-subs+Pt-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -20697.844628 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.043  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.042  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.042  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.070  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.095  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.040  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.040  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.037  ag_us.pseudo
 8    Ag  [  5.830  1.680  4.741]   2   0.001  ag_us.pseudo
 9    Ag  [  2.908  1.679  4.742]   2   0.001  ag_us.pseudo
10    Ag  [  7.284  4.205  4.711]   2   0.003  ag_us.pseudo
11    Ag  [  4.370  4.209  4.741]   2   0.002  ag_us.pseudo
12    Pt  [ -0.099 -0.057  7.104]   1   0.019  pt_us_gga.pseudo
13    Pt  [  3.014 -0.058  7.104]   1   0.022  pt_us_gga.pseudo
14    Pt  [  1.457  2.639  7.104]   1   0.022  pt_us_gga.pseudo
15    Pt  [  4.370  2.523  7.034]   1   0.022  pt_us_gga.pseudo
16     S  [  1.456  0.841  8.511]   0   0.029  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 178.0
Number of bands     = 119
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Au overlayer:

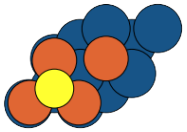
```
---------------------------------
Dacapo calculation from Ag-subs+S/Au-layer/Ag111-subs+Au-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -21416.618577 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8266  0.0000  0.0000] 5.83
a1 [ 2.9133  5.0459  0.0000] 5.83
a2 [ 0.0000  0.0000  19.5147] 19.51
No stress calculated.
Volume = 573.74 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ag  [  0.000  0.000  0.000]   4   0.061  ag_us.pseudo
 1    Ag  [  2.913  0.000  0.000]   4   0.060  ag_us.pseudo
 2    Ag  [  1.457  2.523  0.000]   4   0.060  ag_us.pseudo
 3    Ag  [  4.370  2.523  0.000]   4   0.023  ag_us.pseudo
 4    Ag  [  1.457  0.841  2.379]   3   0.036  ag_us.pseudo
 5    Ag  [  4.370  0.841  2.379]   3   0.134  ag_us.pseudo
 6    Ag  [  2.913  3.364  2.379]   3   0.134  ag_us.pseudo
 7    Ag  [  5.827  3.364  2.379]   3   0.127  ag_us.pseudo
 8    Ag  [  5.843  1.671  4.727]   2   0.015  ag_us.pseudo
 9    Ag  [  2.896  1.672  4.725]   2   0.017  ag_us.pseudo
10    Ag  [  7.283  4.205  4.840]   2   0.043  ag_us.pseudo
11    Ag  [  4.369  4.225  4.727]   2   0.015  ag_us.pseudo
12    Au  [ -0.063 -0.036  7.254]   1   0.030  Au_us_gga.pseudo
13    Au  [  2.974 -0.035  7.248]   1   0.027  Au_us_gga.pseudo
14    Au  [  1.456  2.593  7.248]   1   0.027  Au_us_gga.pseudo
15    Au  [  4.368  2.522  7.017]   1   0.044  Au_us_gga.pseudo
16     S  [  1.458  0.842  8.923]   0   0.014  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 182.0
Number of bands     = 122
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Structures with Ir as the substrate:

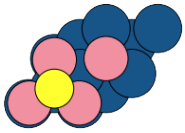
Fe overlayer:

```
---------------------------------
Dacapo calculation from Ir-subs+S/Fe-layer/Ir111-subs+Fe-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -16229.274234 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.384  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.399  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.399  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.579  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.515  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.441  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.441  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.432  ir_us_gga_flocal.pseudo
 8    Ir  [  5.440  1.576  4.477]   2   0.018  ir_us_gga_flocal.pseudo
 9    Ir  [  2.729  1.576  4.476]   2   0.020  ir_us_gga_flocal.pseudo
10    Ir  [  6.810  3.932  4.496]   2   0.047  ir_us_gga_flocal.pseudo
11    Ir  [  4.085  3.923  4.477]   2   0.018  ir_us_gga_flocal.pseudo
12    Fe  [  0.082  0.047  6.476]   1   0.027  Fe_us_gga_d2.1.8.pseudo
13    Fe  [  2.642  0.050  6.475]   1   0.029  Fe_us_gga_d2.1.8.pseudo
14    Fe  [  1.364  2.263  6.475]   1   0.029  Fe_us_gga_d2.1.8.pseudo
15    Fe  [  4.083  2.357  6.450]   1   0.004  Fe_us_gga_d2.1.8.pseudo
16     S  [  1.362  0.786  8.089]   0   0.005  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 146.0
Number of bands     = 98
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



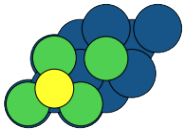
Co overlayer:

```
---------------------------------
Dacapo calculation from Ir-subs+S/Co-layer/Ir111-subs+Co-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -17266.183158 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.362  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.376  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.376  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.542  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.455  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.442  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.442  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.441  ir_us_gga_flocal.pseudo
 8    Ir  [  5.444  1.575  4.442]   2   0.012  ir_us_gga_flocal.pseudo
 9    Ir  [  2.728  1.575  4.441]   2   0.012  ir_us_gga_flocal.pseudo
10    Ir  [  6.810  3.932  4.465]   2   0.037  ir_us_gga_flocal.pseudo
11    Ir  [  4.086  3.927  4.442]   2   0.012  ir_us_gga_flocal.pseudo
12    Co  [  0.050  0.029  6.466]   1   0.009  Co_us_gga.pseudo
13    Co  [  2.672  0.033  6.465]   1   0.010  Co_us_gga.pseudo
14    Co  [  1.364  2.298  6.465]   1   0.010  Co_us_gga.pseudo
15    Co  [  4.085  2.358  6.435]   1   0.018  Co_us_gga.pseudo
16     S  [  1.361  0.785  8.016]   0   0.017  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 150.0
Number of bands     = 101
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



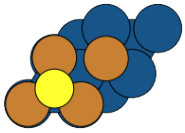
Ni overlayer:

```
---------------------------------
Dacapo calculation from Ir-subs+S/Ni-layer/Ir111-subs+Ni-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -18126.407355 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.381  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.393  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.393  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.416  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.442  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.447  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.447  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.453  ir_us_gga_flocal.pseudo
 8    Ir  [  5.447  1.573  4.410]   2   0.020  ir_us_gga_flocal.pseudo
 9    Ir  [  2.726  1.574  4.410]   2   0.019  ir_us_gga_flocal.pseudo
10    Ir  [  6.810  3.932  4.440]   2   0.012  ir_us_gga_flocal.pseudo
11    Ir  [  4.086  3.930  4.410]   2   0.020  ir_us_gga_flocal.pseudo
12    Ni  [ -0.032 -0.018  6.492]   1   0.027  Ni_us_gga.pseudo
13    Ni  [  2.756 -0.017  6.492]   1   0.025  Ni_us_gga.pseudo
14    Ni  [  1.363  2.395  6.492]   1   0.025  Ni_us_gga.pseudo
15    Ni  [  4.088  2.360  6.433]   1   0.050  Ni_us_gga.pseudo
16     S  [  1.361  0.786  7.919]   0   0.012  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 154.0
Number of bands     = 104
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



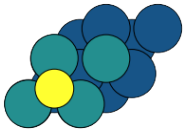
Cu overlayer:

```
---------------------------------
Dacapo calculation from Ir-subs+S/Cu-layer/Ir111-subs+Cu-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19603.497249 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.445  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.446  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.446  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.313  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.431  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.431  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.431  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.426  ir_us_gga_flocal.pseudo
 8    Ir  [  5.451  1.572  4.384]   2   0.041  ir_us_gga_flocal.pseudo
 9    Ir  [  2.723  1.572  4.385]   2   0.040  ir_us_gga_flocal.pseudo
10    Ir  [  6.811  3.932  4.482]   2   0.009  ir_us_gga_flocal.pseudo
11    Ir  [  4.087  3.935  4.384]   2   0.041  ir_us_gga_flocal.pseudo
12    Cu  [ -0.044 -0.026  6.608]   1   0.023  Cu_us_gga.pseudo
13    Cu  [  2.769 -0.026  6.608]   1   0.023  Cu_us_gga.pseudo
14    Cu  [  1.362  2.411  6.608]   1   0.023  Cu_us_gga.pseudo
15    Cu  [  4.087  2.360  6.486]   1   0.013  Cu_us_gga.pseudo
16     S  [  1.362  0.787  8.143]   0   0.027  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 158.0
Number of bands     = 106
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



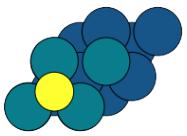
Ru overlayer:

```
---------------------------------
Dacapo calculation from Ir-subs+S/Ru-layer/Ir111-subs+Ru-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -15638.233141 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.350  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.344  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.344  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.518  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.328  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.464  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.464  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.452  ir_us_gga_flocal.pseudo
 8    Ir  [  5.446  1.571  4.459]   2   0.047  ir_us_gga_flocal.pseudo
 9    Ir  [  2.720  1.571  4.459]   2   0.036  ir_us_gga_flocal.pseudo
10    Ir  [  6.811  3.933  4.396]   2   0.020  ir_us_gga_flocal.pseudo
11    Ir  [  4.084  3.931  4.459]   2   0.047  ir_us_gga_flocal.pseudo
12    Ru  [ -0.021 -0.012  6.641]   1   0.028  Ru_us_gga.pseudo
13    Ru  [  2.740 -0.014  6.640]   1   0.032  Ru_us_gga.pseudo
14    Ru  [  1.358  2.380  6.640]   1   0.032  Ru_us_gga.pseudo
15    Ru  [  4.084  2.358  6.609]   1   0.022  Ru_us_gga.pseudo
16     S  [  1.360  0.785  8.365]   0   0.023  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 146.0
Number of bands     = 98
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



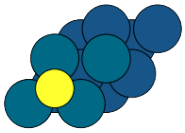
Rh overlayer:

```
---------------------------------
Dacapo calculation from Ir-subs+S/Rh-layer/Ir111-subs+Rh-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -16297.975560 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.339  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.340  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.340  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.474  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.186  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.448  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.448  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.444  ir_us_gga_flocal.pseudo
 8    Ir  [  5.447  1.573  4.417]   2   0.032  ir_us_gga_flocal.pseudo
 9    Ir  [  2.727  1.574  4.418]   2   0.023  ir_us_gga_flocal.pseudo
10    Ir  [  6.809  3.931  4.408]   2   0.016  ir_us_gga_flocal.pseudo
11    Ir  [  4.086  3.931  4.417]   2   0.031  ir_us_gga_flocal.pseudo
12    Rh  [ -0.021 -0.012  6.642]   1   0.030  Rh_us_gga_fl.pseudo
13    Rh  [  2.746 -0.010  6.643]   1   0.027  Rh_us_gga_fl.pseudo
14    Rh  [  1.364  2.383  6.643]   1   0.028  Rh_us_gga_fl.pseudo
15    Rh  [  4.089  2.361  6.612]   1   0.048  Rh_us_gga_fl.pseudo
16     S  [  1.360  0.785  8.288]   0   0.020  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 150.0
Number of bands     = 101
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



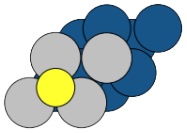
Pd overlayer:

```
---------------------------------
Dacapo calculation from Ir-subs+S/Pd-layer/Ir111-subs+Pd-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -17098.708812 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.431  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.442  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.442  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.401  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.355  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.471  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.471  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.465  ir_us_gga_flocal.pseudo
 8    Ir  [  5.446  1.574  4.380]   2   0.019  ir_us_gga_flocal.pseudo
 9    Ir  [  2.725  1.574  4.380]   2   0.021  ir_us_gga_flocal.pseudo
10    Ir  [  6.810  3.932  4.430]   2   0.006  ir_us_gga_flocal.pseudo
11    Ir  [  4.086  3.930  4.380]   2   0.019  ir_us_gga_flocal.pseudo
12    Pd  [ -0.021 -0.012  6.702]   1   0.019  046-Pd-gpe-n-6projectors-floc.uspp
13    Pd  [  2.747 -0.013  6.702]   1   0.018  046-Pd-gpe-n-6projectors-floc.uspp
14    Pd  [  1.362  2.385  6.702]   1   0.018  046-Pd-gpe-n-6projectors-floc.uspp
15    Pd  [  4.087  2.360  6.668]   1   0.008  046-Pd-gpe-n-6projectors-floc.uspp
16     S  [  1.363  0.787  8.358]   0   0.014  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 154.0
Number of bands     = 104
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



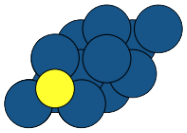
Ag overlayer:

```
---------------------------------
Dacapo calculation from Ir-subs+S/Ag-layer/Ir111-subs+Ag-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -18076.472740 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.468  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.454  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.454  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.273  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.357  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.442  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.442  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.439  ir_us_gga_flocal.pseudo
 8    Ir  [  5.441  1.578  4.374]   2   0.011  ir_us_gga_flocal.pseudo
 9    Ir  [  2.735  1.579  4.376]   2   0.020  ir_us_gga_flocal.pseudo
10    Ir  [  6.810  3.932  4.442]   2   0.009  ir_us_gga_flocal.pseudo
11    Ir  [  4.087  3.923  4.374]   2   0.009  ir_us_gga_flocal.pseudo
12    Ag  [ -0.025 -0.015  6.795]   1   0.045  ag_us.pseudo
13    Ag  [  2.737 -0.015  6.792]   1   0.043  ag_us.pseudo
14    Ag  [  1.356  2.378  6.792]   1   0.042  ag_us.pseudo
15    Ag  [  4.081  2.356  7.409]   1   0.045  ag_us.pseudo
16     S  [  1.362  0.786  8.680]   0   0.005  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 158.0
Number of bands     = 106
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



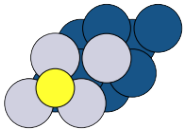
Ir overlayer:

```
---------------------------------
Dacapo calculation from Ir-subs+S/Ir-layer/Ir111-subs+Ir-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -17095.968732 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.334  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.335  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.335  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.480  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.192  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.461  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.461  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.453  ir_us_gga_flocal.pseudo
 8    Ir  [  5.450  1.572  4.423]   2   0.020  ir_us_gga_flocal.pseudo
 9    Ir  [  2.724  1.573  4.423]   2   0.010  ir_us_gga_flocal.pseudo
10    Ir  [  6.808  3.931  4.417]   2   0.007  ir_us_gga_flocal.pseudo
11    Ir  [  4.086  3.934  4.423]   2   0.019  ir_us_gga_flocal.pseudo
12    Ir  [ -0.032 -0.019  6.663]   1   0.039  ir_us_gga_flocal.pseudo
13    Ir  [  2.758 -0.018  6.667]   1   0.041  ir_us_gga_flocal.pseudo
14    Ir  [  1.364  2.398  6.667]   1   0.041  ir_us_gga_flocal.pseudo
15    Ir  [  4.089  2.361  6.606]   1   0.013  ir_us_gga_flocal.pseudo
16     S  [  1.361  0.786  8.337]   0   0.040  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 150.0
Number of bands     = 101
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



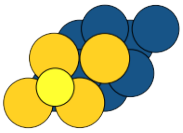
Pt overlayer:

```
---------------------------------
Dacapo calculation from Ir-subs+S/Pt-layer/Ir111-subs+Pt-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -17749.727244 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.432  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.438  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.438  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.375  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.358  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.451  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.451  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.444  ir_us_gga_flocal.pseudo
 8    Ir  [  5.450  1.571  4.370]   2   0.007  ir_us_gga_flocal.pseudo
 9    Ir  [  2.722  1.571  4.370]   2   0.007  ir_us_gga_flocal.pseudo
10    Ir  [  6.809  3.931  4.458]   2   0.016  ir_us_gga_flocal.pseudo
11    Ir  [  4.086  3.934  4.370]   2   0.007  ir_us_gga_flocal.pseudo
12    Pt  [ -0.027 -0.016  6.776]   1   0.031  pt_us_gga.pseudo
13    Pt  [  2.748 -0.016  6.774]   1   0.030  pt_us_gga.pseudo
14    Pt  [  1.360  2.388  6.774]   1   0.030  pt_us_gga.pseudo
15    Pt  [  4.085  2.358  6.664]   1   0.011  pt_us_gga.pseudo
16     S  [  1.362  0.786  8.490]   0   0.013  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 154.0
Number of bands     = 104
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Au overlayer:

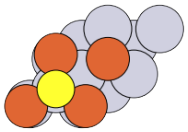
```
---------------------------------
Dacapo calculation from Ir-subs+S/Au-layer/Ir111-subs+Au-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -18466.737218 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.4490  0.0000  0.0000] 5.45
a1 [ 2.7245  4.7189  0.0000] 5.45
a2 [ 0.0000  0.0000  18.8981] 18.90
No stress calculated.
Volume = 485.93 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Ir  [  0.000  0.000  0.000]   4   0.433  ir_us_gga_flocal.pseudo
 1    Ir  [  2.724  0.000  0.000]   4   0.438  ir_us_gga_flocal.pseudo
 2    Ir  [  1.362  2.359  0.000]   4   0.438  ir_us_gga_flocal.pseudo
 3    Ir  [  4.087  2.359  0.000]   4   0.387  ir_us_gga_flocal.pseudo
 4    Ir  [  1.362  0.786  2.225]   3   0.591  ir_us_gga_flocal.pseudo
 5    Ir  [  4.087  0.786  2.225]   3   0.425  ir_us_gga_flocal.pseudo
 6    Ir  [  2.724  3.146  2.225]   3   0.425  ir_us_gga_flocal.pseudo
 7    Ir  [  5.449  3.146  2.225]   3   0.403  ir_us_gga_flocal.pseudo
 8    Ir  [  5.459  1.563  4.359]   2   0.023  ir_us_gga_flocal.pseudo
 9    Ir  [  2.712  1.566  4.354]   2   0.015  ir_us_gga_flocal.pseudo
10    Ir  [  6.813  3.934  4.506]   2   0.005  ir_us_gga_flocal.pseudo
11    Ir  [  4.083  3.947  4.359]   2   0.023  ir_us_gga_flocal.pseudo
12    Au  [ -0.040 -0.023  7.083]   1   0.044  Au_us_gga.pseudo
13    Au  [  2.730 -0.019  6.941]   1   0.009  Au_us_gga.pseudo
14    Au  [  1.348  2.374  6.941]   1   0.009  Au_us_gga.pseudo
15    Au  [  4.075  2.353  6.669]   1   0.007  Au_us_gga.pseudo
16     S  [  1.407  0.812  8.847]   0   0.013  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 158.0
Number of bands     = 106
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Structures with Pt as the substrate:

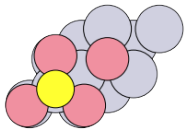
Fe overlayer:

```
---------------------------------
Dacapo calculation from Pt-subs+S/Fe-layer/Pt111-subs+Fe-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -18189.528871 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.306  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.303  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.303  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.327  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.550  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.289  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.289  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.280  pt_us_gga.pseudo
 8    Pt  [  5.640  1.626  4.692]   2   0.017  pt_us_gga.pseudo
 9    Pt  [  2.817  1.627  4.693]   2   0.016  pt_us_gga.pseudo
10    Pt  [  7.046  4.068  4.571]   2   0.034  pt_us_gga.pseudo
11    Pt  [  4.228  4.071  4.692]   2   0.018  pt_us_gga.pseudo
12    Fe  [ -0.208 -0.120  6.696]   1   0.020  Fe_us_gga_d2.1.8.pseudo
13    Fe  [  3.024 -0.122  6.697]   1   0.021  Fe_us_gga_d2.1.8.pseudo
14    Fe  [  1.406  2.679  6.697]   1   0.021  Fe_us_gga_d2.1.8.pseudo
15    Fe  [  4.232  2.443  6.643]   1   0.012  Fe_us_gga_d2.1.8.pseudo
16     S  [  1.407  0.813  7.872]   0   0.030  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 158.0
Number of bands     = 106
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



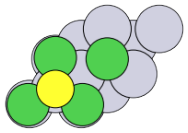
Co overlayer:

```
---------------------------------
Dacapo calculation from Pt-subs+S/Co-layer/Pt111-subs+Co-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19226.783999 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.269  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.268  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.268  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.322  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.460  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.278  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.278  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.277  pt_us_gga.pseudo
 8    Pt  [  5.642  1.625  4.669]   2   0.020  pt_us_gga.pseudo
 9    Pt  [  2.816  1.626  4.667]   2   0.021  pt_us_gga.pseudo
10    Pt  [  7.047  4.069  4.610]   2   0.038  pt_us_gga.pseudo
11    Pt  [  4.228  4.074  4.669]   2   0.020  pt_us_gga.pseudo
12    Co  [ -0.150 -0.087  6.712]   1   0.037  Co_us_gga.pseudo
13    Co  [  2.966 -0.084  6.712]   1   0.035  Co_us_gga.pseudo
14    Co  [  1.410  2.611  6.712]   1   0.035  Co_us_gga.pseudo
15    Co  [  4.226  2.440  6.610]   1   0.031  Co_us_gga.pseudo
16     S  [  1.407  0.812  7.891]   0   0.013  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 162.0
Number of bands     = 109
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



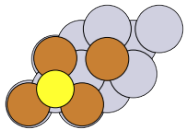
Ni overlayer:

```
---------------------------------
Dacapo calculation from Pt-subs+S/Ni-layer/Pt111-subs+Ni-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -20087.496406 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.246  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.242  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.242  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.329  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.289  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.243  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.243  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.239  pt_us_gga.pseudo
 8    Pt  [  5.642  1.627  4.636]   2   0.011  pt_us_gga.pseudo
 9    Pt  [  2.817  1.626  4.635]   2   0.015  pt_us_gga.pseudo
10    Pt  [  7.049  4.070  4.660]   2   0.020  pt_us_gga.pseudo
11    Pt  [  4.230  4.072  4.636]   2   0.012  pt_us_gga.pseudo
12    Ni  [ -0.065 -0.038  6.712]   1   0.036  Ni_us_gga.pseudo
13    Ni  [  2.882 -0.038  6.711]   1   0.038  Ni_us_gga.pseudo
14    Ni  [  1.408  2.514  6.711]   1   0.038  Ni_us_gga.pseudo
15    Ni  [  4.226  2.440  6.607]   1   0.011  Ni_us_gga.pseudo
16     S  [  1.409  0.813  8.005]   0   0.036  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 166.0
Number of bands     = 111
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



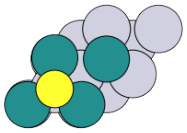
Cu overlayer:

```
---------------------------------
Dacapo calculation from Pt-subs+S/Cu-layer/Pt111-subs+Cu-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -21565.595464 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.213  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.216  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.216  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.448  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.282  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.326  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.326  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.329  pt_us_gga.pseudo
 8    Pt  [  5.640  1.627  4.643]   2   0.045  pt_us_gga.pseudo
 9    Pt  [  2.818  1.627  4.642]   2   0.048  pt_us_gga.pseudo
10    Pt  [  7.049  4.070  4.730]   2   0.020  pt_us_gga.pseudo
11    Pt  [  4.229  4.071  4.643]   2   0.045  pt_us_gga.pseudo
12    Cu  [ -0.041 -0.024  6.824]   1   0.012  Cu_us_gga.pseudo
13    Cu  [  2.860 -0.025  6.824]   1   0.012  Cu_us_gga.pseudo
14    Cu  [  1.408  2.489  6.824]   1   0.012  Cu_us_gga.pseudo
15    Cu  [  4.227  2.441  6.706]   1   0.043  Cu_us_gga.pseudo
16     S  [  1.410  0.814  8.294]   0   0.046  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 170.0
Number of bands     = 114
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



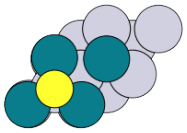
Ru overlayer:

```
---------------------------------
Dacapo calculation from Pt-subs+S/Ru-layer/Pt111-subs+Ru-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -17598.727045 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.320  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.318  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.318  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.255  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.478  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.251  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.251  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.253  pt_us_gga.pseudo
 8    Pt  [  5.639  1.626  4.646]   2   0.022  pt_us_gga.pseudo
 9    Pt  [  2.816  1.626  4.643]   2   0.019  pt_us_gga.pseudo
10    Pt  [  7.046  4.068  4.575]   2   0.001  pt_us_gga.pseudo
11    Pt  [  4.228  4.071  4.646]   2   0.022  pt_us_gga.pseudo
12    Ru  [ -0.068 -0.039  6.854]   1   0.006  Ru_us_gga.pseudo
13    Ru  [  2.886 -0.032  6.853]   1   0.008  Ru_us_gga.pseudo
14    Ru  [  1.415  2.515  6.853]   1   0.008  Ru_us_gga.pseudo
15    Ru  [  4.222  2.438  6.788]   1   0.012  Ru_us_gga.pseudo
16     S  [  1.407  0.812  8.452]   0   0.008  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 158.0
Number of bands     = 106
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



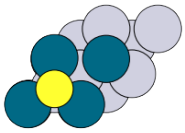
Rh overlayer:

```
---------------------------------
Dacapo calculation from Pt-subs+S/Rh-layer/Pt111-subs+Rh-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -18258.752445 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.261  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.256  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.256  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.287  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.392  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.193  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.193  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.185  pt_us_gga.pseudo
 8    Pt  [  5.642  1.624  4.625]   2   0.049  pt_us_gga.pseudo
 9    Pt  [  2.814  1.625  4.629]   2   0.050  pt_us_gga.pseudo
10    Pt  [  7.046  4.068  4.630]   2   0.027  pt_us_gga.pseudo
11    Pt  [  4.227  4.074  4.625]   2   0.050  pt_us_gga.pseudo
12    Rh  [ -0.065 -0.038  6.904]   1   0.007  Rh_us_gga_fl.pseudo
13    Rh  [  2.881 -0.040  6.905]   1   0.009  Rh_us_gga_fl.pseudo
14    Rh  [  1.406  2.515  6.905]   1   0.009  Rh_us_gga_fl.pseudo
15    Rh  [  4.233  2.444  6.791]   1   0.025  Rh_us_gga_fl.pseudo
16     S  [  1.409  0.813  8.383]   0   0.005  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 162.0
Number of bands     = 109
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



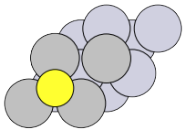
Pd overlayer:

```
---------------------------------
Dacapo calculation from Pt-subs+S/Pd-layer/Pt111-subs+Pd-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19060.386723 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.208  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.207  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.207  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.295  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.250  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.214  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.214  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.215  pt_us_gga.pseudo
 8    Pt  [  5.637  1.628  4.619]   2   0.026  pt_us_gga.pseudo
 9    Pt  [  2.818  1.627  4.618]   2   0.028  pt_us_gga.pseudo
10    Pt  [  7.048  4.069  4.674]   2   0.034  pt_us_gga.pseudo
11    Pt  [  4.228  4.068  4.619]   2   0.027  pt_us_gga.pseudo
12    Pd  [ -0.044 -0.025  6.951]   1   0.011  046-Pd-gpe-n-6projectors-floc.uspp
13    Pd  [  2.861 -0.025  6.950]   1   0.008  046-Pd-gpe-n-6projectors-floc.uspp
14    Pd  [  1.408  2.490  6.950]   1   0.008  046-Pd-gpe-n-6projectors-floc.uspp
15    Pd  [  4.225  2.440  6.878]   1   0.045  046-Pd-gpe-n-6projectors-floc.uspp
16     S  [  1.408  0.813  8.463]   0   0.022  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 166.0
Number of bands     = 111
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



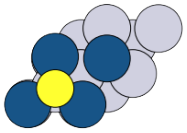
Ag overlayer:

```
---------------------------------
Dacapo calculation from Pt-subs+S/Ag-layer/Pt111-subs+Ag-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -20039.505580 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.214  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.220  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.220  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.432  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.184  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.281  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.281  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.284  pt_us_gga.pseudo
 8    Pt  [  5.639  1.628  4.624]   2   0.027  pt_us_gga.pseudo
 9    Pt  [  2.818  1.627  4.623]   2   0.018  pt_us_gga.pseudo
10    Pt  [  7.049  4.070  4.720]   2   0.016  pt_us_gga.pseudo
11    Pt  [  4.229  4.070  4.624]   2   0.026  pt_us_gga.pseudo
12    Ag  [ -0.029 -0.017  7.054]   1   0.026  ag_us.pseudo
13    Ag  [  2.839 -0.020  7.052]   1   0.016  ag_us.pseudo
14    Ag  [  1.402  2.469  7.052]   1   0.016  ag_us.pseudo
15    Ag  [  4.219  2.436  7.019]   1   0.014  ag_us.pseudo
16     S  [  1.409  0.814  8.835]   0   0.015  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 170.0
Number of bands     = 114
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



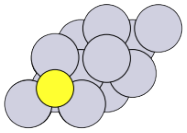
Ir overlayer:

```
---------------------------------
Dacapo calculation from Pt-subs+S/Ir-layer/Pt111-subs+Ir-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19056.436326 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.255  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.248  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.248  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.297  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.439  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.193  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.193  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.179  pt_us_gga.pseudo
 8    Pt  [  5.647  1.621  4.626]   2   0.045  pt_us_gga.pseudo
 9    Pt  [  2.810  1.623  4.630]   2   0.045  pt_us_gga.pseudo
10    Pt  [  7.046  4.068  4.618]   2   0.019  pt_us_gga.pseudo
11    Pt  [  4.227  4.080  4.626]   2   0.045  pt_us_gga.pseudo
12    Ir  [ -0.091 -0.052  6.925]   1   0.010  ir_us_gga_flocal.pseudo
13    Ir  [  2.906 -0.056  6.926]   1   0.009  ir_us_gga_flocal.pseudo
14    Ir  [  1.405  2.544  6.926]   1   0.009  ir_us_gga_flocal.pseudo
15    Ir  [  4.233  2.444  6.773]   1   0.024  ir_us_gga_flocal.pseudo
16     S  [  1.409  0.813  8.419]   0   0.018  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 162.0
Number of bands     = 109
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



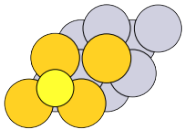
Pt overlayer:

```
---------------------------------
Dacapo calculation from Pt-subs+S/Pt-layer/Pt111-subs+Pt-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19711.342782 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.170  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.174  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.174  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.343  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.226  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.195  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.195  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.196  pt_us_gga.pseudo
 8    Pt  [  5.642  1.625  4.603]   2   0.039  pt_us_gga.pseudo
 9    Pt  [  2.813  1.624  4.601]   2   0.041  pt_us_gga.pseudo
10    Pt  [  7.049  4.070  4.688]   2   0.049  pt_us_gga.pseudo
11    Pt  [  4.229  4.074  4.603]   2   0.039  pt_us_gga.pseudo
12    Pt  [ -0.050 -0.029  7.023]   1   0.025  pt_us_gga.pseudo
13    Pt  [  2.868 -0.029  7.021]   1   0.025  pt_us_gga.pseudo
14    Pt  [  1.409  2.498  7.021]   1   0.025  pt_us_gga.pseudo
15    Pt  [  4.227  2.441  6.877]   1   0.002  pt_us_gga.pseudo
16     S  [  1.410  0.814  8.575]   0   0.006  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 166.0
Number of bands     = 111
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Au overlayer:

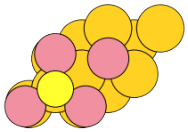
```
---------------------------------
Dacapo calculation from Pt-subs+S/Au-layer/Pt111-subs+Au-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -20429.643618 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.6385  0.0000  0.0000] 5.64
a1 [ 2.8192  4.8831  0.0000] 5.64
a2 [ 0.0000  0.0000  19.2076] 19.21
No stress calculated.
Volume = 528.84 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Pt  [  0.000  0.000  0.000]   4   0.175  pt_us_gga.pseudo
 1    Pt  [  2.819  0.000  0.000]   4   0.183  pt_us_gga.pseudo
 2    Pt  [  1.410  2.442  0.000]   4   0.183  pt_us_gga.pseudo
 3    Pt  [  4.229  2.442  0.000]   4   0.438  pt_us_gga.pseudo
 4    Pt  [  1.410  0.814  2.302]   3   0.096  pt_us_gga.pseudo
 5    Pt  [  4.229  0.814  2.302]   3   0.308  pt_us_gga.pseudo
 6    Pt  [  2.819  3.255  2.302]   3   0.308  pt_us_gga.pseudo
 7    Pt  [  5.638  3.255  2.302]   3   0.305  pt_us_gga.pseudo
 8    Pt  [  5.649  1.622  4.604]   2   0.030  pt_us_gga.pseudo
 9    Pt  [  2.810  1.623  4.603]   2   0.017  pt_us_gga.pseudo
10    Pt  [  7.049  4.070  4.752]   2   0.015  pt_us_gga.pseudo
11    Pt  [  4.229  4.081  4.604]   2   0.030  pt_us_gga.pseudo
12    Au  [ -0.038 -0.022  7.153]   1   0.041  Au_us_gga.pseudo
13    Au  [  2.844 -0.021  7.143]   1   0.040  Au_us_gga.pseudo
14    Au  [  1.404  2.474  7.143]   1   0.040  Au_us_gga.pseudo
15    Au  [  4.223  2.438  6.941]   1   0.016  Au_us_gga.pseudo
16     S  [  1.407  0.812  8.913]   0   0.026  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 170.0
Number of bands     = 114
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Structures with Au as the substrate:

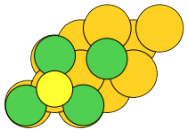
Co overlayer:

```
--------------------------------
Dacapo calculation from Au-subs+S/Co-layer/Au111-subs+Co-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -21383.121647 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.142  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.144  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.144  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.094  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.269  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.154  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.154  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.149  Au_us_gga.pseudo
 8    Au  [  5.898  1.697  4.876]   2   0.020  Au_us_gga.pseudo
 9    Au  [  2.944  1.700  4.893]   2   0.024  Au_us_gga.pseudo
10    Au  [  7.368  4.254  4.708]   2   0.003  Au_us_gga.pseudo
11    Au  [  4.419  4.259  4.876]   2   0.020  Au_us_gga.pseudo
12    Co  [ -0.224 -0.130  6.896]   1   0.022  Co_us_gga.pseudo
13    Co  [  3.164 -0.137  6.899]   1   0.024  Co_us_gga.pseudo
14    Co  [  1.464  2.808  6.899]   1   0.024  Co_us_gga.pseudo
15    Co  [  4.436  2.561  6.873]   1   0.012  Co_us_gga.pseudo
16     S  [  1.469  0.848  7.862]   0   0.038  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 174.0
Number of bands     = 117
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
--------------------------------
```



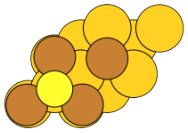
Ni overlayer:

```
---------------------------------
Dacapo calculation from Au-subs+S/Ni-layer/Au111-subs+Ni-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -22244.446187 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.123  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.131  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.131  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.153  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.214  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.110  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.110  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.121  Au_us_gga.pseudo
 8    Au  [  5.898  1.703  4.856]   2   0.018  Au_us_gga.pseudo
 9    Au  [  2.945  1.701  4.843]   2   0.031  Au_us_gga.pseudo
10    Au  [  7.372  4.256  4.777]   2   0.014  Au_us_gga.pseudo
11    Au  [  4.424  4.256  4.856]   2   0.018  Au_us_gga.pseudo
12    Ni  [ -0.136 -0.078  6.905]   1   0.041  Ni_us_gga.pseudo
13    Ni  [  3.090 -0.065  6.904]   1   0.046  Ni_us_gga.pseudo
14    Ni  [  1.489  2.708  6.904]   1   0.046  Ni_us_gga.pseudo
15    Ni  [  4.406  2.544  6.865]   1   0.034  Ni_us_gga.pseudo
16     S  [  1.473  0.851  7.988]   0   0.020  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 178.0
Number of bands     = 119
Kpoint grid         = 36 kpts
Spin-polarized      = True
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



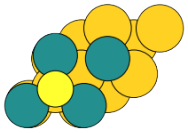
Cu overlayer:

```
---------------------------------
Dacapo calculation from Au-subs+S/Cu-layer/Au111-subs+Cu-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -23723.258216 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.142  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.157  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.157  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.053  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.162  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.201  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.201  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.200  Au_us_gga.pseudo
 8    Au  [  5.905  1.698  4.842]   2   0.011  Au_us_gga.pseudo
 9    Au  [  2.942  1.699  4.836]   2   0.008  Au_us_gga.pseudo
10    Au  [  7.372  4.256  4.911]   2   0.001  Au_us_gga.pseudo
11    Au  [  4.423  4.265  4.842]   2   0.011  Au_us_gga.pseudo
12    Cu  [ -0.086 -0.050  7.023]   1   0.047  Cu_us_gga.pseudo
13    Cu  [  3.034 -0.044  7.023]   1   0.049  Cu_us_gga.pseudo
14    Cu  [  1.479  2.650  7.023]   1   0.049  Cu_us_gga.pseudo
15    Cu  [  4.419  2.551  6.864]   1   0.010  Cu_us_gga.pseudo
16     S  [  1.474  0.851  8.346]   0   0.026  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 182.0
Number of bands     = 122
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



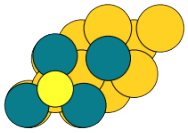
Ru overlayer:

```
---------------------------------
Dacapo calculation from Au-subs+S/Ru-layer/Au111-subs+Ru-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -19754.782933 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.105  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.111  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.111  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.083  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.255  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.183  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.183  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.183  Au_us_gga.pseudo
 8    Au  [  5.901  1.698  4.842]   2   0.005  Au_us_gga.pseudo
 9    Au  [  2.937  1.696  4.846]   2   0.008  Au_us_gga.pseudo
10    Au  [  7.370  4.255  4.702]   2   0.008  Au_us_gga.pseudo
11    Au  [  4.421  4.261  4.842]   2   0.005  Au_us_gga.pseudo
12    Ru  [ -0.142 -0.082  7.071]   1   0.004  Ru_us_gga.pseudo
13    Ru  [  3.098 -0.089  7.076]   1   0.006  Ru_us_gga.pseudo
14    Ru  [  1.472  2.728  7.076]   1   0.006  Ru_us_gga.pseudo
15    Ru  [  4.422  2.553  7.029]   1   0.049  Ru_us_gga.pseudo
16     S  [  1.476  0.852  8.452]   0   0.030  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 170.0
Number of bands     = 114
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



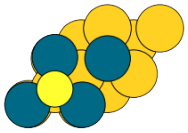
Rh overlayer:

```
---------------------------------
Dacapo calculation from Au-subs+S/Rh-layer/Au111-subs+Rh-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -20415.854401 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.095  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.093  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.093  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.128  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.210  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.120  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.120  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.114  Au_us_gga.pseudo
 8    Au  [  5.901  1.700  4.836]   2   0.031  Au_us_gga.pseudo
 9    Au  [  2.947  1.701  4.854]   2   0.032  Au_us_gga.pseudo
10    Au  [  7.371  4.256  4.750]   2   0.015  Au_us_gga.pseudo
11    Au  [  4.423  4.260  4.836]   2   0.029  Au_us_gga.pseudo
12    Rh  [ -0.123 -0.071  7.092]   1   0.003  Rh_us_gga_fl.pseudo
13    Rh  [  3.078 -0.080  7.101]   1   0.006  Rh_us_gga_fl.pseudo
14    Rh  [  1.470  2.706  7.101]   1   0.006  Rh_us_gga_fl.pseudo
15    Rh  [  4.450  2.569  7.062]   1   0.015  Rh_us_gga_fl.pseudo
16     S  [  1.477  0.853  8.375]   0   0.003  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 174.0
Number of bands     = 117
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



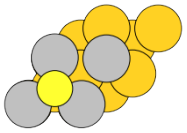
Pd overlayer:

```
---------------------------------
Dacapo calculation from Au-subs+S/Pd-layer/Au111-subs+Pd-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -21218.590956 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.112  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.109  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.109  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.199  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.178  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.114  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.114  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.111  Au_us_gga.pseudo
 8    Au  [  5.896  1.704  4.822]   2   0.014  Au_us_gga.pseudo
 9    Au  [  2.950  1.703  4.826]   2   0.005  Au_us_gga.pseudo
10    Au  [  7.373  4.257  4.816]   2   0.014  Au_us_gga.pseudo
11    Au  [  4.423  4.254  4.822]   2   0.014  Au_us_gga.pseudo
12    Pd  [ -0.072 -0.042  7.116]   1   0.027  046-Pd-gpe-n-6projectors-floc.uspp
13    Pd  [  3.021 -0.040  7.118]   1   0.026  046-Pd-gpe-n-6projectors-floc.uspp
14    Pd  [  1.476  2.636  7.118]   1   0.026  046-Pd-gpe-n-6projectors-floc.uspp
15    Pd  [  4.434  2.560  7.092]   1   0.038  046-Pd-gpe-n-6projectors-floc.uspp
16     S  [  1.472  0.850  8.512]   0   0.019  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 178.0
Number of bands     = 119
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



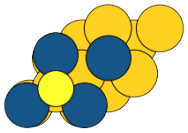
Ag overlayer:

```
---------------------------------
Dacapo calculation from Au-subs+S/Ag-layer/Au111-subs+Ag-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -22198.037456 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.130  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.138  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.138  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.040  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.029  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.127  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.127  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.118  Au_us_gga.pseudo
 8    Au  [  5.901  1.699  4.807]   2   0.015  Au_us_gga.pseudo
 9    Au  [  2.944  1.700  4.806]   2   0.010  Au_us_gga.pseudo
10    Au  [  7.372  4.256  4.894]   2   0.008  Au_us_gga.pseudo
11    Au  [  4.422  4.260  4.807]   2   0.015  Au_us_gga.pseudo
12    Ag  [ -0.055 -0.032  7.220]   1   0.023  ag_us.pseudo
13    Ag  [  3.001 -0.033  7.219]   1   0.027  ag_us.pseudo
14    Ag  [  1.472  2.616  7.219]   1   0.027  ag_us.pseudo
15    Ag  [  4.418  2.551  7.122]   1   0.049  ag_us.pseudo
16     S  [  1.475  0.851  8.888]   0   0.014  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 182.0
Number of bands     = 122
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



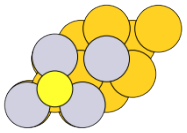
Ir overlayer:

```
---------------------------------
Dacapo calculation from Au-subs+S/Ir-layer/Au111-subs+Ir-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -21212.962253 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.106  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.101  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.101  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.115  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.243  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.151  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.151  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.139  Au_us_gga.pseudo
 8    Au  [  5.903  1.695  4.832]   2   0.048  Au_us_gga.pseudo
 9    Au  [  2.941  1.698  4.864]   2   0.039  Au_us_gga.pseudo
10    Au  [  7.369  4.255  4.721]   2   0.005  Au_us_gga.pseudo
11    Au  [  4.420  4.265  4.832]   2   0.050  Au_us_gga.pseudo
12    Ir  [ -0.167 -0.097  7.109]   1   0.006  ir_us_gga_flocal.pseudo
13    Ir  [  3.106 -0.107  7.116]   1   0.010  ir_us_gga_flocal.pseudo
14    Ir  [  1.460  2.744  7.116]   1   0.010  ir_us_gga_flocal.pseudo
15    Ir  [  4.456  2.573  7.043]   1   0.024  ir_us_gga_flocal.pseudo
16     S  [  1.471  0.849  8.406]   0   0.021  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 174.0
Number of bands     = 117
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Pt overlayer:

```
---------------------------------
Dacapo calculation from Au-subs+S/Pt-layer/Au111-subs+Pt-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -21869.379647 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.122  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.121  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.121  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.189  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.193  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.140  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.140  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.136  Au_us_gga.pseudo
 8    Au  [  5.902  1.699  4.817]   2   0.020  Au_us_gga.pseudo
 9    Au  [  2.941  1.698  4.820]   2   0.015  Au_us_gga.pseudo
10    Au  [  7.372  4.256  4.802]   2   0.030  Au_us_gga.pseudo
11    Au  [  4.422  4.262  4.817]   2   0.020  Au_us_gga.pseudo
12    Pt  [ -0.099 -0.057  7.189]   1   0.031  pt_us_gga.pseudo
13    Pt  [  3.049 -0.057  7.190]   1   0.035  pt_us_gga.pseudo
14    Pt  [  1.475  2.669  7.190]   1   0.035  pt_us_gga.pseudo
15    Pt  [  4.424  2.554  7.115]   1   0.021  pt_us_gga.pseudo
16     S  [  1.473  0.851  8.567]   0   0.046  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 178.0
Number of bands     = 119
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```



Au overlayer:

```
---------------------------------
Dacapo calculation from Au-subs+S/Au-layer/Au111-subs+Au-overlayer+S-relaxed-DOS.nc
status = finished
version = ifc ser v2-3-3
Energy = -22588.437689 eV

Unit Cell vectors (angstroms)
       x        y       z   length
a0 [ 5.8973  0.0000  0.0000] 5.90
a1 [ 2.9486  5.1072  0.0000] 5.90
a2 [ 0.0000  0.0000  19.6302] 19.63
No stress calculated.
Volume = 591.23 A^3

Atom,  sym, position (in x,y,z),     tag, rmsForce and psp
 0    Au  [  0.000  0.000  0.000]   4   0.126  Au_us_gga.pseudo
 1    Au  [  2.949  0.000  0.000]   4   0.139  Au_us_gga.pseudo
 2    Au  [  1.474  2.554  0.000]   4   0.139  Au_us_gga.pseudo
 3    Au  [  4.423  2.554  0.000]   4   0.033  Au_us_gga.pseudo
 4    Au  [  1.474  0.851  2.408]   3   0.025  Au_us_gga.pseudo
 5    Au  [  4.423  0.851  2.408]   3   0.168  Au_us_gga.pseudo
 6    Au  [  2.949  3.405  2.408]   3   0.168  Au_us_gga.pseudo
 7    Au  [  5.897  3.405  2.408]   3   0.159  Au_us_gga.pseudo
 8    Au  [  5.912  1.694  4.782]   2   0.048  Au_us_gga.pseudo
 9    Au  [  2.935  1.695  4.777]   2   0.043  Au_us_gga.pseudo
10    Au  [  7.372  4.256  4.909]   2   0.024  Au_us_gga.pseudo
11    Au  [  4.423  4.273  4.782]   2   0.046  Au_us_gga.pseudo
12    Au  [ -0.072 -0.041  7.315]   1   0.009  Au_us_gga.pseudo
13    Au  [  3.017 -0.041  7.311]   1   0.011  Au_us_gga.pseudo
14    Au  [  1.473  2.633  7.311]   1   0.010  Au_us_gga.pseudo
15    Au  [  4.420  2.552  7.060]   1   0.026  Au_us_gga.pseudo
16     S  [  1.475  0.852  8.924]   0   0.033  S_tm.pseudo

Details:
XCfunctional        = PW91
Planewavecutoff     = 340 eV
Densitywavecutoff   = 340 eV
FermiTemperature    = 0.100000 kT
Number of electrons = 182.0
Number of bands     = 122
Kpoint grid         = 36 kpts
Spin-polarized      = False
Dipole correction   = False
Symmetry            = False
Constraints         = []
---------------------------------
```