Propriedades Quânticas de Nanomateriais utilizando a Teoria do Funcional Densidade (DFT)

Pedro Venezuela

Marcio Costa

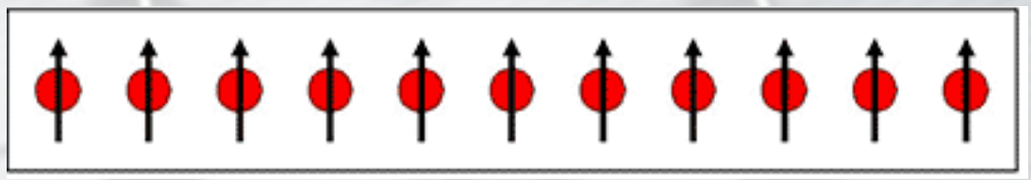
Instituto de Física
Universidade Federal Fluminense

Practical Part

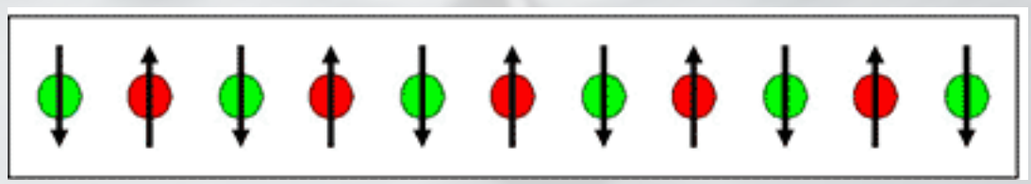
2D Magnetic Material - FeSe

- Band structure
- DOS and PDOS
- Magnetic ground state - AFM x FM

Ferromagnetic - FM



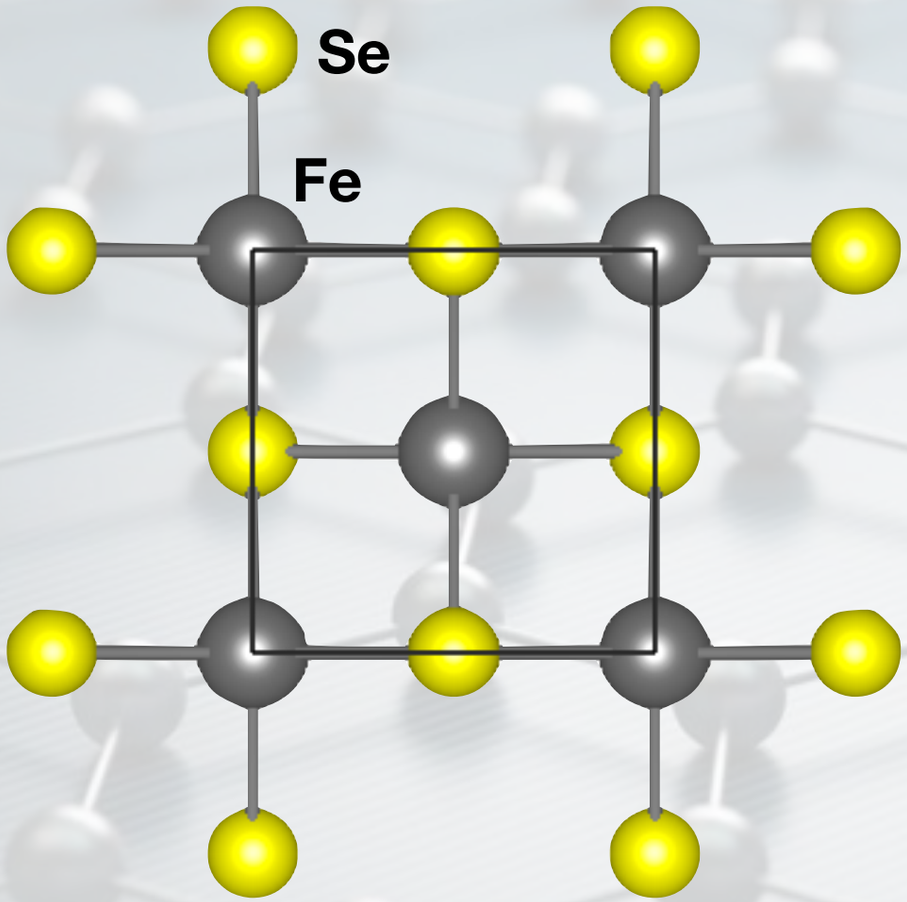
Antiferromagnetic - AFM



- Spin polarized density

FeSe

Top



FeSe

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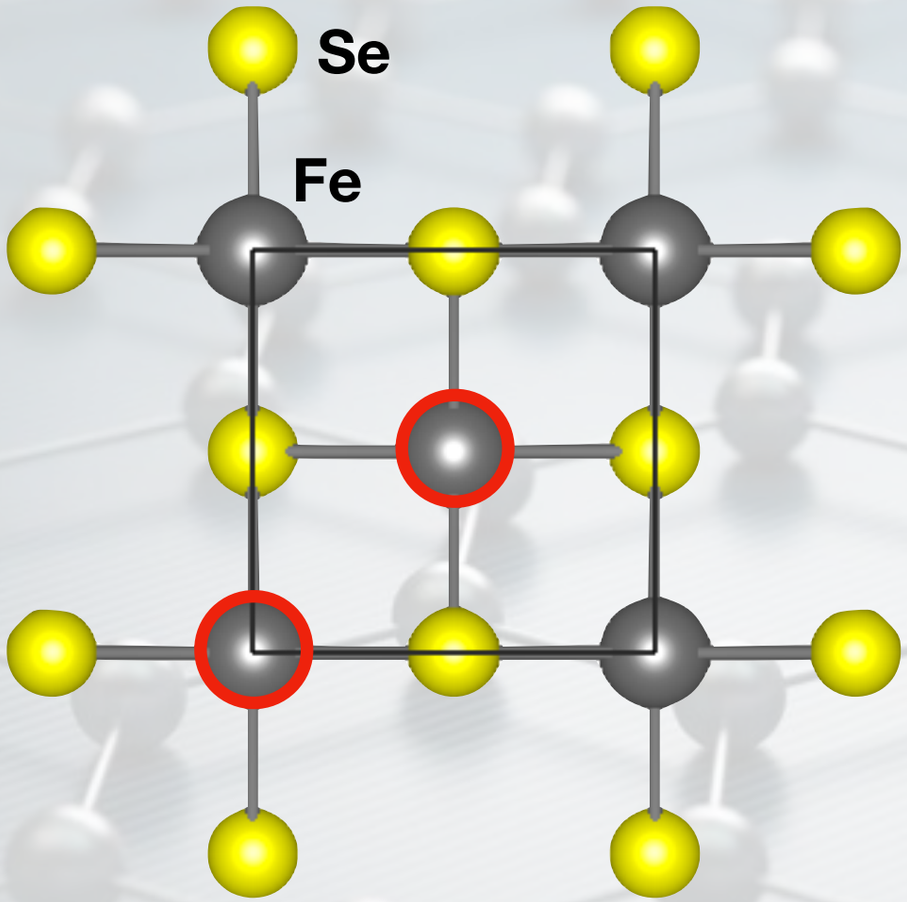
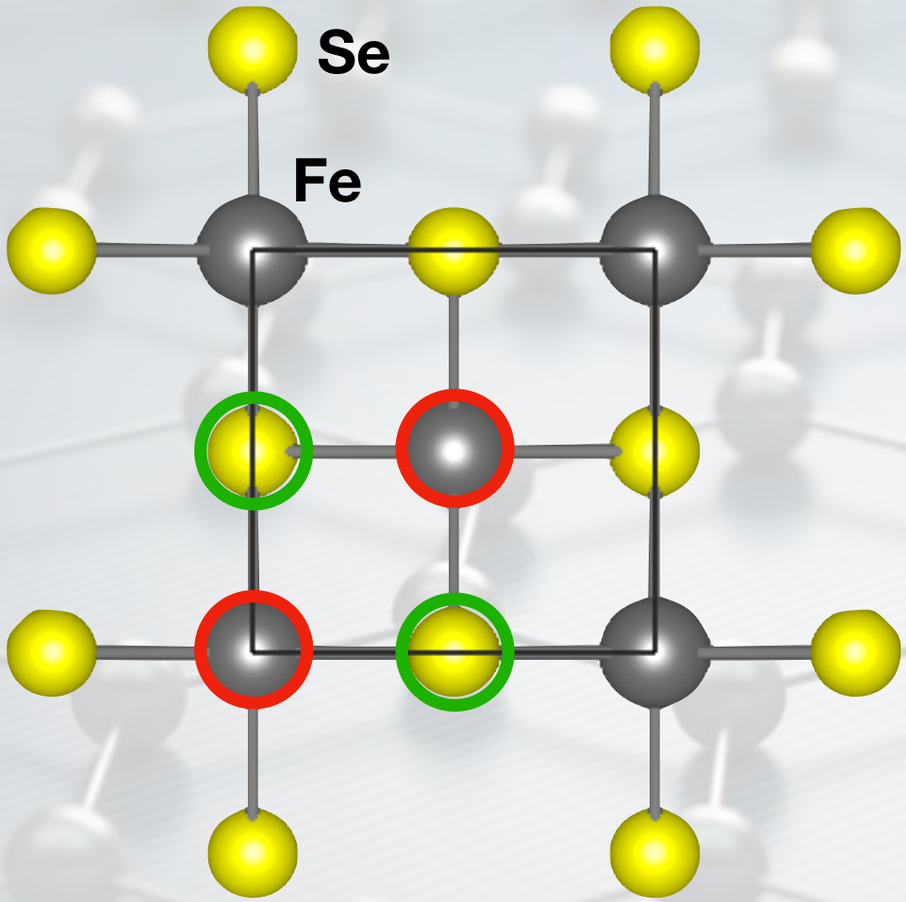
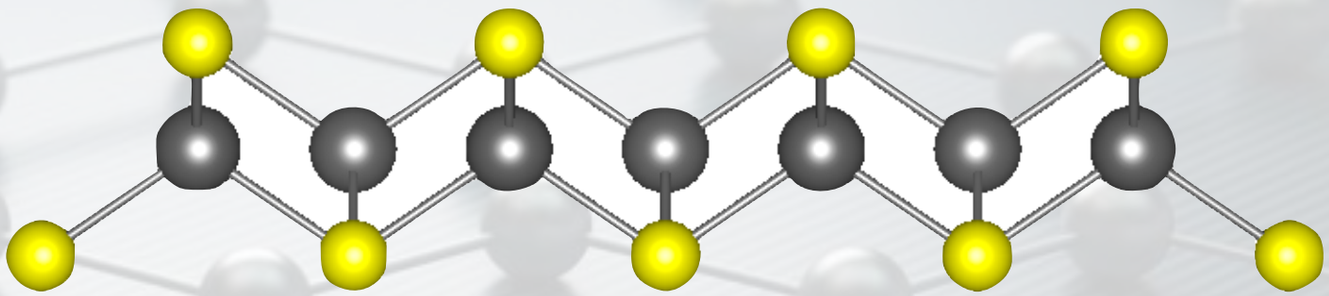


FeSe

Top



Side



FeSe

PHYSICAL REVIEW B **84**, 020503(R) (2011)

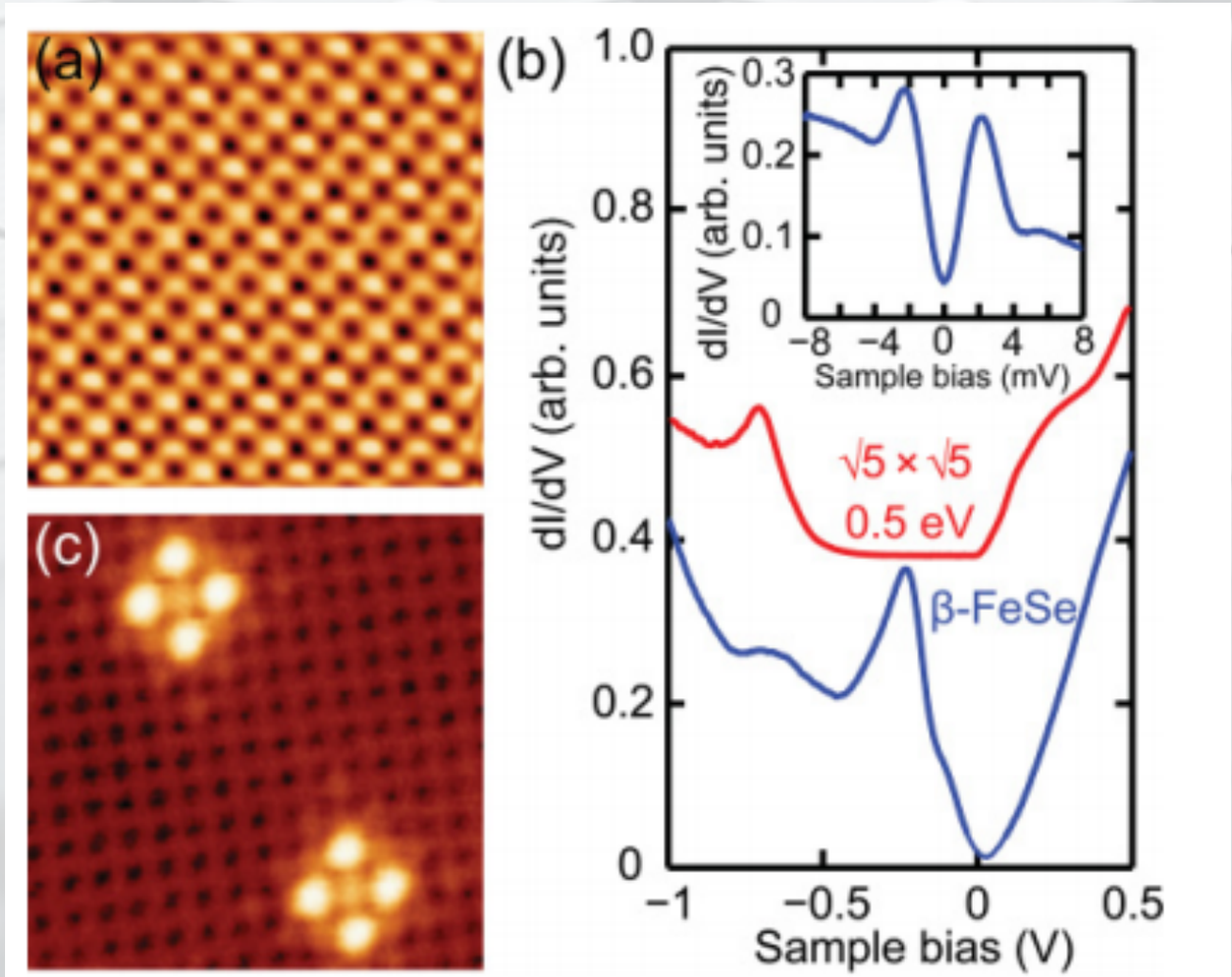
Molecular-beam epitaxy and robust superconductivity of stoichiometric FeSe crystalline films on bilayer graphene

Can-Li Song,[1,2] Yi-Lin Wang,[1] Ye-Ping Jiang,[1,2] Zhi Li,[1] Lili Wang,[1] Ke He,[1] Xi Chen,[2] Xu-Cun Ma,[1,*] and Qi-Kun Xue[1,2,†]

[1]*State Key Laboratory for Surface Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*

[2]*State Key Laboratory for Low-Dimensional Quantum Physics, Department of Physics, Tsinghua University, Beijing 100084, China*

(Received 19 May 2011; revised manuscript received 10 June 2011; published 12 July 2011)



FeSe

Computational 2D materials database

C2DB
The Computational 2D Materials Database

Search formula e.g. MoS2

Material class : All

Dynamic stability : medium - high

Thermodynamic stability : medium - high

Magnetic state : -

Band gap range [eV] : - PBE

Help with constructing advanced search queries ...

Toggle list of keys ...

https://cmrdb.fysik.dtu.dk/c2db/

FeSe

Fe_2Se_2

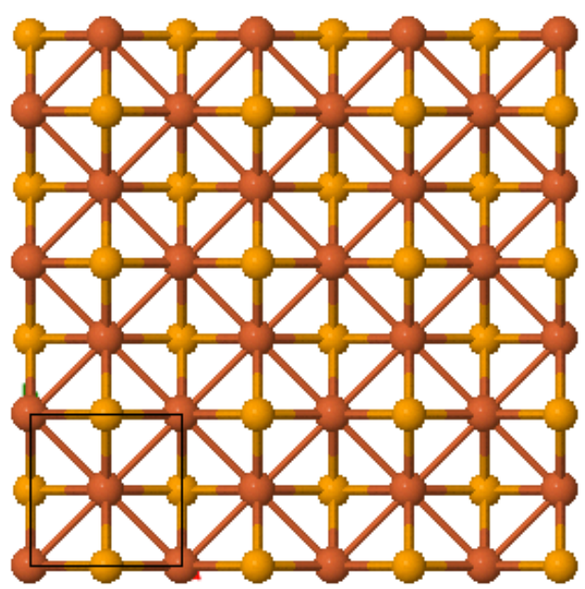
C2DB
The Computational 2D Materials Database

Summary

Structure info	Value
Crystal prototype	AB-129-bc
Space group	P4/nmm
Space group number	129
Monolayer reported DOI	10.1103/PhysRevB.84.020503

Stability

Thermodynamic	HIGH
Dynamical (phonons)	HIGH
Dynamical (stiffness)	HIGH



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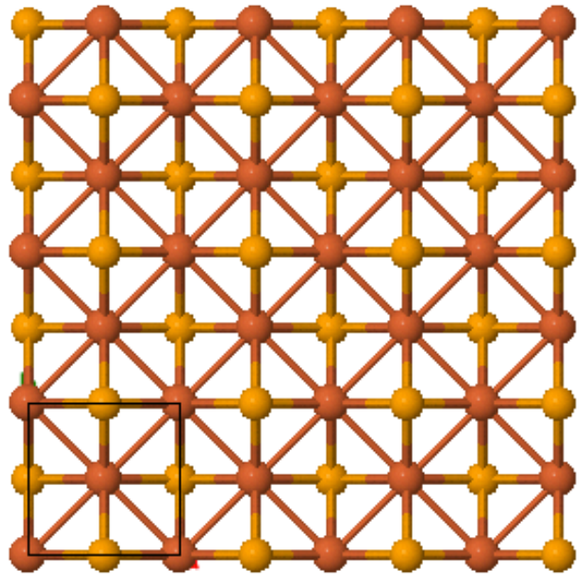

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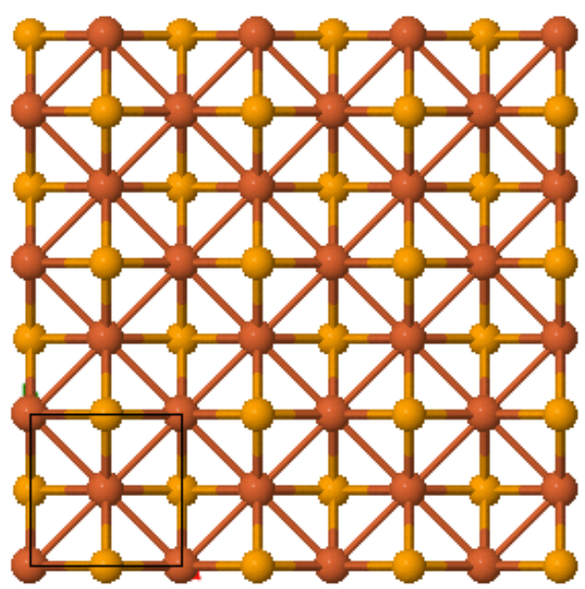

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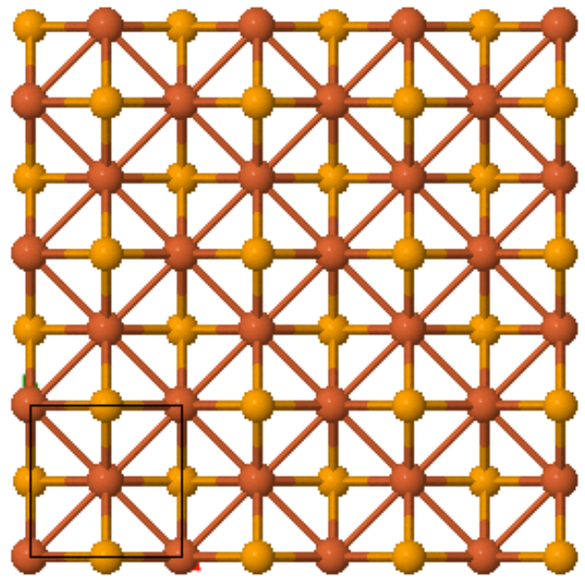

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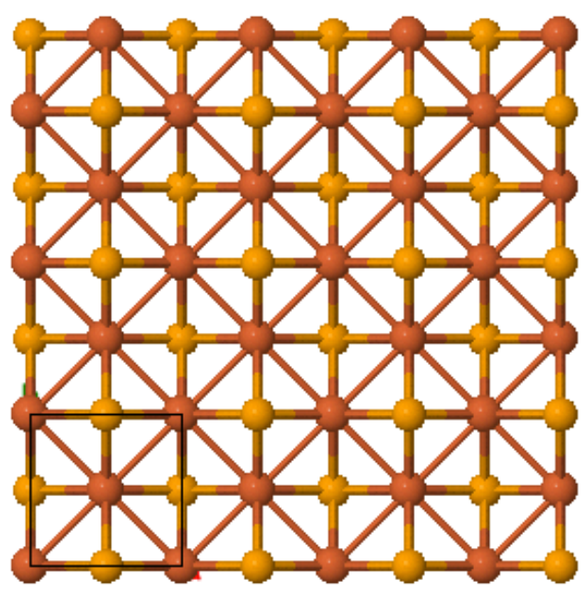

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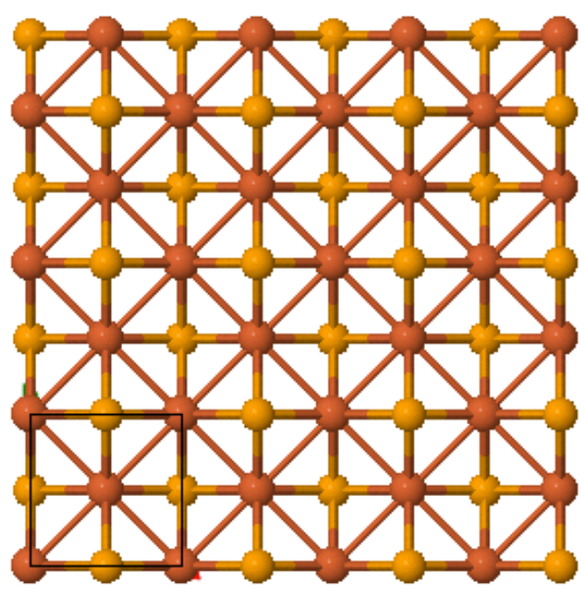

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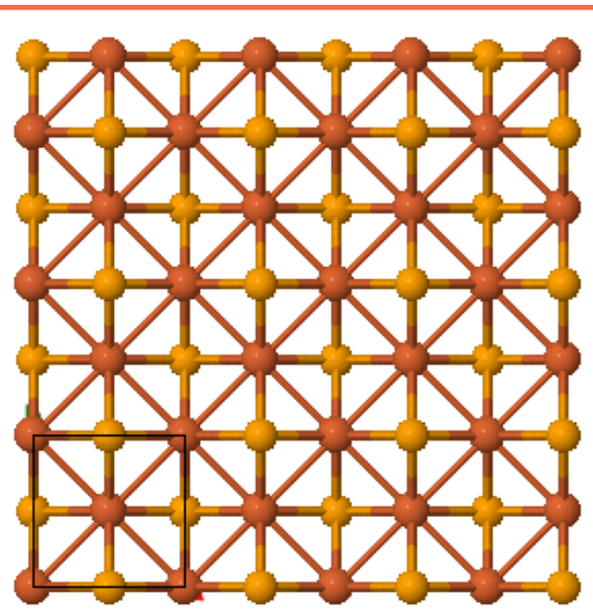
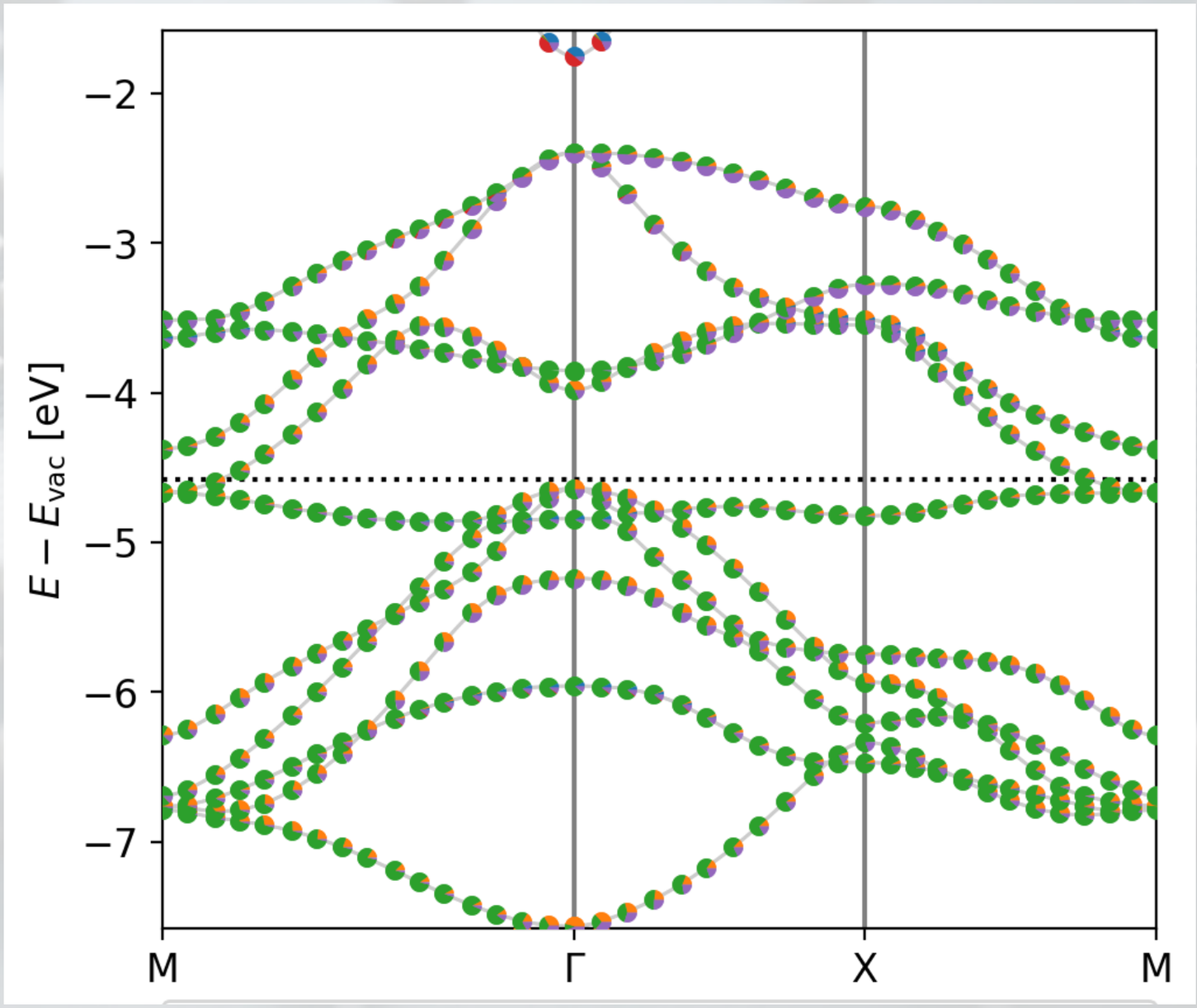


FeSe

Electronic properties

Magnetic state	AFM
Band gap (PBE)	0.00 eV
Band gap (HSE)	0.03 eV



FeSe

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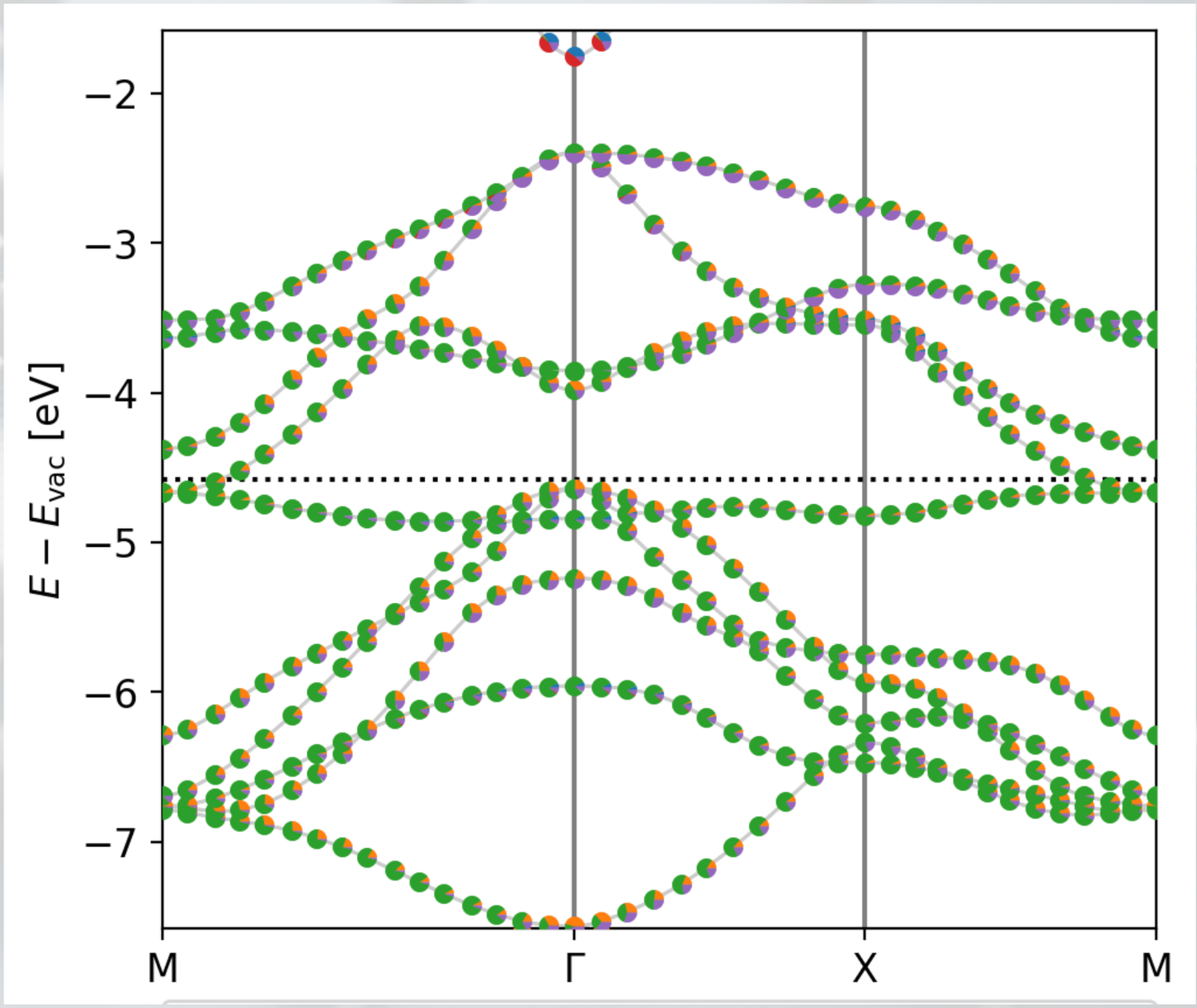

FeSe

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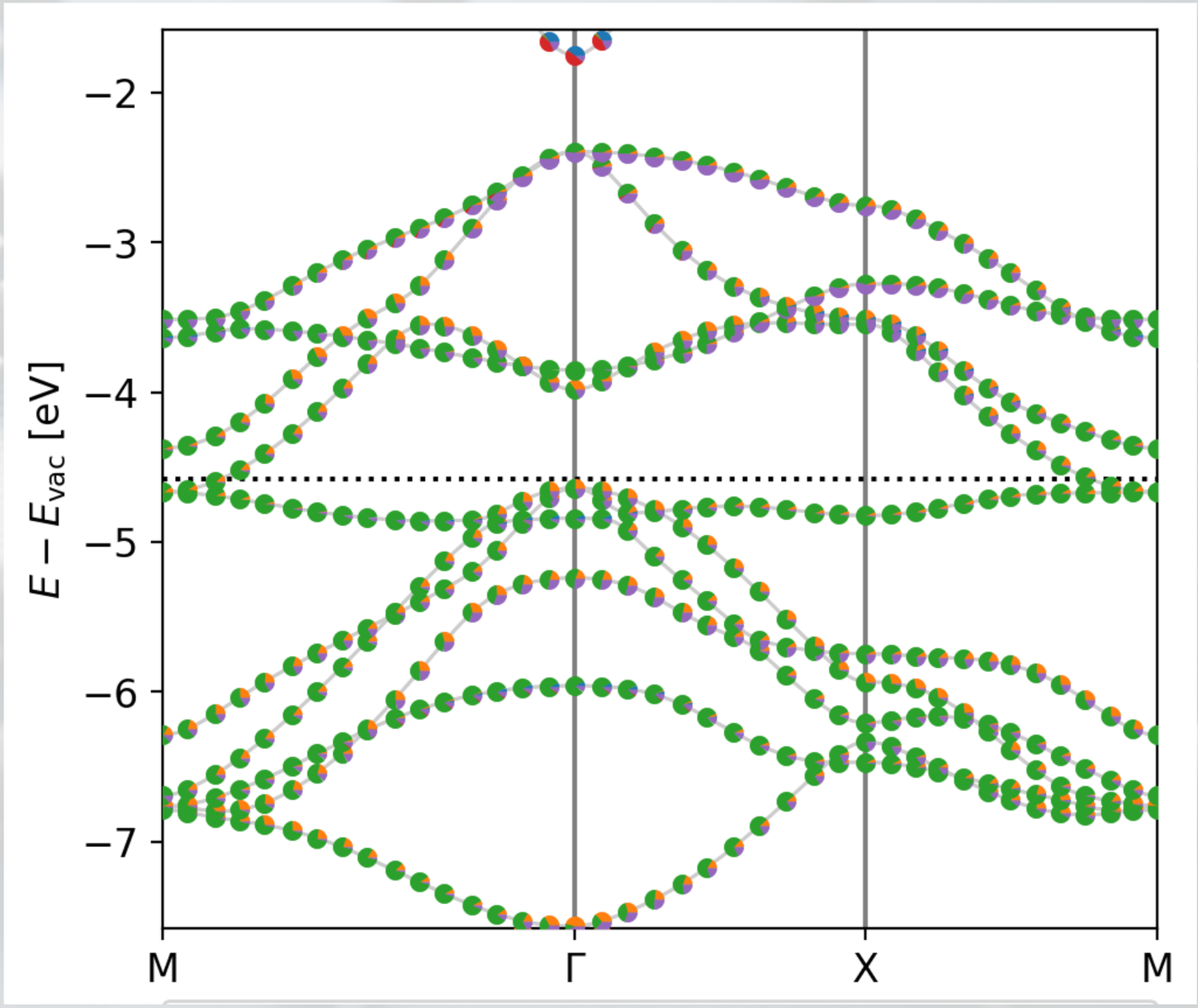

FeSe

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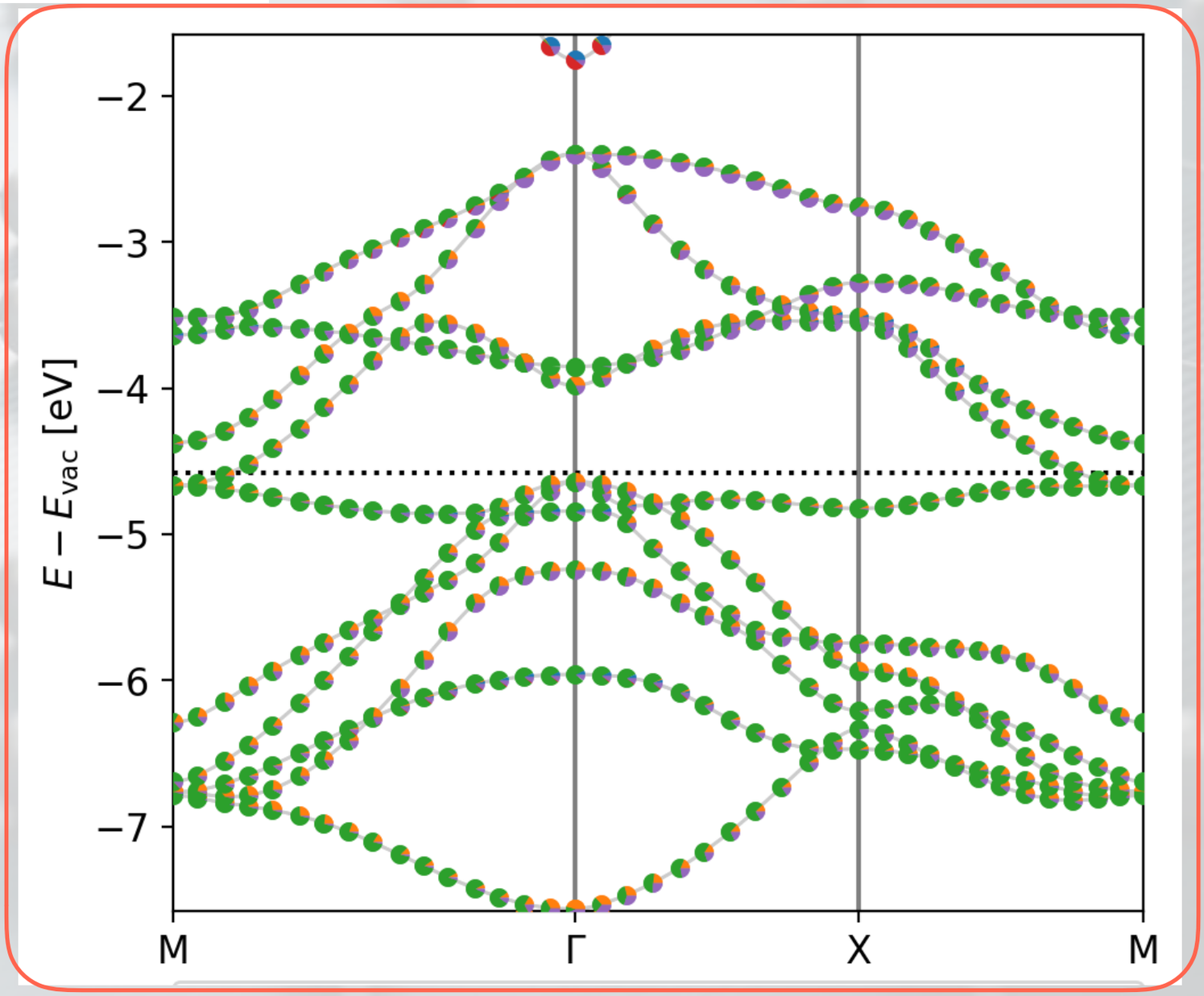


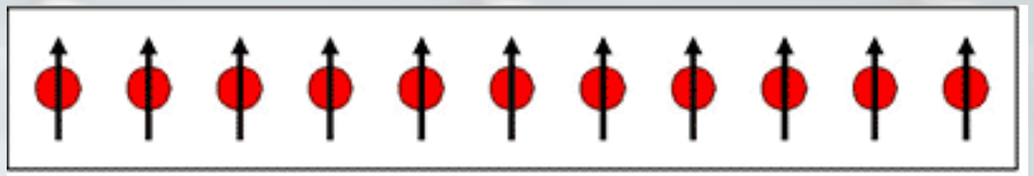
FeSe

Magnetic ground state - AFM x FM

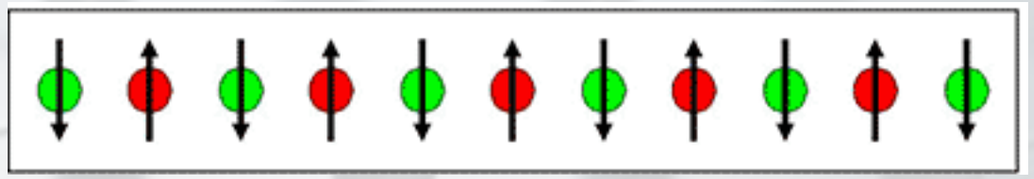
FeSe

Magnetic ground state - AFM x FM

Ferromagnetic - FM



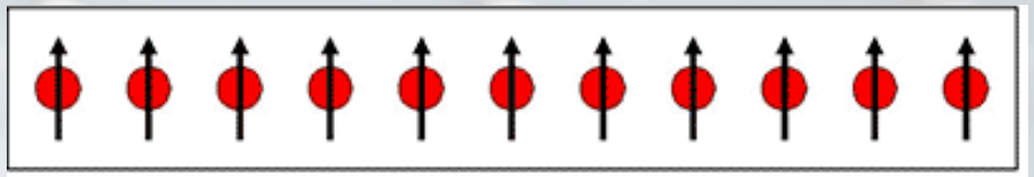
Antiferromagnetic - AFM



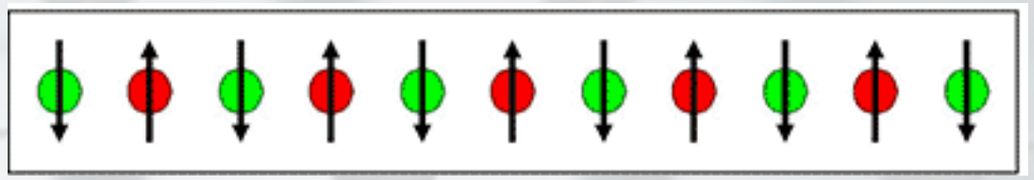
FeSe

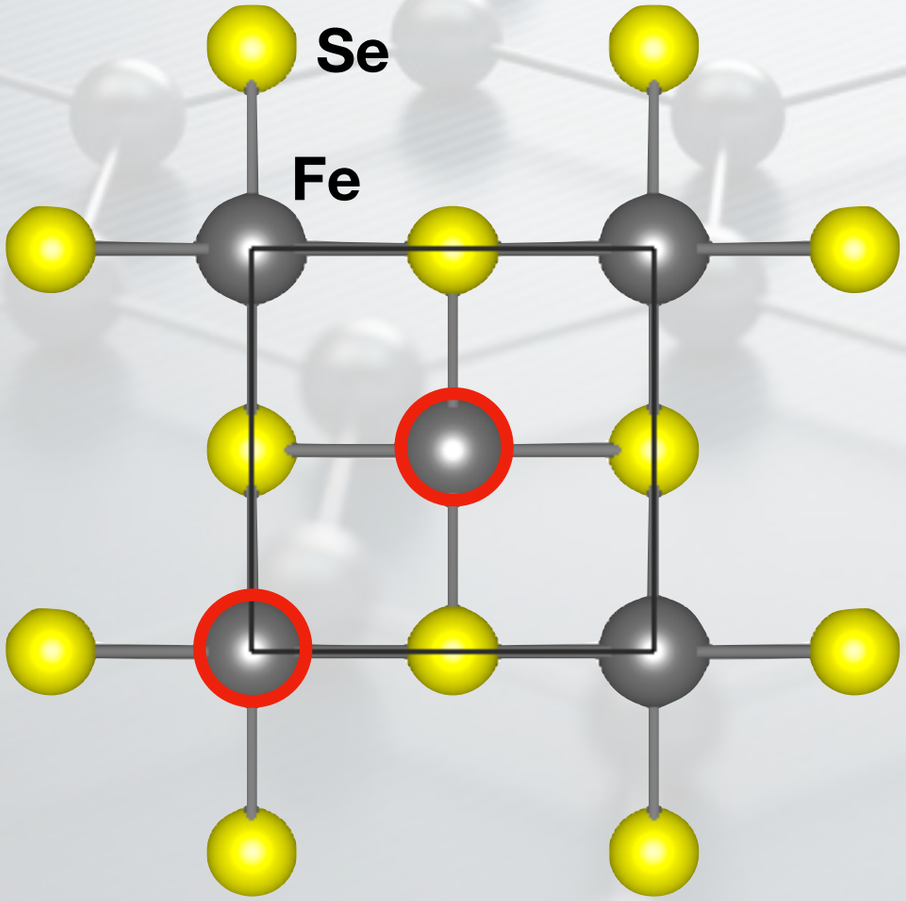
Magnetic ground state - AFM x FM

Ferromagnetic - FM



Antiferromagnetic - AFM





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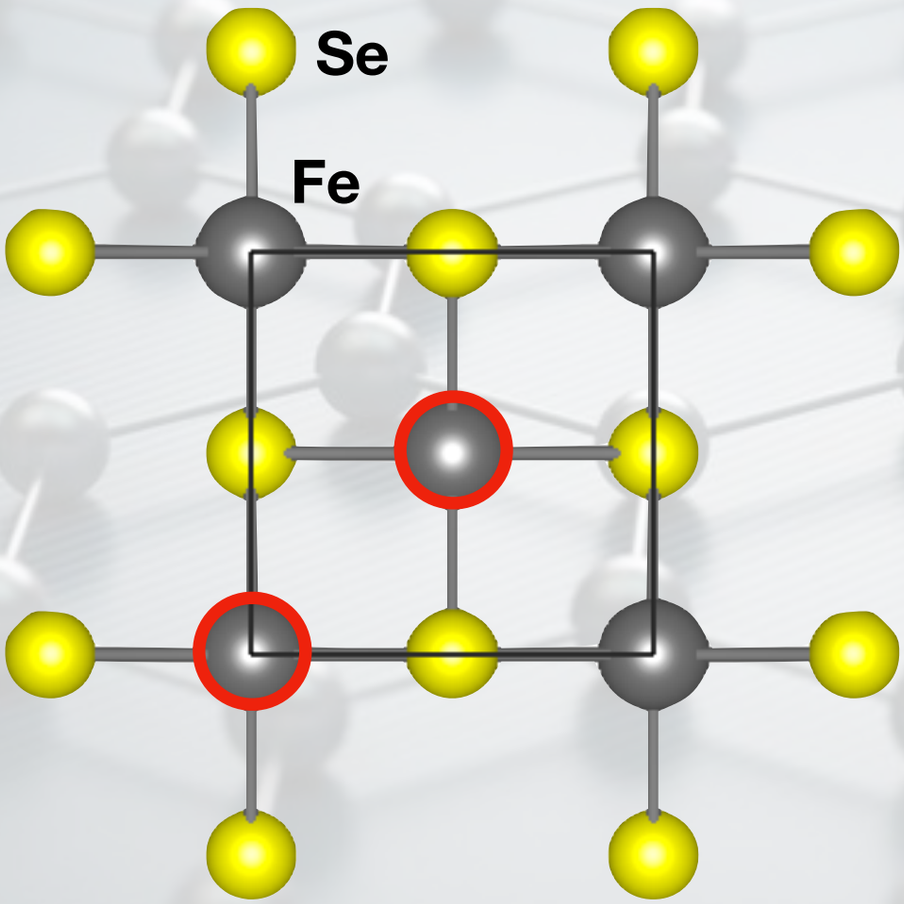

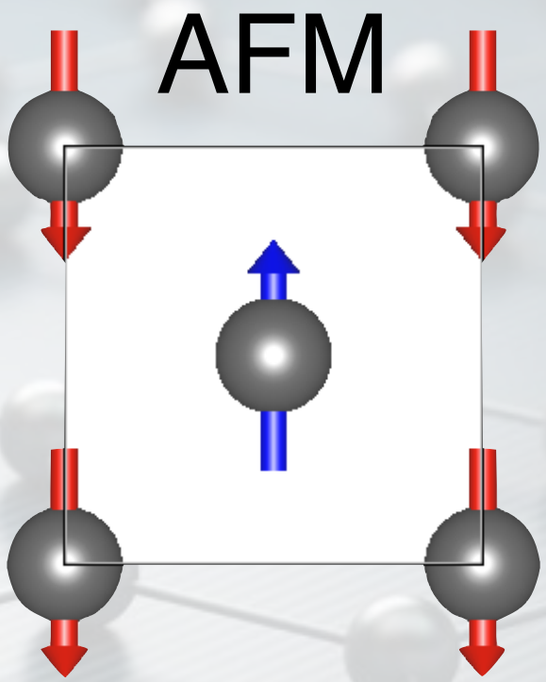

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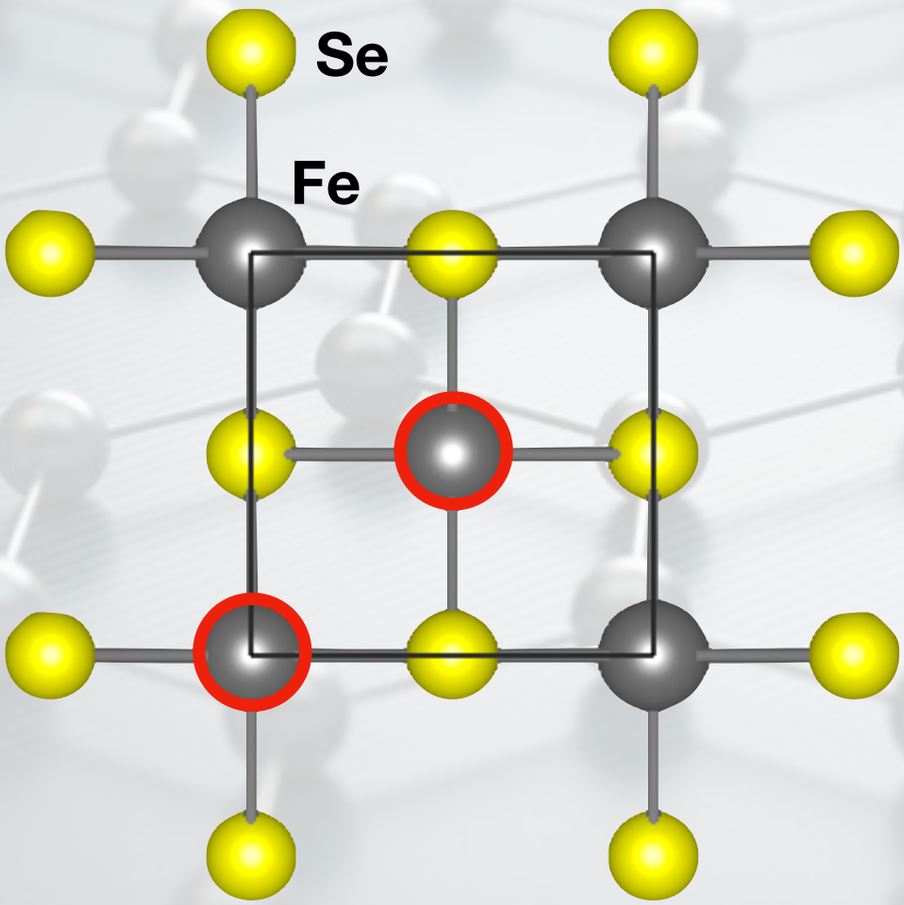
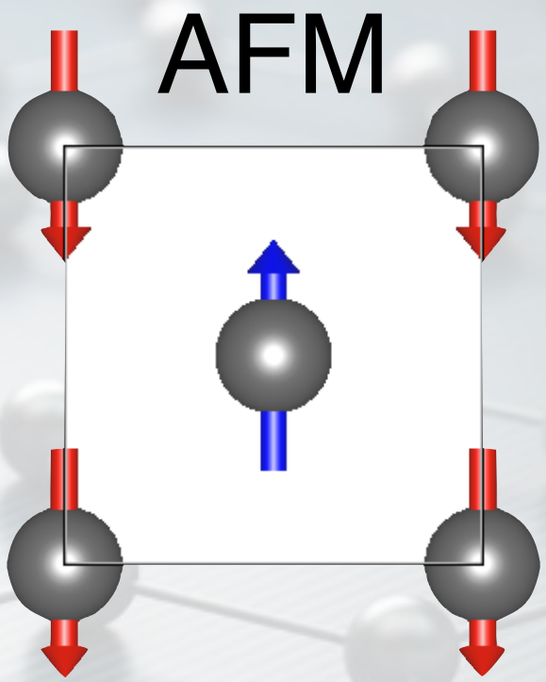
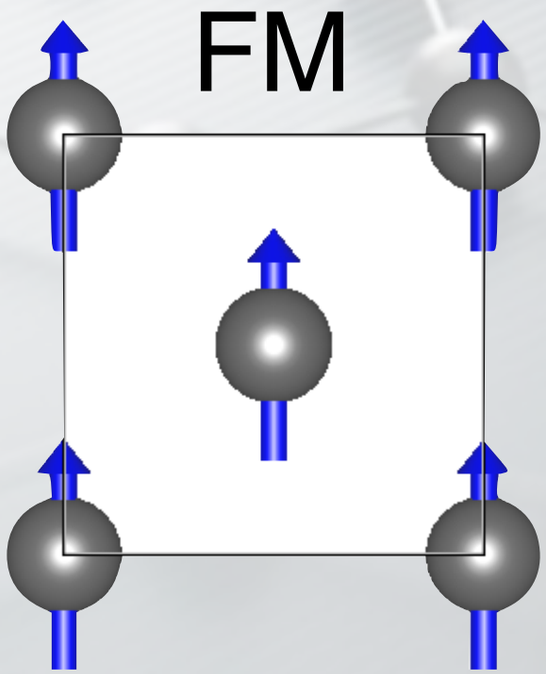


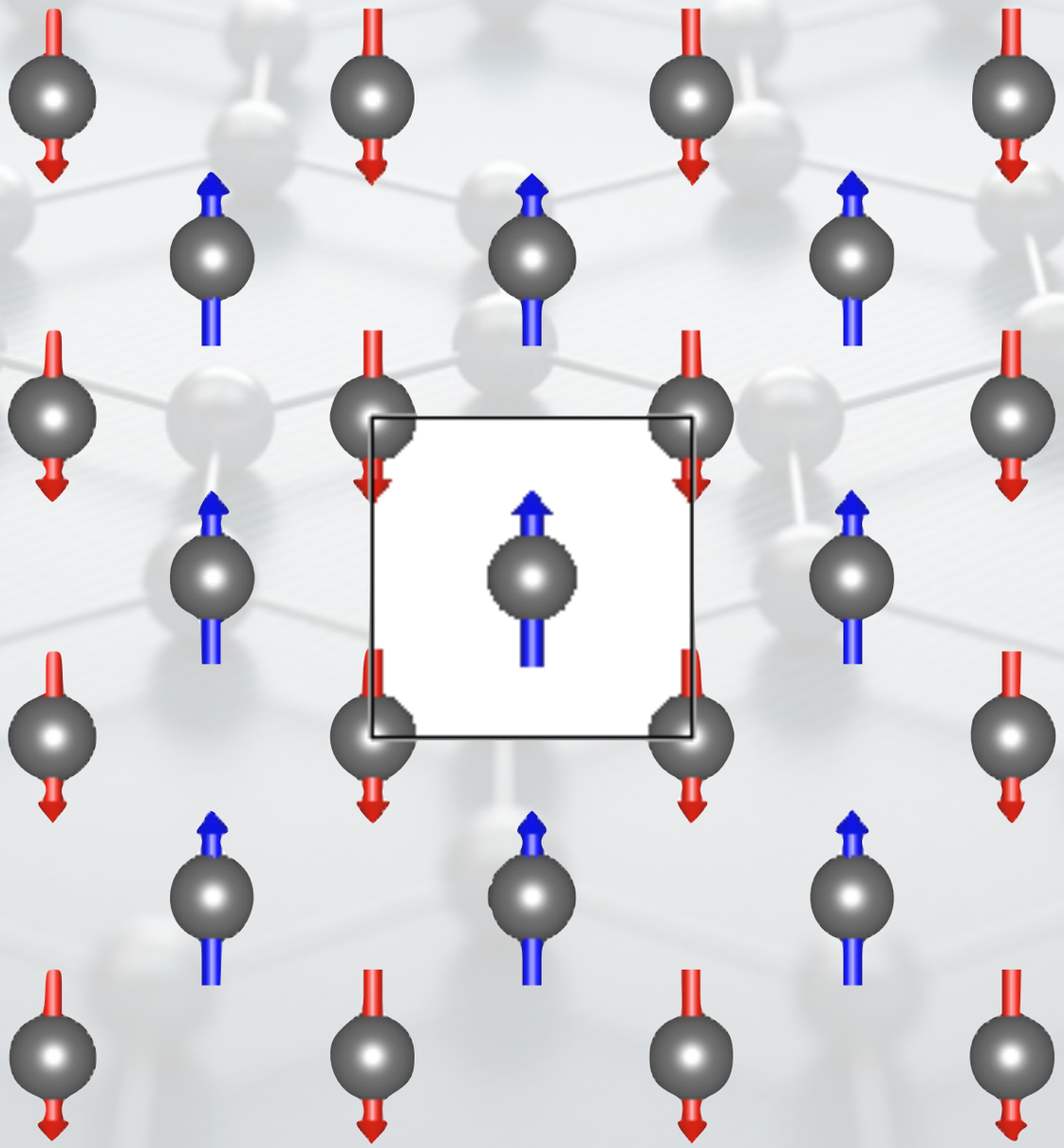




FeSe

Magnetic ground state - AFM x FM

AFM



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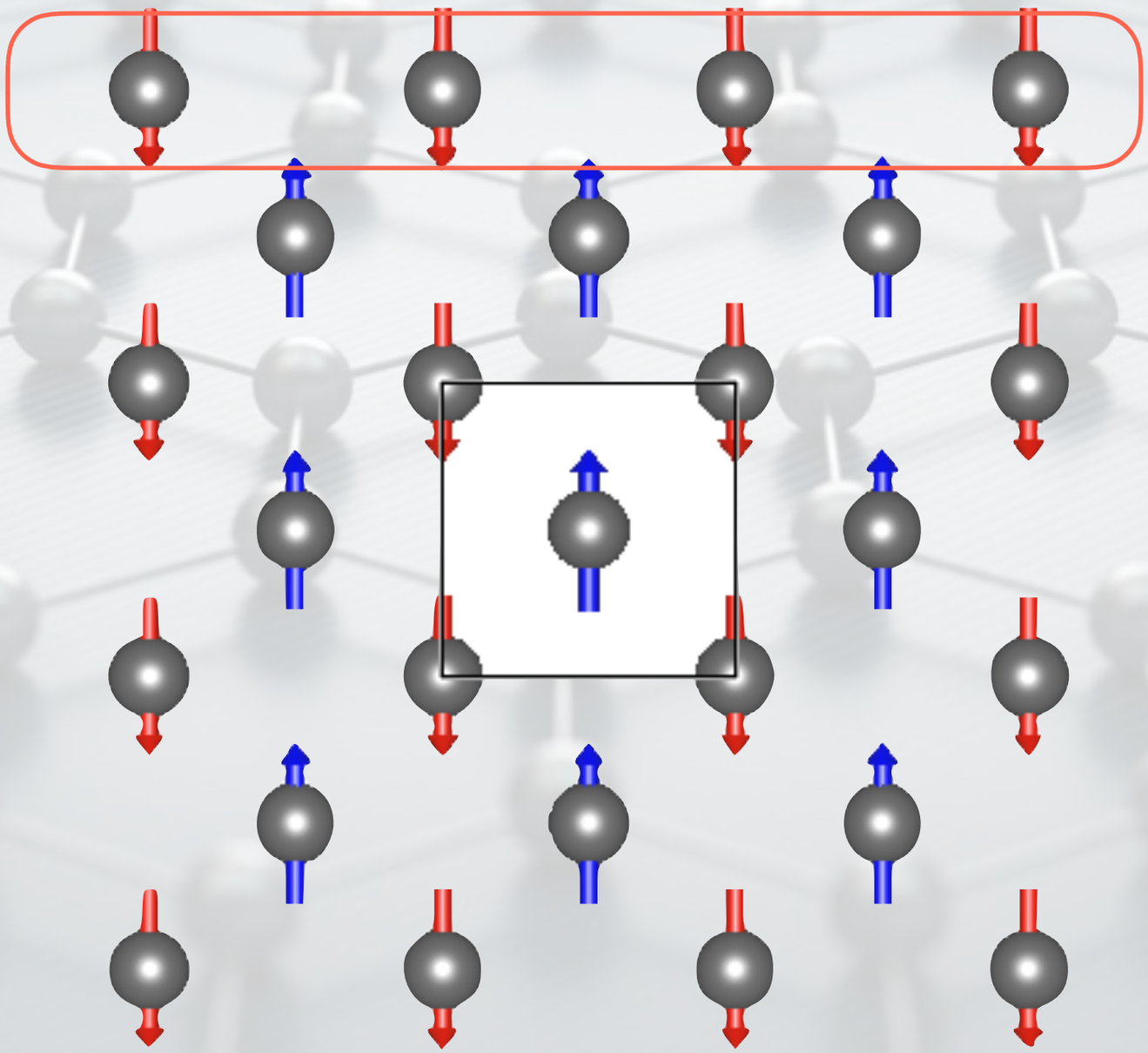

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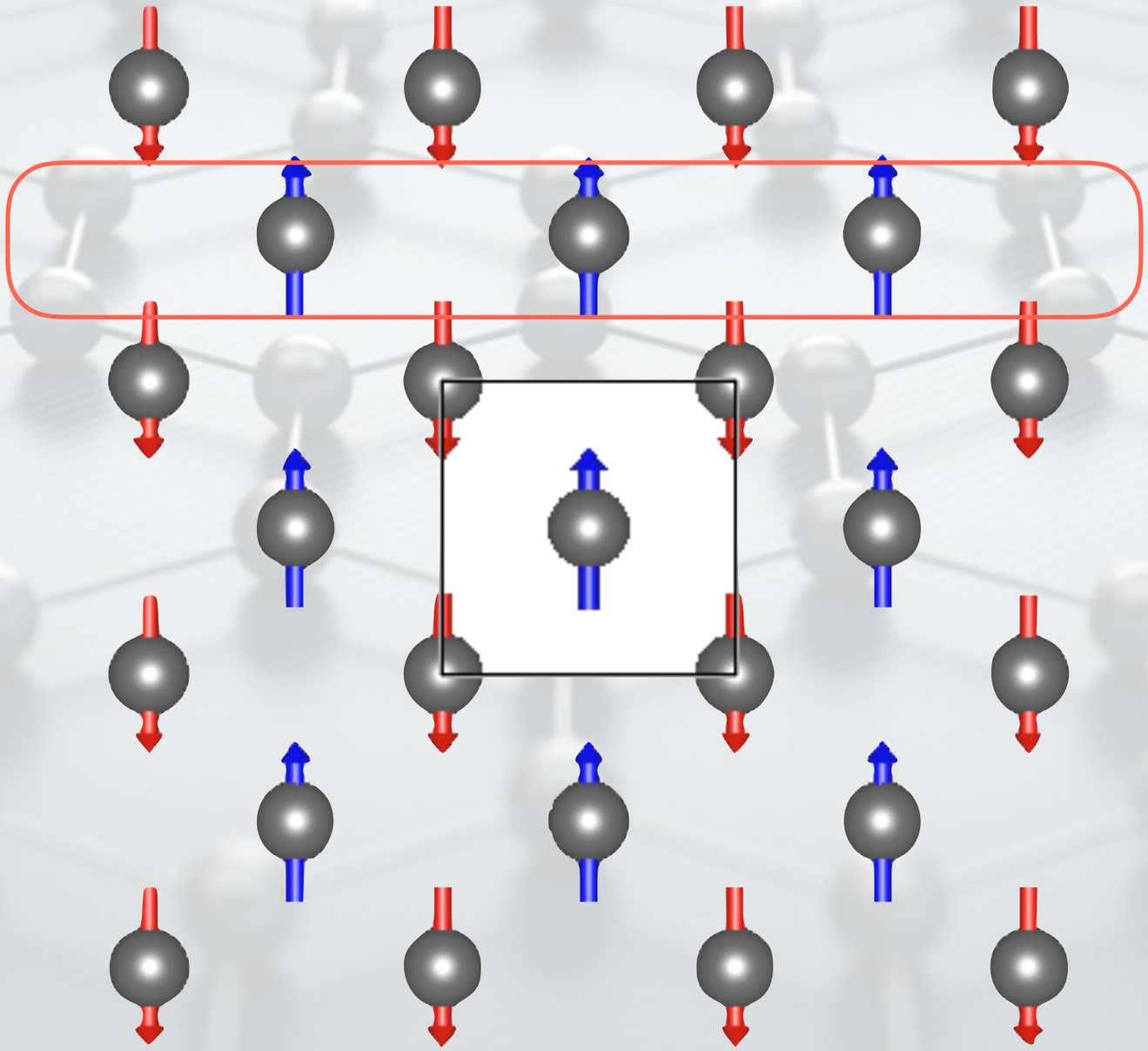

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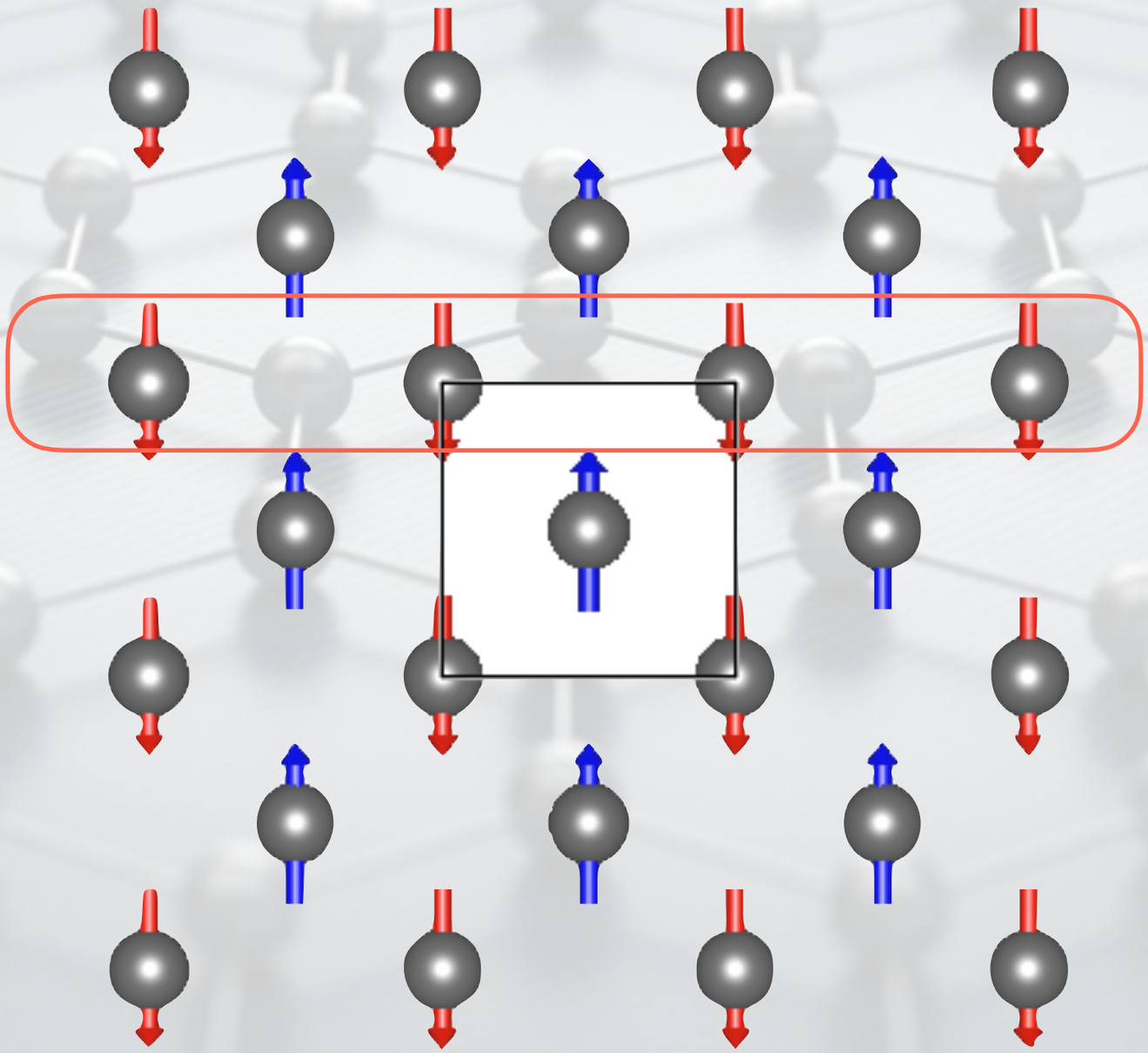

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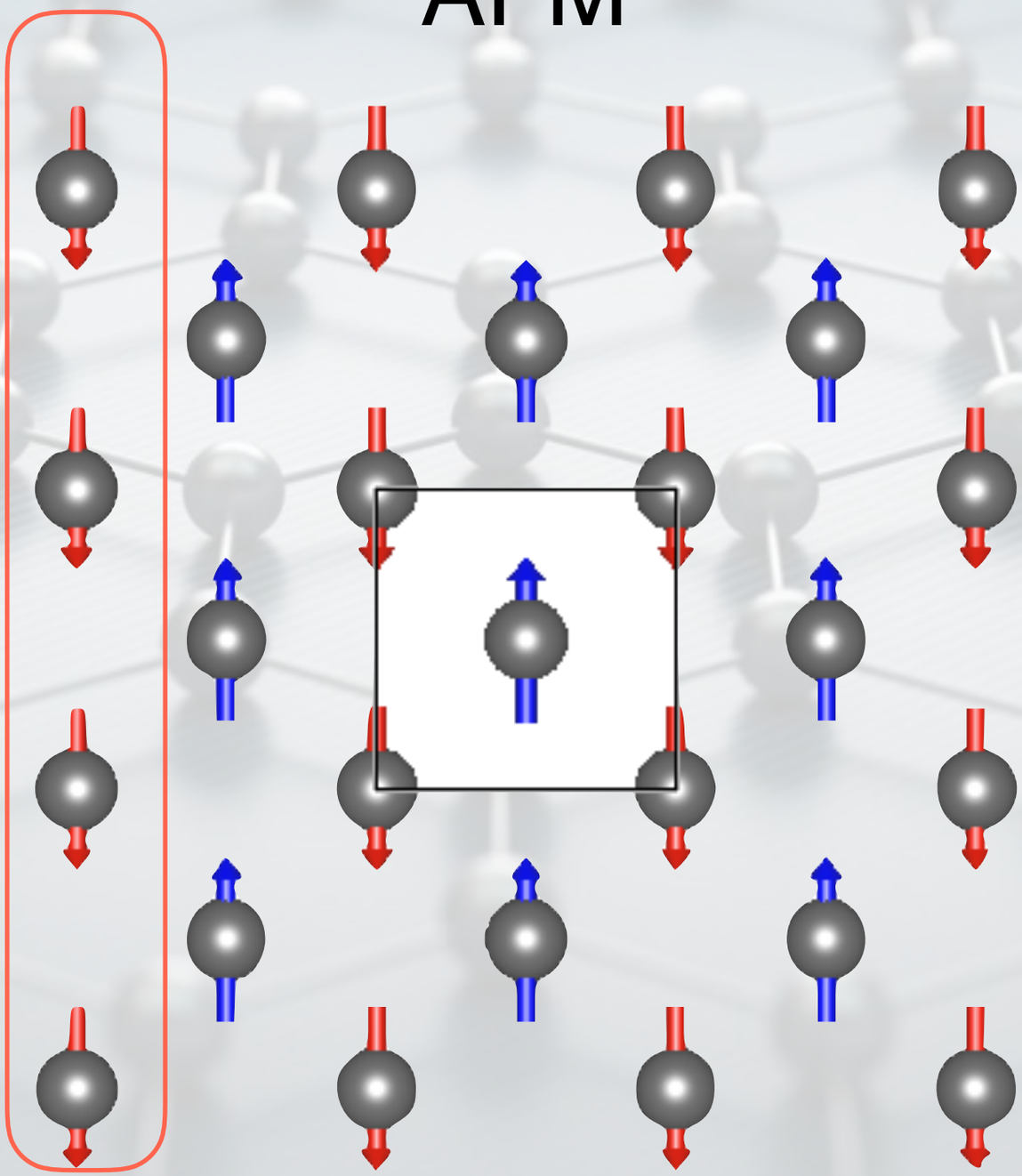

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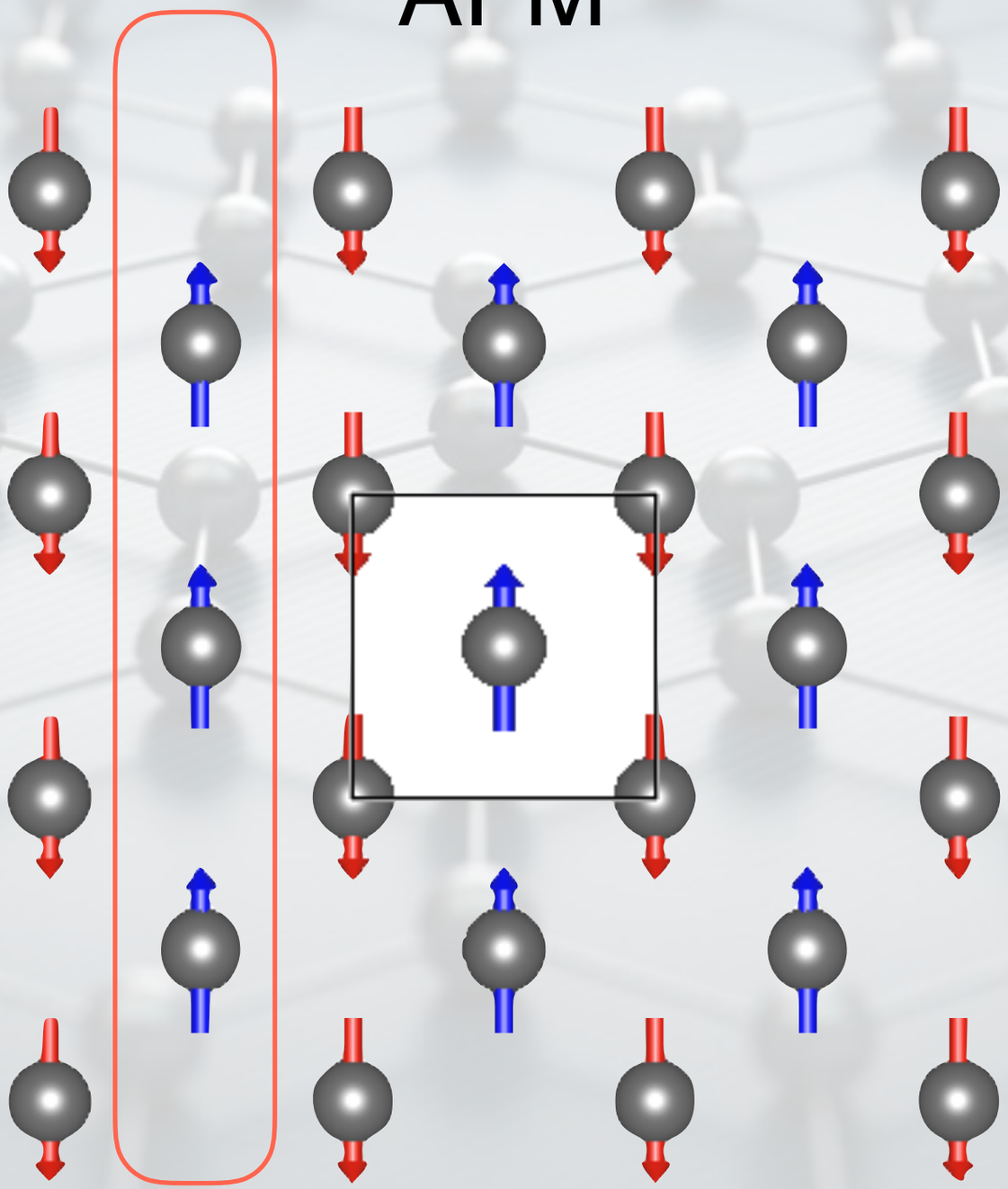

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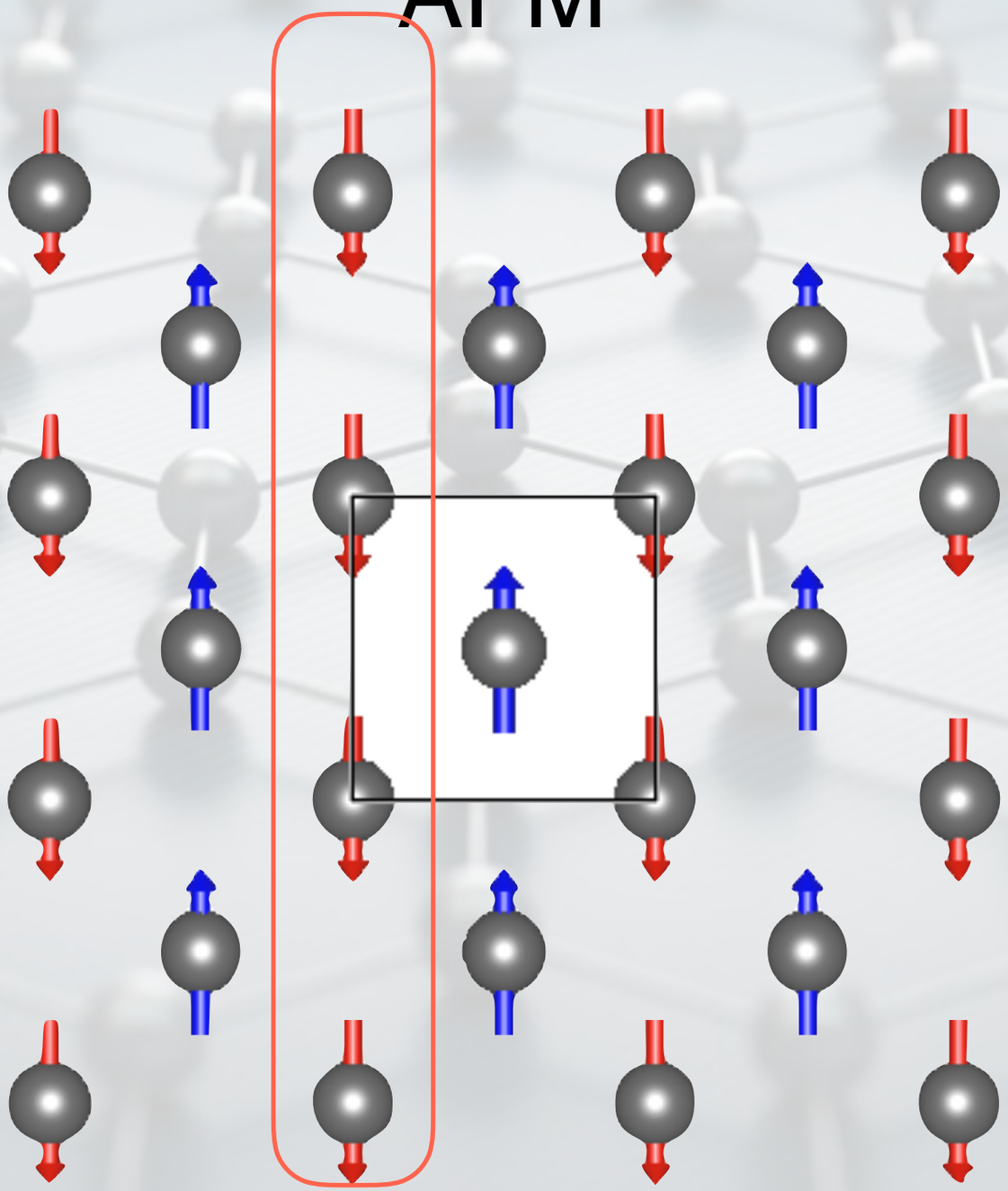

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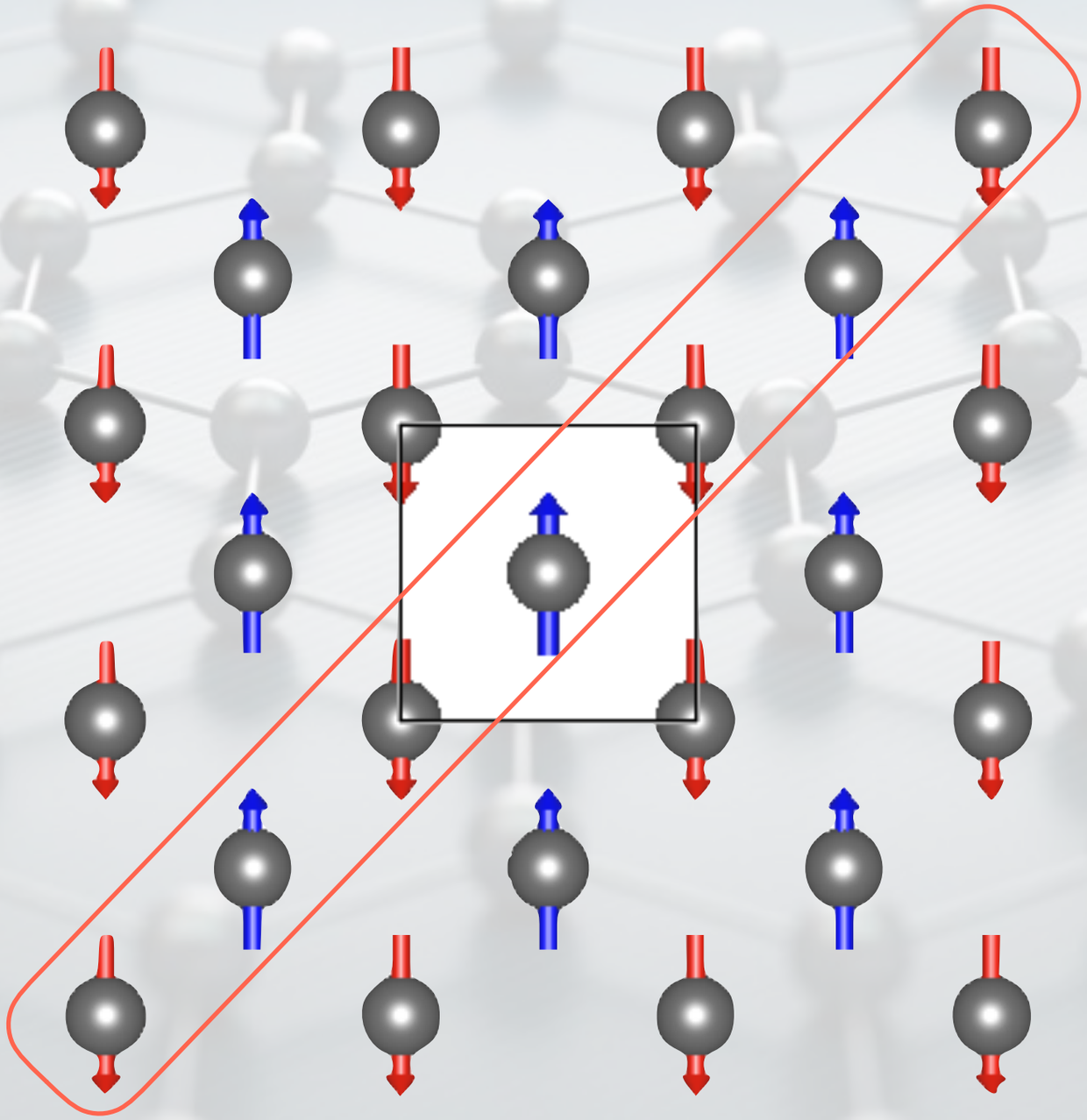

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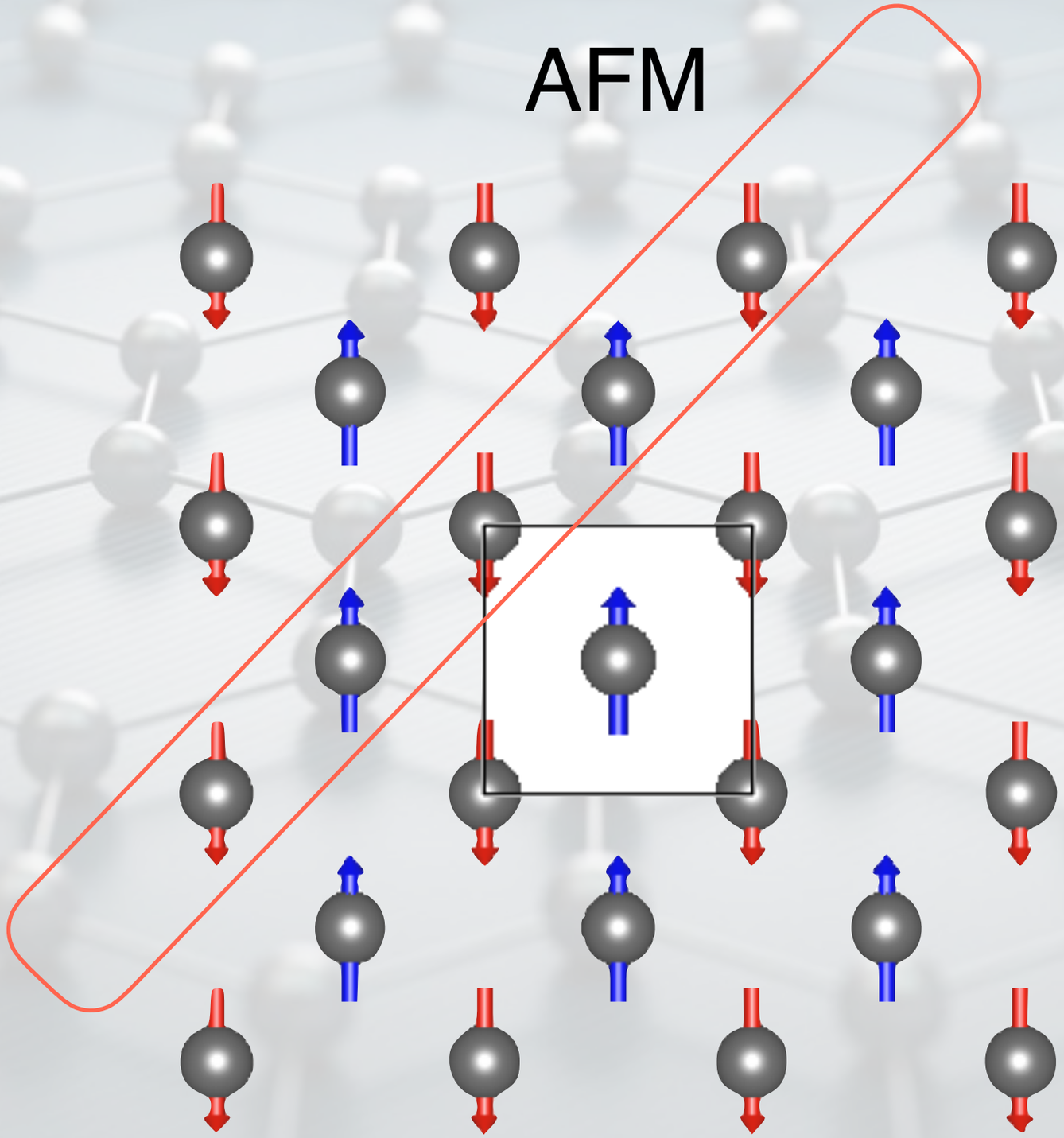

FeSe

```
&control
    calculation = 'relax'
   prefix      = 'Fe2Se2-FeSe'
    tprnfor = .true.
    pseudo_dir = '/home/mcosta/codes/pseudo/qe/pbe-no-soc/',
    outdir='./'
    verbosity = 'high'
    wf_collect=.true.
    forc_conv_thr= 0.000735294117647
/
&system
    ibrav=  0
    nat=  4
    ntyp=  3
    ecutwfc =  60.000
    ecutrho =  600.000
    occupations='smearing', smearing='methfessel-paxton', degauss=0.00073529411765
    nspin=2
    starting_magnetization(2)=  0.500
    starting_magnetization(3)= -0.500
/
&electrons
conv_thr= 1.D-8
mixing_beta = 0.1
/
&ions
/
CELL_PARAMETERS angstrom
 3.382000      0.00000000000         0.00000000000
 0.00000000    3.382000000000000           0.00000000000
 0.00000000    0.00000000           17.910
ATOMIC_SPECIES
Se  0.0 Se.pbe-n-kjpaw_psl.1.0.0.UPF
Fe1  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
Fe2  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
ATOMIC_POSITIONS angstrom
Fe1      -0.00000000       0.00000000       8.95499994
Fe2       1.85826050       1.85826049       8.95499993
Se       -0.00000000       1.85826049       7.49452840
Se        1.85826050      -0.00000000      10.41547176
K_POINTS (automatic)
 12 12 1 0 0 0
```

Why 3? We have only Fe and Se

FeSe

```
&control
    calculation = 'relax'
   prefix      = 'Fe2Se2-FeSe'
    tprnfor = .true.
    pseudo_dir = '/home/mcosta/codes/pseudo/qe/pbe-no-soc/',
    outdir='./'
    verbosity = 'high'
    wf_collect=.true.
    forc_conv_thr= 0.000735294117647
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&system
    ibrav=  0
    nat=  4
    ntyp=  3
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 0.00000000    3.382000000000000           0.00000000000
 0.00000000    0.00000000            17.910
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Fe1  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
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ATOMIC_POSITIONS angstrom
Fe1      -0.00000000       0.00000000       8.95499994
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Se       -0.00000000       1.85826049       7.49452840
Se        1.85826050      -0.00000000      10.41547176
K_POINTS (automatic)
 12 12 1 0 0 0
```

switch on spin polarization

FeSe

```
&control
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   prefix      = 'Fe2Se2-FeSe'
    tprnfor = .true.
    pseudo_dir = '/home/mcosta/codes/pseudo/qe/pbe-no-soc/',
    outdir='./'
    verbosity = 'high'
    wf_collect=.true.
    forc_conv_thr= 0.000735294117647
/
&system
    ibrav=
    nat=  4
    ntyp=  3
    ecutwfc
    ecutrho
    occupat
    nspin=2
    starting
    starting
/
&electrons
conv_thr=
mixing_be
/
&ions
/
CELL_PARAMETERS angstrom
 3.382000      0.00000000000        0.00000000000
 0.00000000    3.382000000000000          0.00000000000
 0.00000000    0.00000000          17.910
ATOMIC_SPECIES
Se  0.0 Se.pbe-n-kjpaw_psl.1.0.0.UPF
Fe1  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
Fe2  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
ATOMIC_POSITIONS angstrom
Fe1      -0.00000000      0.00000000      8.95499994
Fe2       1.85826050      1.85826049      8.95499993
Se       -0.00000000      1.85826049      7.49452840
Se        1.85826050     -0.00000000     10.41547176
K_POINTS (automatic)
 12 12 1 0 0 0
```
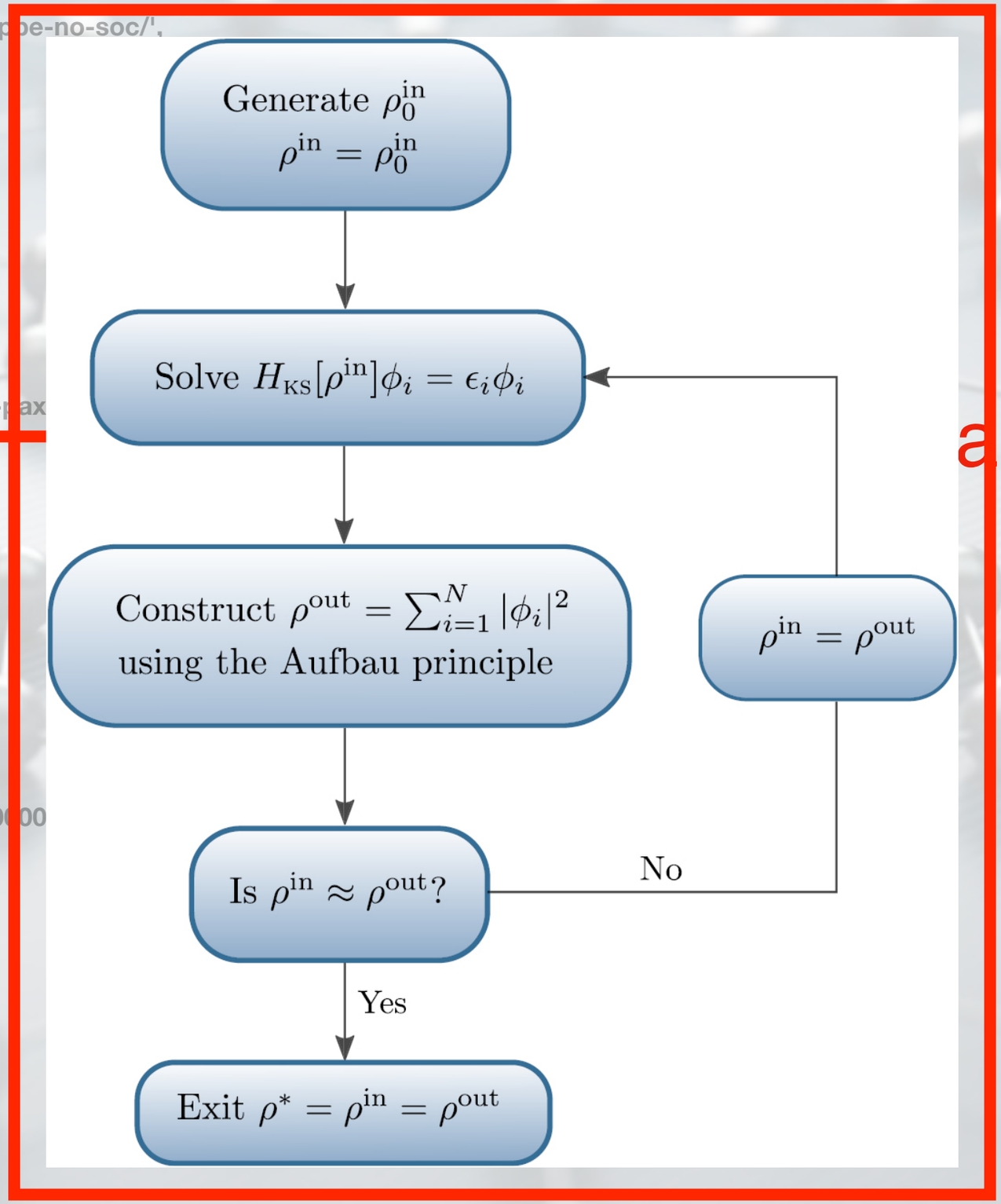

nspin	INTEGER
Default:	1

```
nspin = 1 :  non-polarized calculation (default)

nspin = 2 :  spin-polarized calculation, LSDA
             (magnetization along z axis)

nspin = 4 :  spin-polarized calculation, noncollinear
             (magnetization in generic direction)
             DO NOT specify nspin in this case;
             specify noncolin=.TRUE. instead
```

FeSe

```
&control
    calculation = 'relax'
   prefix      = 'Fe2Se2-FeSe'
    tprnfor = .true.
    pseudo_dir = '/home/mcosta/codes/pseudo/qe/pbe-no-soc/',
    outdir='./'
    verbosity = 'high'
    wf_collect=.true.
    forc_conv_thr= 0.000735294117647
/
&system
    ibrav=  0
    nat=  4
    ntyp=  3
    ecutwfc =  60.000
    ecutrho =  600.000
    occupations='smearing', smearing='methfessel-pax
    nspin=2
    starting_magnetization(2)=  0.500
    starting_magnetization(3)= -0.500
/
&electrons
conv_thr= 1.D-8
mixing_beta = 0.1
/
&ions
/
CELL_PARAMETERS angstrom
 3.382000      0.00000000000         0.00000000000
 0.00000000    3.382000000000000           0.000000000
 0.00000000    0.00000000          17.910
ATOMIC_SPECIES
Se  0.0 Se.pbe-n-kjpaw_psl.1.0.0.UPF
Fe1  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
Fe2  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
ATOMIC_POSITIONS angstrom
Fe1      -0.00000000      0.00000000      8.95499994
Fe2       1.85826050      1.85826049      8.95499993
Se       -0.00000000      1.85826049      7.49452840
Se        1.85826050     -0.00000000     10.41547176
K_POINTS (automatic)
 12 12 1 0 0 0
```

SCF cycle

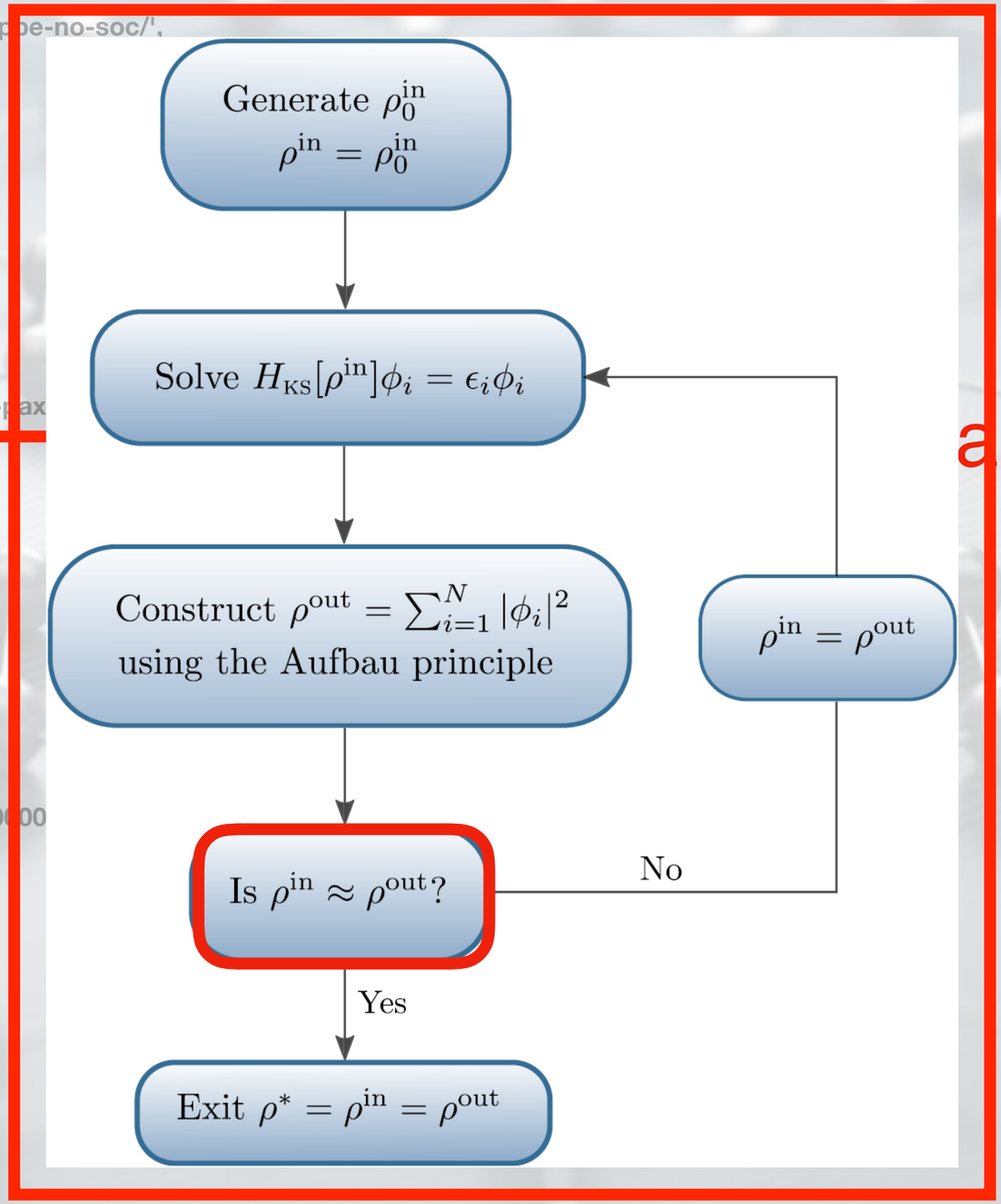


arization

FeSe

```
&control
    calculation = 'relax'
   prefix      = 'Fe2Se2-FeSe'
    tprnfor = .true.
    pseudo_dir = '/home/mcosta/codes/pseudo/qe/pbe-no-soc/',
    outdir='./'
    verbosity = 'high'
    wf_collect=.true.
    forc_conv_thr= 0.000735294117647
/
&system
    ibrav=  0
    nat=  4
    ntyp=  3
    ecutwfc =  60.000
    ecutrho =  600.000
    occupations='smearing', smearing='methfessel-pax
    nspin=2
    starting_magnetization(2)=  0.500
    starting_magnetization(3)= -0.500
/
&electrons
conv_thr= 1.D-8
mixing_beta = 0.1
/
&ions
/
CELL_PARAMETERS angstrom
 3.382000      0.00000000000         0.00000000000
 0.00000000    3.382000000000000             0.000000000
 0.00000000    0.00000000          17.910
ATOMIC_SPECIES
Se  0.0 Se.pbe-n-kjpaw_psl.1.0.0.UPF
Fe1  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
Fe2  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
ATOMIC_POSITIONS angstrom
Fe1      -0.00000000      0.00000000      8.95499994
Fe2       1.85826050      1.85826049      8.95499993
Se       -0.00000000      1.85826049      7.49452840
Se        1.85826050     -0.00000000     10.41547176
K_POINTS (automatic)
 12 12 1 0 0 0
```

SCF cycle



arization

FeSe

```
&control
    calculation = 'relax'
   prefix      = 'Fe2Se2-FeSe'
    tprnfor = .true.
    pseudo_dir = '/home/mcosta/codes/pseudo/qe/pbe-no-soc/',
    outdir='./'
    verbosity = 'high'
    wf_collect=.true.
    forc_conv_thr= 0.000735294117647
/
&system
    ibrav=  0
    nat=  4
    ntyp=  3
    ecutwfc =  60.000
    ecutrho =  600.000
    occupations='smearing', smearing='methfessel-paxton', degauss=0.00073529411765
    nspin=2
    starting_magnetization(2)=  0.500
    starting_magnetization(3)= -0.500
/
&electrons
conv_thr= 1.D-8
mixing_beta = 0.1
/
&ions
/
CELL_PARAMETERS angstrom
 3.382000      0.00000000000         0.00000000000
 0.00000000    3.382000000000000           0.00000000000
 0.00000000    0.00000000          17.910
ATOMIC_SPECIES
Se  0.0 Se.pbe-n-kjpaw_psl.1.0.0.UPF
Fe1  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
Fe2  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
ATOMIC_POSITIONS angstrom
Fe1      -0.00000000       0.00000000       8.95499994
Fe2       1.85826050       1.85826049       8.95499993
Se       -0.00000000       1.85826049       7.49452840
Se        1.85826050      -0.00000000      10.41547176
K_POINTS (automatic)
 12 12 1 0 0 0
```

species 2 magnetization

FeSe

```
&control
    calculation = 'relax'
   prefix      = 'Fe2Se2-FeSe'
    tprnfor = .true.
    pseudo_dir = '/home/mcosta/codes/pseudo/qe/pbe-no-soc/',
    outdir='./'
    verbosity = 'high'
    wf_collect=.true.
    forc_conv_thr= 0.000735294117647
/
&system
    ibrav=  0
    nat=  4
    ntyp=  3
    ecutwfc =  60.000
    ecutrho =  600.000
    occupations='smearing', smearing='methfessel-paxton', degauss=0.00073529411765
    nspin=2
    starting_magnetization(2)=  0.500
    starting_magnetization(3)= -0.500
/
&electrons
conv_thr= 1.D-8
mixing_beta = 0.1
/
&ions
/
CELL_PARAMETERS angstrom
 3.382000      0.00000000000         0.00000000000
 0.00000000    3.382000000000000           0.00000000000
 0.00000000    0.00000000          17.910
ATOMIC_SPECIES
Se  0.0 Se.pbe-n-kjpaw_psl.1.0.0.UPF
Fe1  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
Fe2  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
ATOMIC_POSITIONS angstrom
Fe1      -0.00000000       0.00000000       8.95499994
Fe2       1.85826050       1.85826049       8.95499993
Se       -0.00000000       1.85826049       7.49452840
Se        1.85826050      -0.00000000      10.41547176
K_POINTS (automatic)
 12 12 1 0 0 0
```

species 3 magnetization

FeSe

```
&control
    calculation = 'relax'
   prefix      = 'Fe2Se2-FeSe'
    tprnfor = .true.
    pseudo_dir = '/home/mcosta/codes/pseudo/qe/pbe-no-soc/',
    outdir='./'
    verbosity = 'high'
    wf_collect=.true.
    forc_conv_thr= 0.000735294117647
/
&system
    ibrav=  0
    nat=  4
    ntyp=  3
    ecutwfc =  60.000
    ecutrho =  600.000
    occupations='smearing', smearing='methfessel-paxton', degauss=0.00073529411765
    nspin=2
    starting_magnetization(2)=  0.500
    starting_magnetization(3)= -0.500
/
&electrons
conv_thr= 1.D-8
mixing_beta = 0.1
/
&ions
/
CELL_PARAMETERS angstrom
 3.382000      0.00000000000         0.00000000000
 0.00000000    3.382000000000000           0.00000000000
 0.00000000    0.00000000          17.910
ATOMIC_SPECIES
Se  0.0 Se.pbe-n-kjpaw_psl.1.0.0.UPF
Fe1  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
Fe2  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
ATOMIC_POSITIONS angstrom
Fe1      -0.00000000      0.00000000      8.95499994
Fe2       1.85826050      1.85826049      8.95499993
Se       -0.00000000      1.85826049      7.49452840
Se        1.85826050     -0.00000000     10.41547176
K_POINTS (automatic)
 12 12 1 0 0 0
```

specie 2

FeSe

```
&control
    calculation = 'relax'
   prefix      = 'Fe2Se2-FeSe'
    tprnfor = .true.
    pseudo_dir = '/home/mcosta/codes/pseudo/qe/pbe-no-soc/',
    outdir='./'
    verbosity = 'high'
    wf_collect=.true.
    forc_conv_thr= 0.000735294117647
/
&system
    ibrav=  0
    nat=  4
    ntyp=  3
    ecutwfc =  60.000
    ecutrho =  600.000
    occupations='smearing', smearing='methfessel-paxton', degauss=0.00073529411765
    nspin=2
    starting_magnetization(2)=  0.500
    starting_magnetization(3)= -0.500
/
&electrons
conv_thr= 1.D-8
mixing_beta = 0.1
/
&ions
/
CELL_PARAMETERS angstrom
 3.382000      0.00000000000         0.00000000000
 0.00000000    3.382000000000000           0.00000000000
 0.00000000    0.00000000          17.910
ATOMIC_SPECIES
Se  0.0 Se.pbe-n-kjpaw_psl.1.0.0.UPF
Fe1  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
Fe2  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
ATOMIC_POSITIONS angstrom
Fe1      -0.00000000       0.00000000       8.95499994
Fe2       1.85826050       1.85826049       8.95499993
Se       -0.00000000       1.85826049       7.49452840
Se        1.85826050      -0.00000000      10.41547176
K_POINTS (automatic)
 12 12 1 0 0 0
```

specie 3

FeSe

```
&control
    calculation = 'relax'
   prefix      = 'Fe2Se2-FeSe'
    tprnfor = .true.
    pseudo_dir = '/home/mcosta/codes/pseudo/qe/pbe-no-soc/',
    outdir='./'
    verbosity = 'high'
    wf_collect=.true.
    forc_conv_thr= 0.000735294117647
/
&system
    ibrav=  0
    nat=  4
    ntyp=  3
    ecutwfc =  60.000
    ecutrho =  600.000
    occupations='smearing', smearing='methfessel-paxton', degauss=0.00073529411765
    nspin=2
    starting_magnetization(2)=  0.500
    starting_magnetization(3)= -0.500
/
&electrons
conv_thr= 1.D-8
mixing_beta = 0.1
/
&ions
/
CELL_PARAMETERS angstrom
 3.382000      0.00000000000         0.00000000000
 0.00000000    3.382000000000000           0.00000000000
 0.00000000    0.00000000           17.910
ATOMIC_SPECIES
Se  0.0 Se.pbe-n-kjpaw_psl.1.0.0.UPF
Fe1  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
Fe2  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
ATOMIC_POSITIONS angstrom
Fe1      -0.00000000       0.00000000       8.95499994
Fe2       1.85826050       1.85826049       8.95499993
Se       -0.00000000       1.85826049       7.49452840
Se        1.85826050      -0.00000000      10.41547176
K_POINTS (automatic)
 12 12 1 0 0 0
```

ibrav=0

FeSe

```
&control
    calculation = 'relax'
   prefix      = 'Fe2Se2-FeSe'
    tprnfor = .true.
    pseudo_dir = '/home/mcosta/codes/pseudo/qe/pbe-no-soc/',
    outdir='./'
    verbosity = 'high'
    wf_collect=.true.
    forc_conv_thr= 0.000735294117647
/
&system
    ibrav=  0
    nat=  4
    ntyp=  3
    ecutwfc =  60.000
    ecutrho =  600.000
    occupations='smearing', smearing='methfessel-paxton', degauss=0.00073529411765
    nspin=2
    starting_magnetization(2)=  0.500
    starting_magnetization(3)= -0.500
/
&electrons
conv_thr= 1.D-8
mixing_beta = 0.1
/
&ions
/
CELL_PARAMETERS angstrom
 3.382000      0.00000000000         0.00000000000
 0.00000000    3.382000000000000           0.00000000000
 0.00000000    0.00000000          17.910
ATOMIC_SPECIES
Se  0.0 Se.pbe-n-kjpaw_psl.1.0.0.UPF
Fe1  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
Fe2  0.0 Fe.pbe-n-kjpaw_psl.1.0.0.UPF
ATOMIC_POSITIONS angstrom
Fe1      -0.00000000       0.00000000       8.95499994
Fe2       1.85826050       1.85826049       8.95499993
Se       -0.00000000       1.85826049       7.49452840
Se        1.85826050      -0.00000000      10.41547176
K_POINTS (automatic)
 12 12 1 0 0 0
```

cell_parameters

FeSe

Self-consistent Calculation

iteration # 1 ecut= 60.00 Ry beta= 0.10
Davidson diagonalization with overlap
ethr = 1.00E-06, avg # of iterations = 3.2

negative rho (up, down): 2.550E-05 2.591E-05

total cpu time spent up to now is 225.9 secs

total energy = -662.24688877 Ry
Harris-Foulkes estimate = -662.24831901 Ry
estimated scf accuracy < 0.00006976 Ry

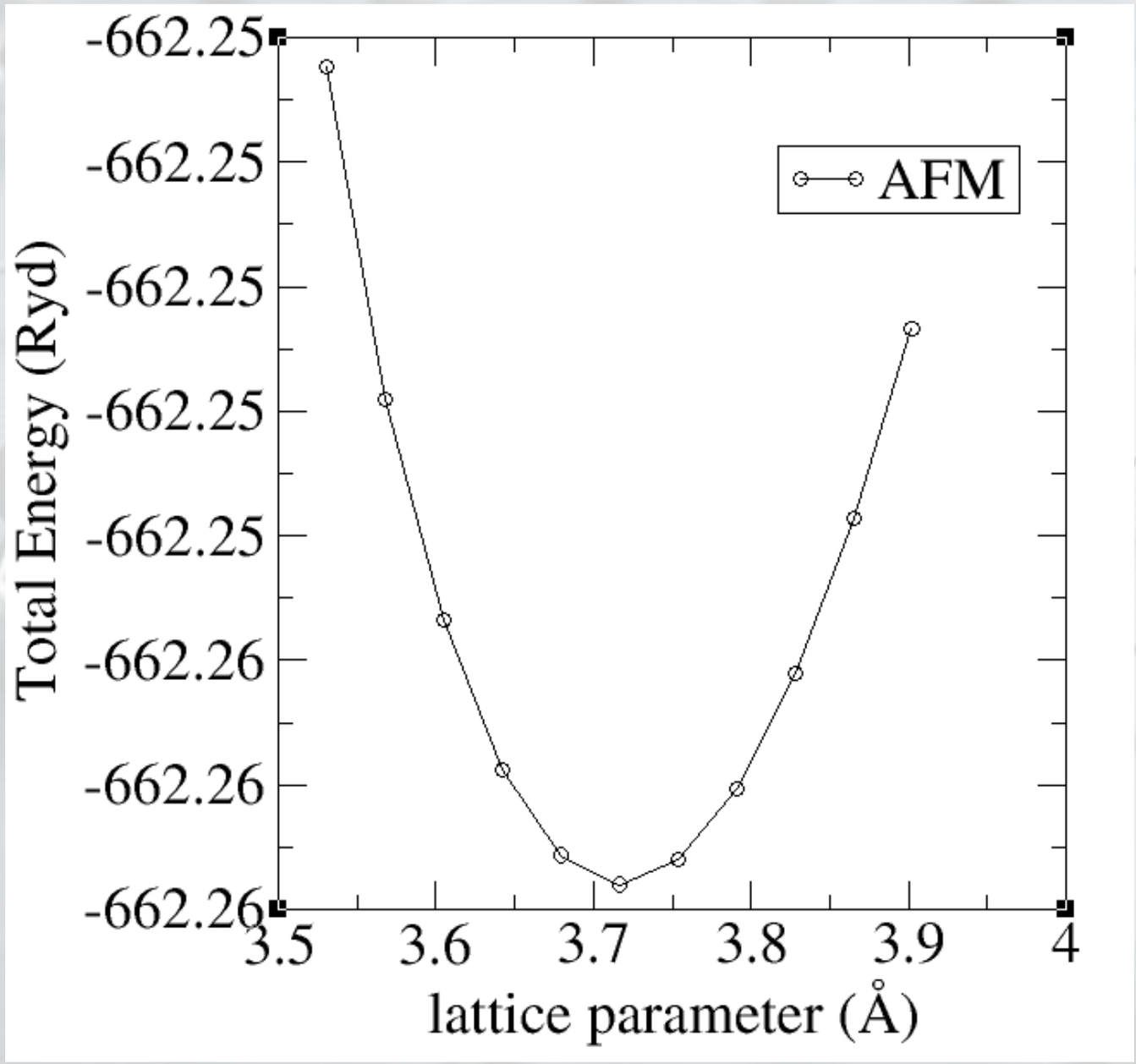
total magnetization = 0.00 Bohr mag/cell
absolute magnetization = 3.36 Bohr mag/cell

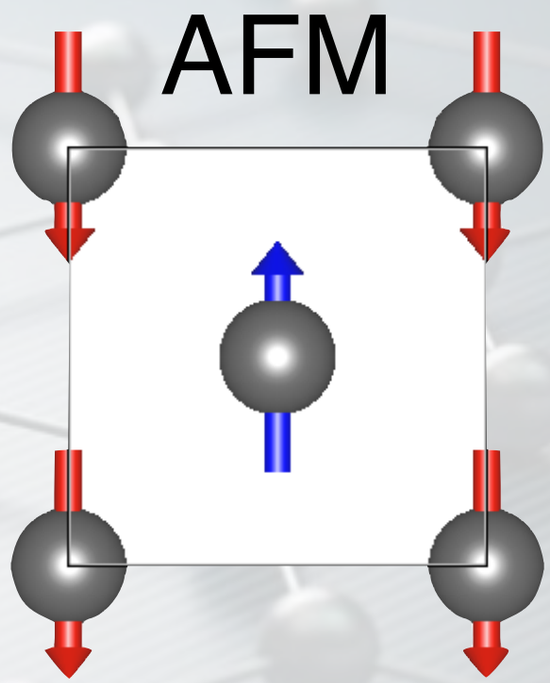
total magnetization

iteration # 2 ecut= 60.00 Ry beta= 0.10
Davidson diagonalization with overlap
ethr = 2.49E-07, avg # of iterations = 1.0

FeSe

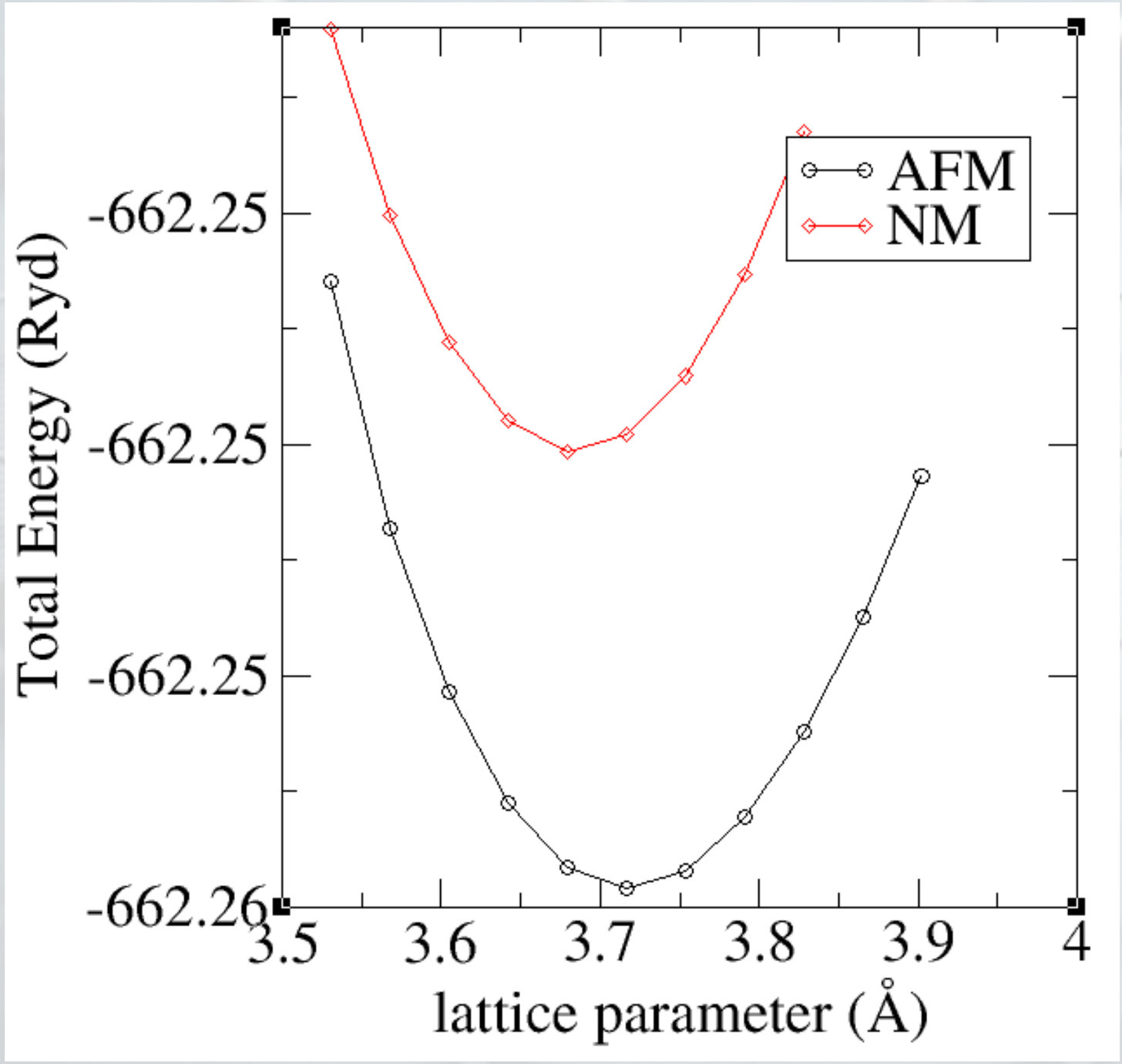
Lattice Parameter

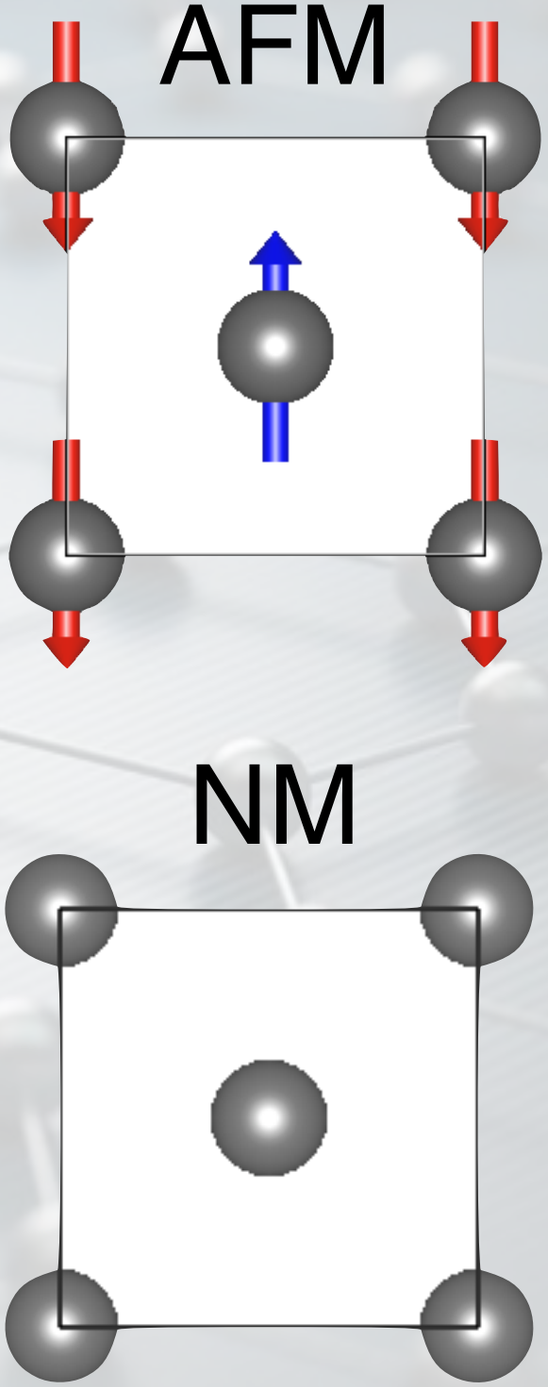




FeSe

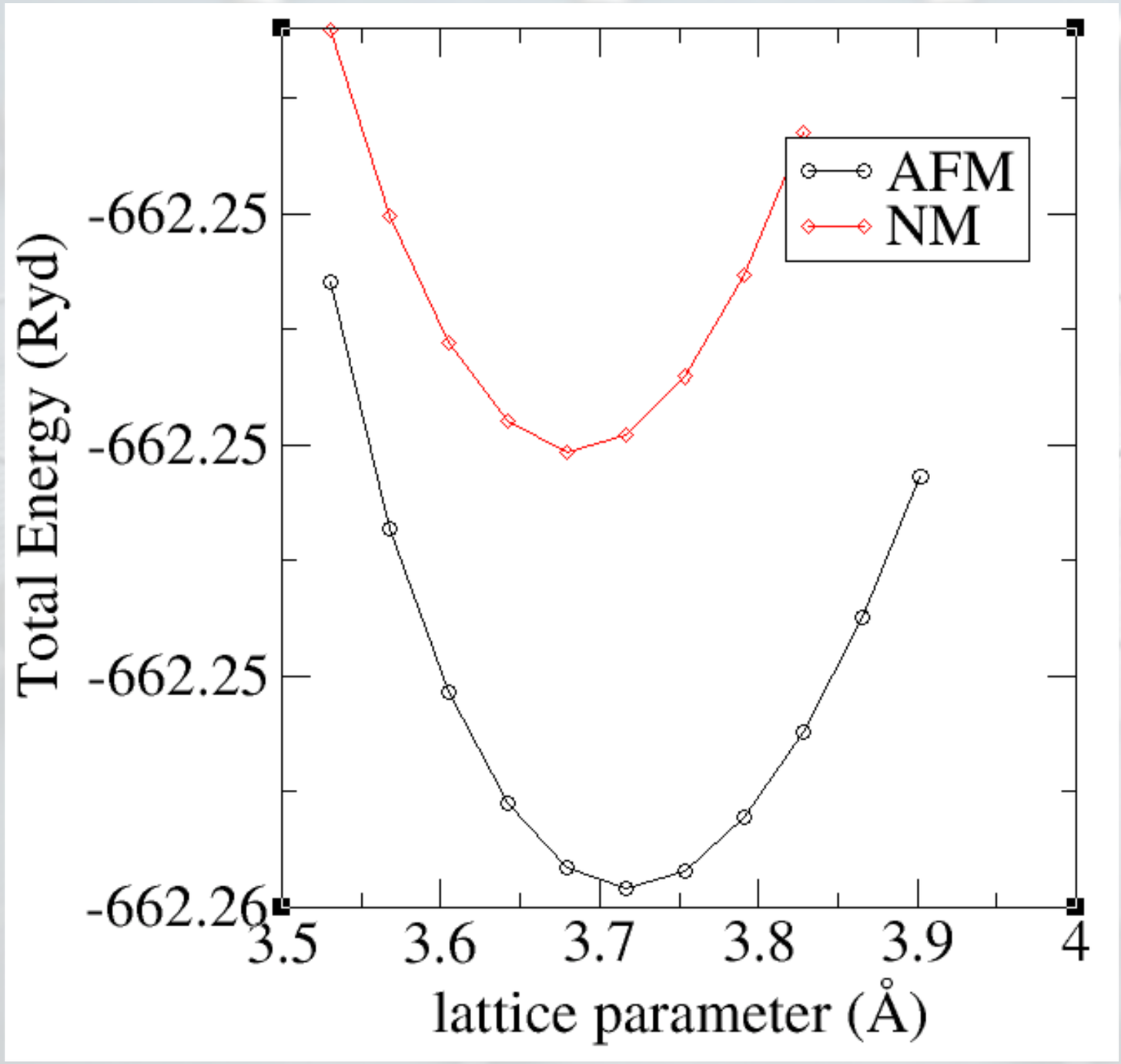
Lattice Parameter

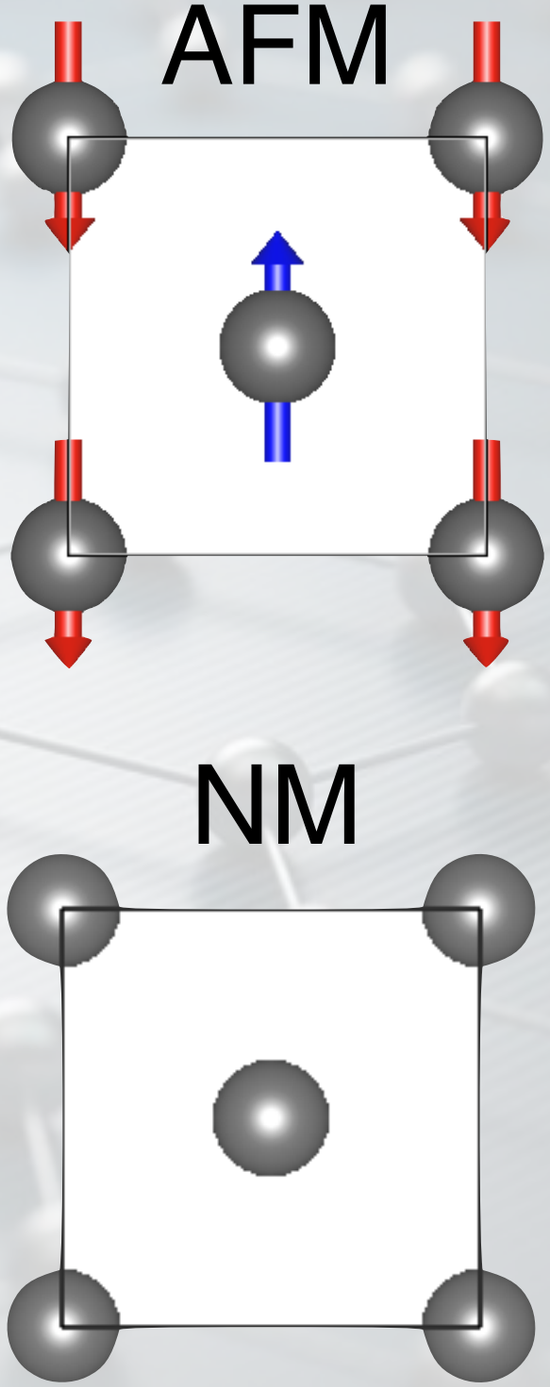




FeSe

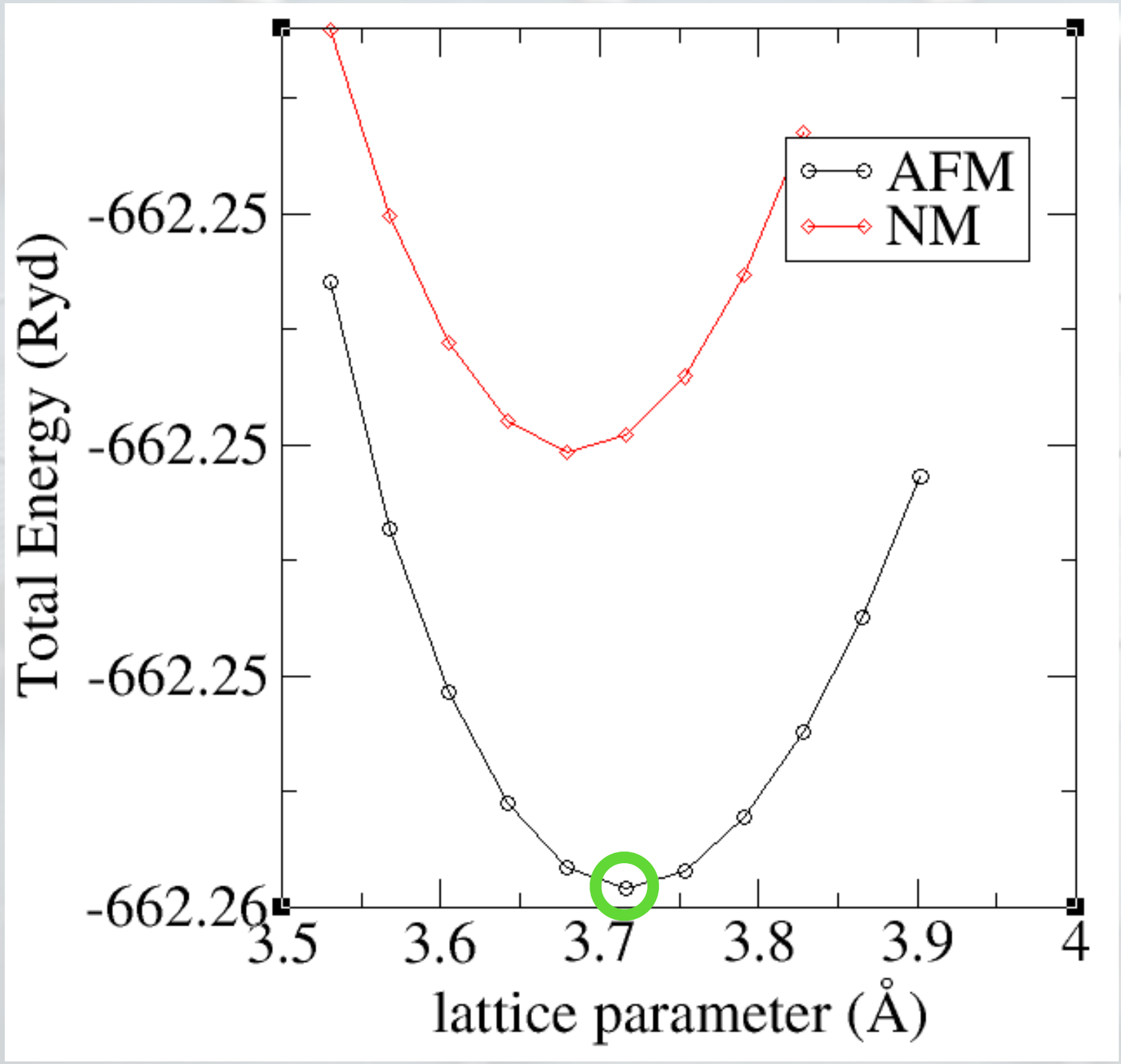
Lattice Parameter

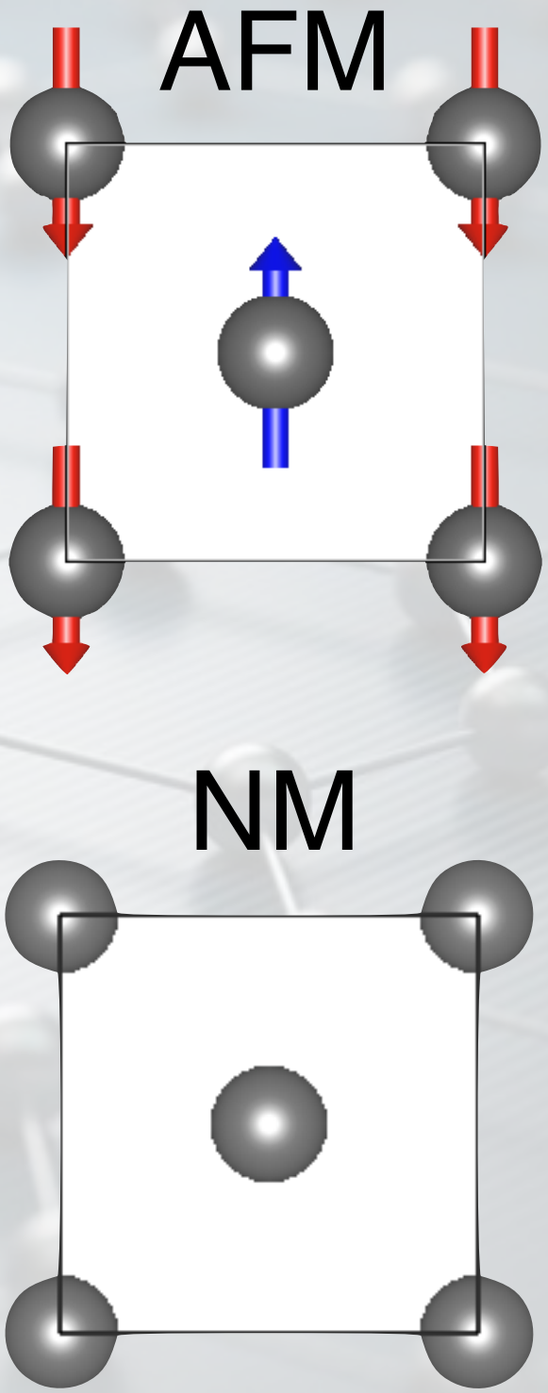




FeSe

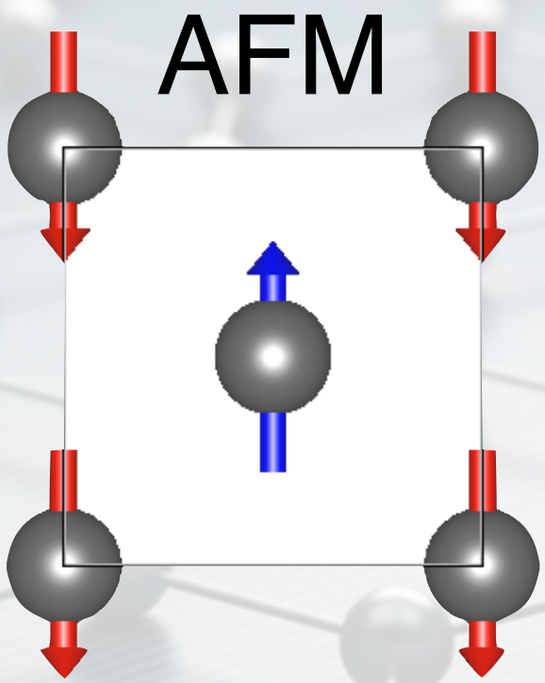
Lattice Parameter

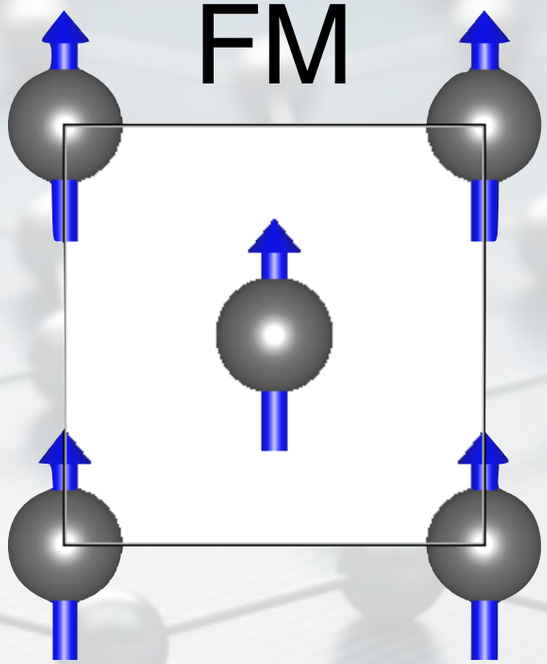




FeSe

Magnetic ground state - AFM x FM



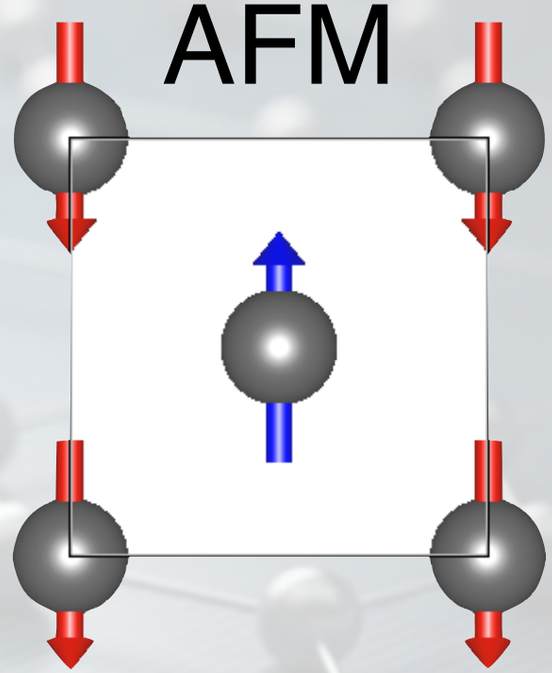


$$E^{AFM-FM} = -78.24meV$$

FeSe

Site projected magnetic moment

projwfc.x

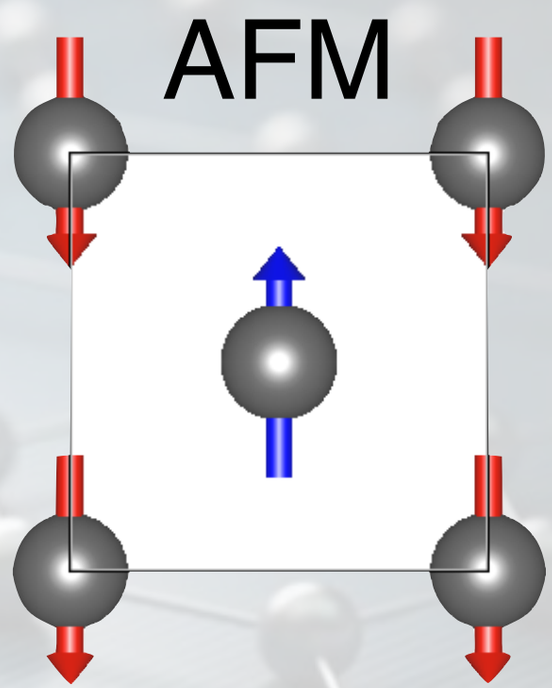



```
&projwfc
   prefix      = 'Fe2Se2-FeSe'
   outdir='./'
  filpdos      = 'Fe2Se2-FeSe'
   lwrite_overlaps = .false.
   lbinary_data  = .false.
/
```

FeSe

Site projected magnetic moment

projwfc.x



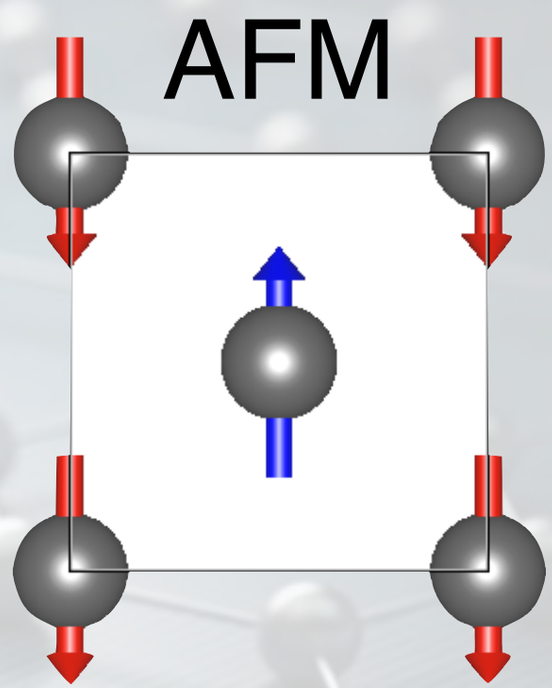
Atom # 1: total charge = 8.3161, s = 0.3653, p = 1.0349, d = 6.9158,
spin up = 4.9766, s = 0.1926,
spin up = 4.9766, p = 0.5313,
spin up = 4.9766, d = 4.2526,
spin down = 3.3395, s = 0.1727,
spin down = 3.3395, p = 0.5036,
spin down = 3.3395, d = 2.6632,
polarization = 1.6370, s = 0.0199, p = 0.0277, d = 1.5894,

Atom # 2: total charge = 8.3162, s = 0.3653, p = 1.0349, d = 6.9159,
spin up = 3.3396, s = 0.1727,
spin up = 3.3396, p = 0.5036,
spin up = 3.3396, d = 2.6633,
spin down = 4.9766, s = 0.1926,
spin down = 4.9766, p = 0.5313,
spin down = 4.9766, d = 4.2527,
polarization = -1.6370, s = -0.0199, p = -0.0277, d = -1.5894,

FeSe

Site projected magnetic moment

projwfc.x



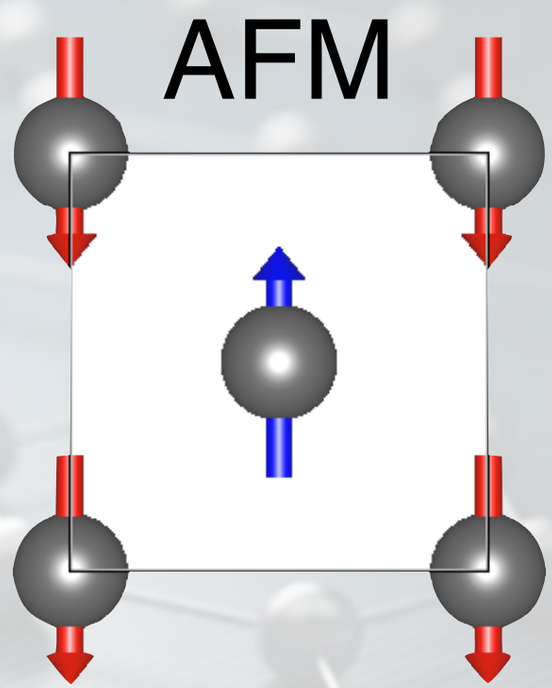
Atom # 1: total charge = 8.3161, s = 0.3653, p = 1.0349, d = 6.9158,
spin up = 4.9766, s = 0.1926,
spin up = 4.9766, p = 0.5313,
spin up = 4.9766, d = 4.2526,
spin down = 3.3395, s = 0.1727,
spin down = 3.3395, p = 0.5036,
spin down = 3.3395, d = 2.6632,
polarization = 1.6370, s = 0.0199, p = 0.0277, d = 1.5894,

Atom # 2: total charge = 8.3162, s = 0.3653, p = 1.0349, d = 6.9159,
spin up = 3.3396, s = 0.1727,
spin up = 3.3396, p = 0.5036,
spin up = 3.3396, d = 2.6633,
spin down = 4.9766, s = 0.1926,
spin down = 4.9766, p = 0.5313,
spin down = 4.9766, d = 4.2527,
polarization = -1.6370, s = -0.0199, p = -0.0277, d = -1.5894,

FeSe

Site projected magnetic moment

projwfc.x

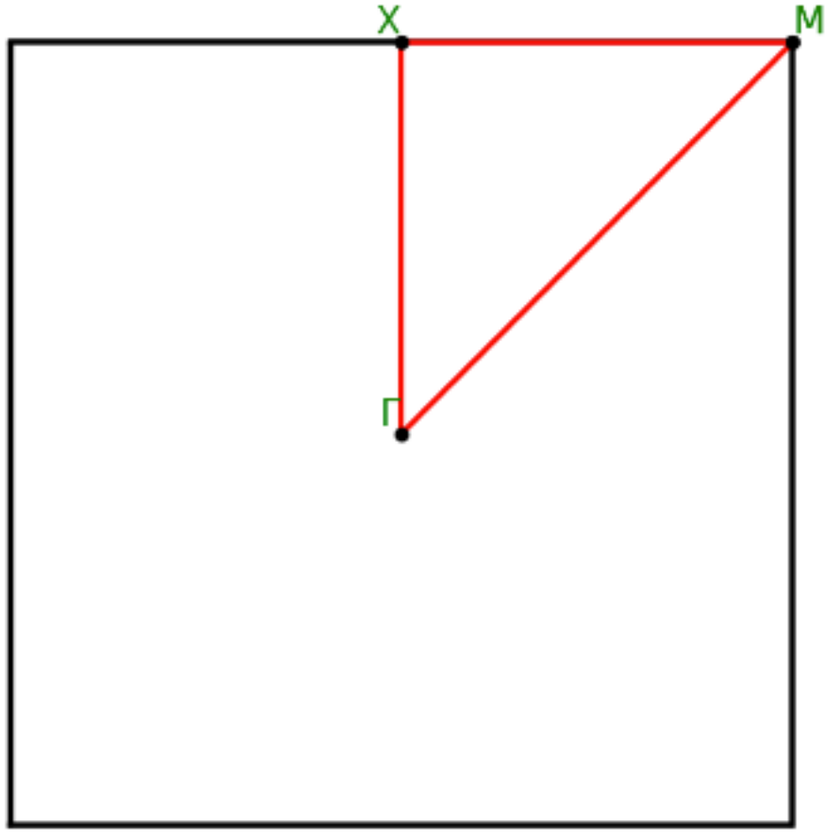


Atom # 1: total charge = 8.3161, s = 0.3653, p = 1.0349, d = 6.9158,
spin up = 4.9766, s = 0.1926,
spin up = 4.9766, p = 0.5313,
spin up = 4.9766, d = 4.2526,
spin down = 3.3395, s = 0.1727,
spin down = 3.3395, p = 0.5036,
spin down = 3.3395, d = 2.6632,
polarization = 1.6370, s = 0.0199, p = 0.0277, d = 1.5894,

Atom # 2: total charge = 8.3162, s = 0.3653, p = 1.0349, d = 6.9159,
spin up = 3.3396, s = 0.1727,
spin up = 3.3396, p = 0.5036,
spin up = 3.3396, d = 2.6633,
spin down = 4.9766, s = 0.1926,
spin down = 4.9766, p = 0.5313,
spin down = 4.9766, d = 4.2527,
polarization = -1.6370, s = -0.0199, p = -0.0277, d = -1.5894,

FeSe - Bandstructure

High Symmetry Path




```
K_POINTS crystal_b
4
   0.5000   0.5000   0.0000 20  ! M
   0.0000   0.0000   0.0000 20  ! \Gamma
   0.5000   0.0000   0.0000 20  ! X
   0.5000   0.5000   0.0000 20  ! M
```

FeSe

Spin Polarized - AFM