ESpinS

A program for classical Monte-Carlo simulations of spin systems

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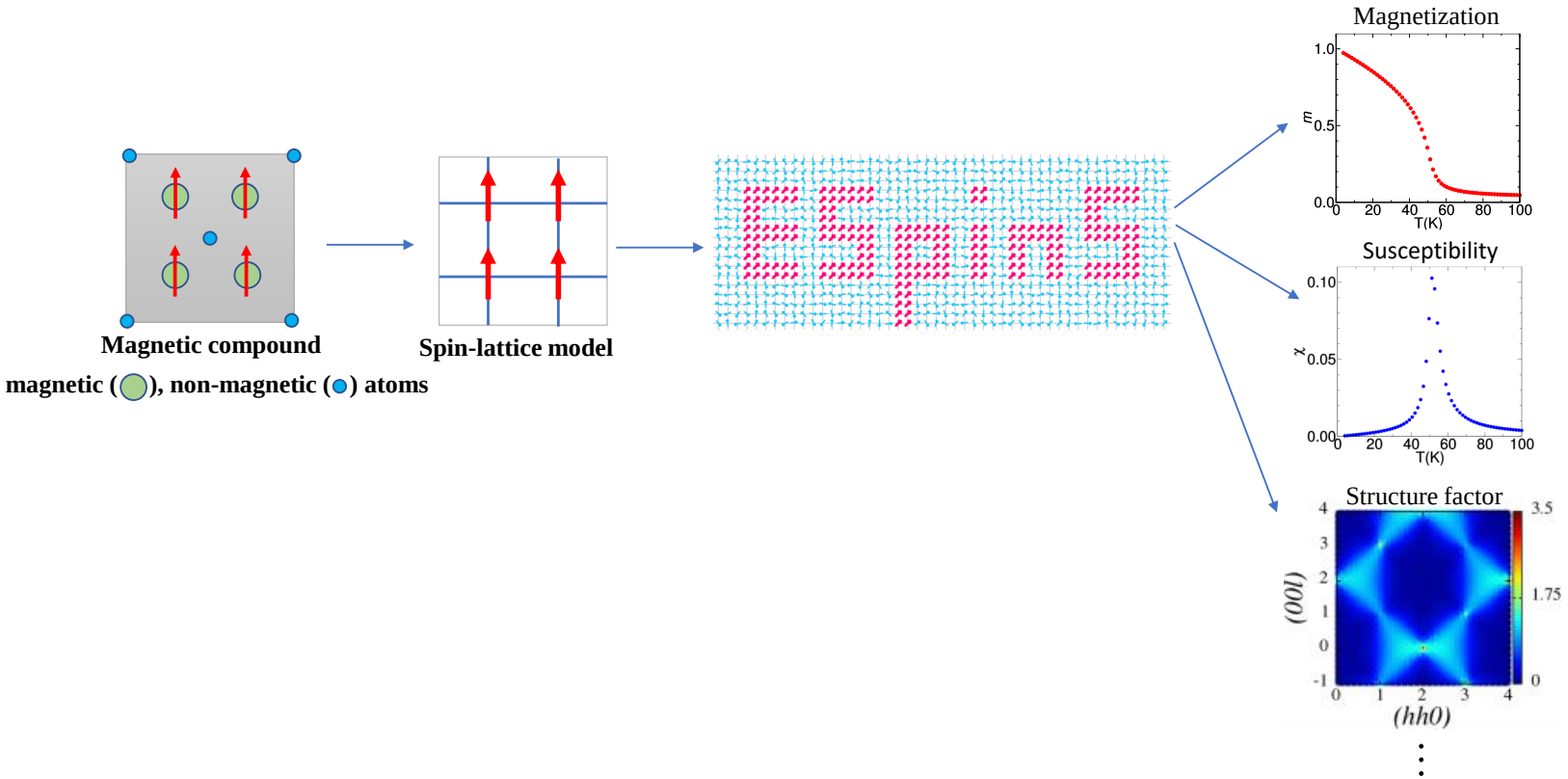
EspinS?



- The main parts of the code are written in Fortran.
- Dr. Nafise Rezaei mainly developed the code for three years.
- The code is still under development.
- GitHub: https://github.com/nafiserb/ESpinS
- Paper: Computational Materials Science, 202, 110947 (2022)

Spin Hamiltonian

$$\mathcal{H} = \mathcal{H}_{\text{Heis}} + \mathcal{H}_{\text{bi-qu}} + \mathcal{H}_{\text{DM}} + \mathcal{H}_{\text{single-ion}}$$

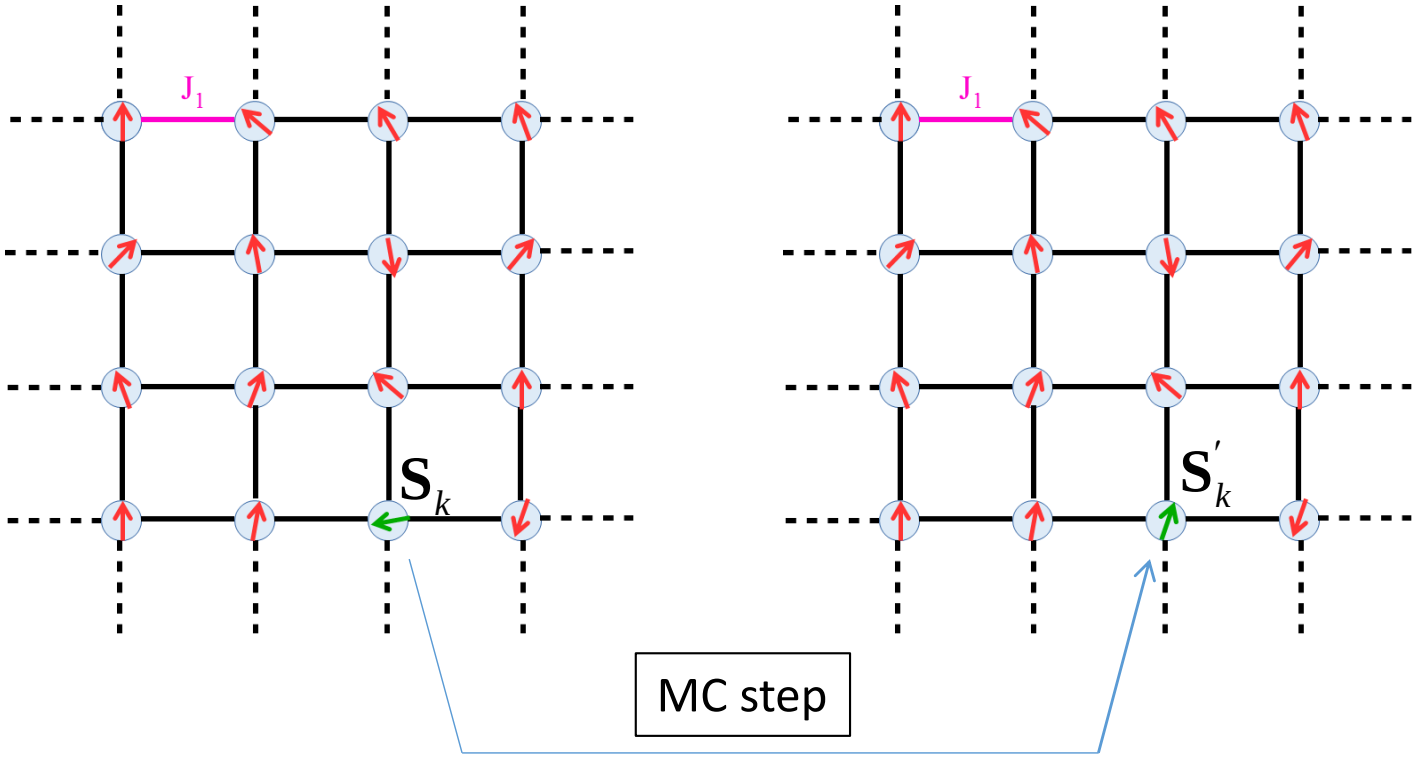
$$\mathcal{H}_{\text{Heis}} = -\frac{1}{2}\sum_{i,j} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j,$$

$$\mathcal{H}_{\text{bi-qu}} = \frac{1}{2}\sum_{ij} B_{ij}(\mathbf{S}_i \cdot \mathbf{S}_j)^2,$$

$$\begin{aligned} \mathcal{H}_{\text{DM}} &= \frac{D}{2}\sum_{ij} \hat{\mathbf{D}}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j), \\ \mathcal{H}_{\text{single-ion}} &= \Delta \sum_i (\mathbf{S}_i \cdot \hat{\mathbf{d}}_i)^2 \end{aligned}$$

Monte Carlo: Local update metropolis algorithm

$$X_i = \{\mathbf{S}_1, \mathbf{S}_2, \mathbf{S}_3, ..., \mathbf{S}_k, ...\} \qquad X_j = \{\mathbf{S}_1, \mathbf{S}_2, \mathbf{S}_3, ..., \mathbf{S}'_k, ...\}$$



$$\mathcal{A}\left(X_i \to X_j\right) = \min\left[\frac{P_{eq}\left(X_j\right)}{P_{eq}\left(X_i\right)}, 1\right] = \min\left[e^{-\beta\Delta E}, 1\right]$$

$$\Delta E = H(X_j) - H(X_i) = E_j - E_i$$

Simple example: Ising

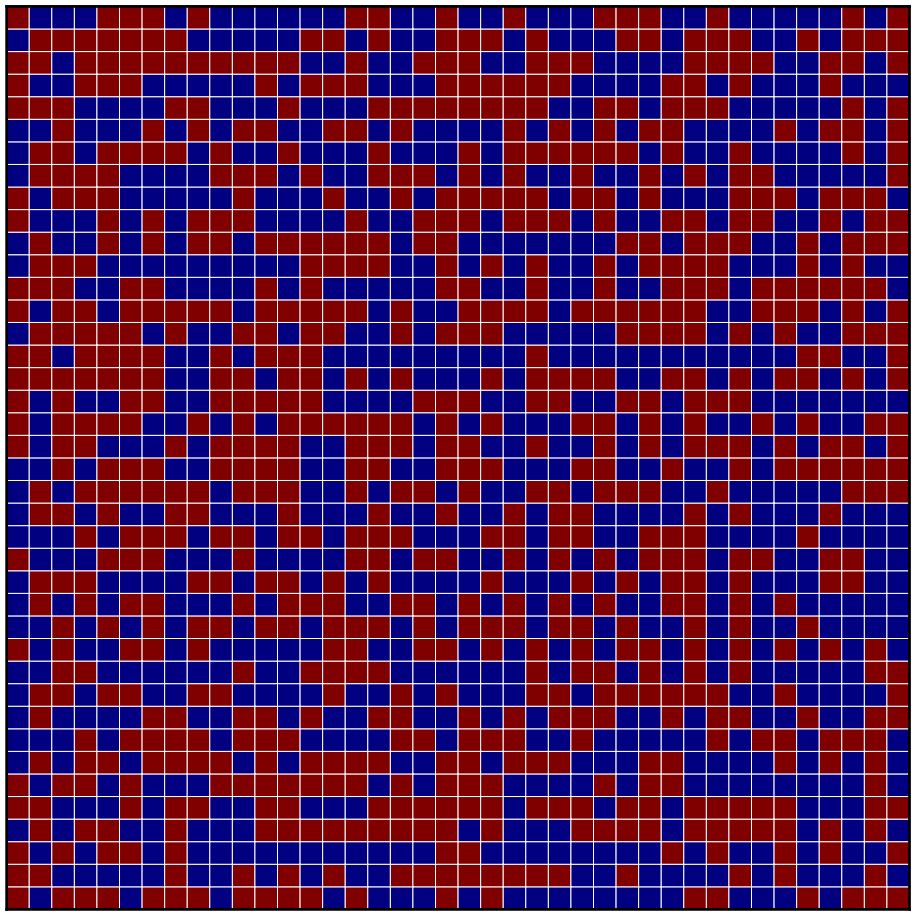
$$H = -\sum_{<i,j>} J_{i,j}\sigma_i\sigma_j$$

$$\sigma_i = \pm 1$$

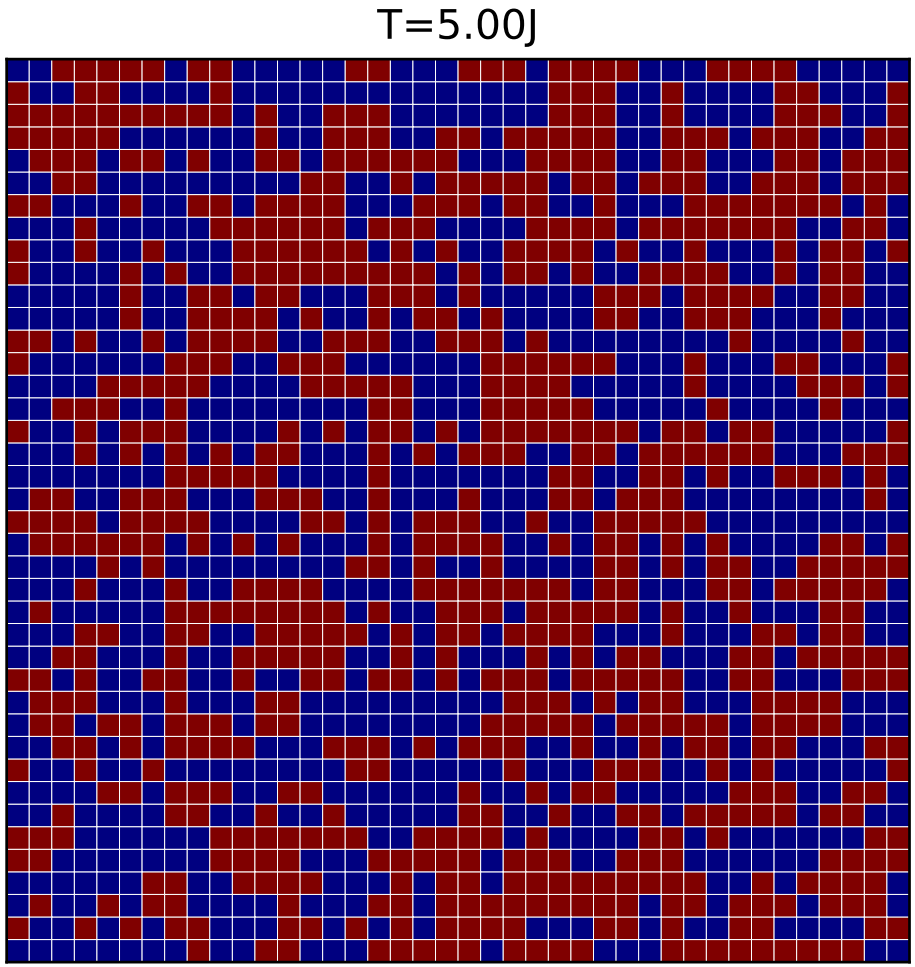
Simple example: Ising

$\sigma_i = +1 \equiv \uparrow \equiv$ 

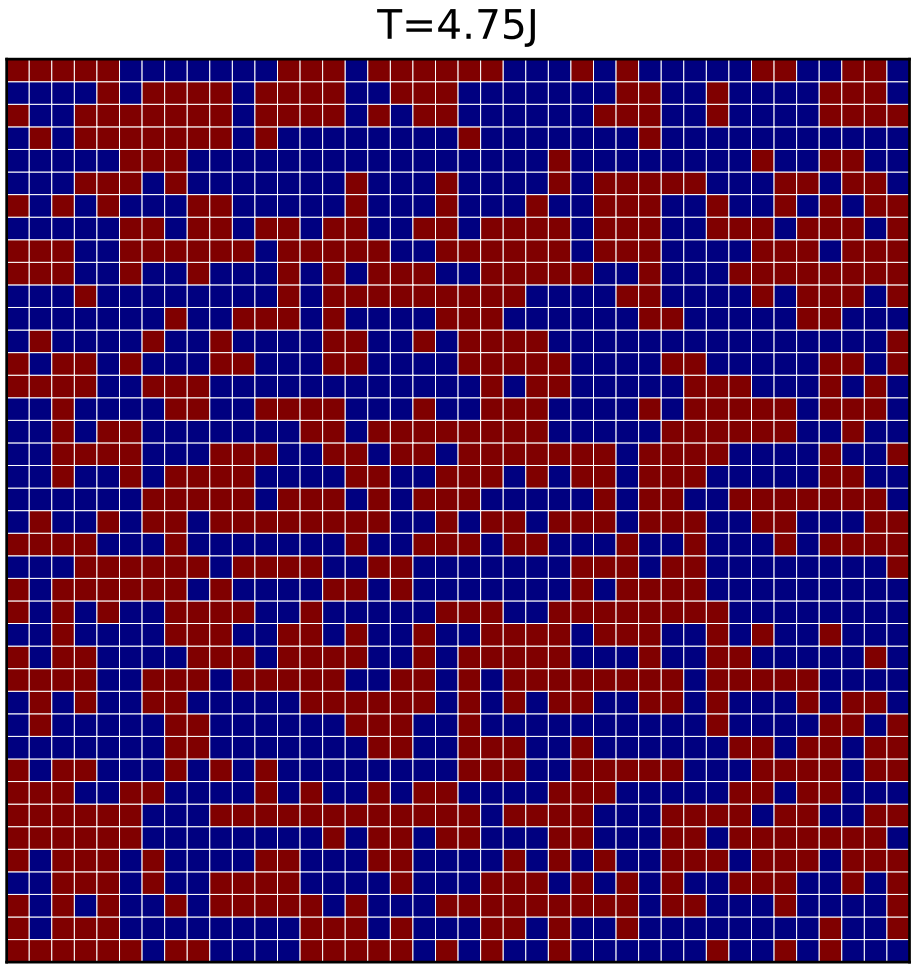
$\sigma_i = -1 \equiv \downarrow \equiv$ 



Simple example: Ising



Simple example: Ising



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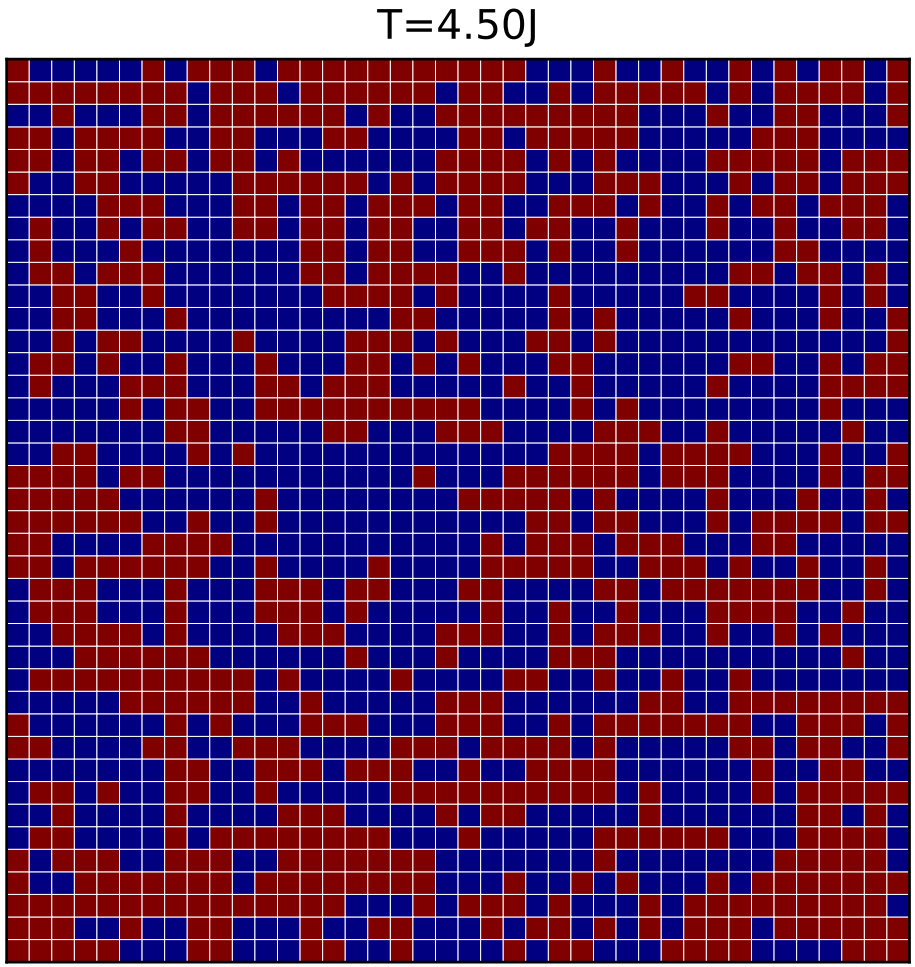
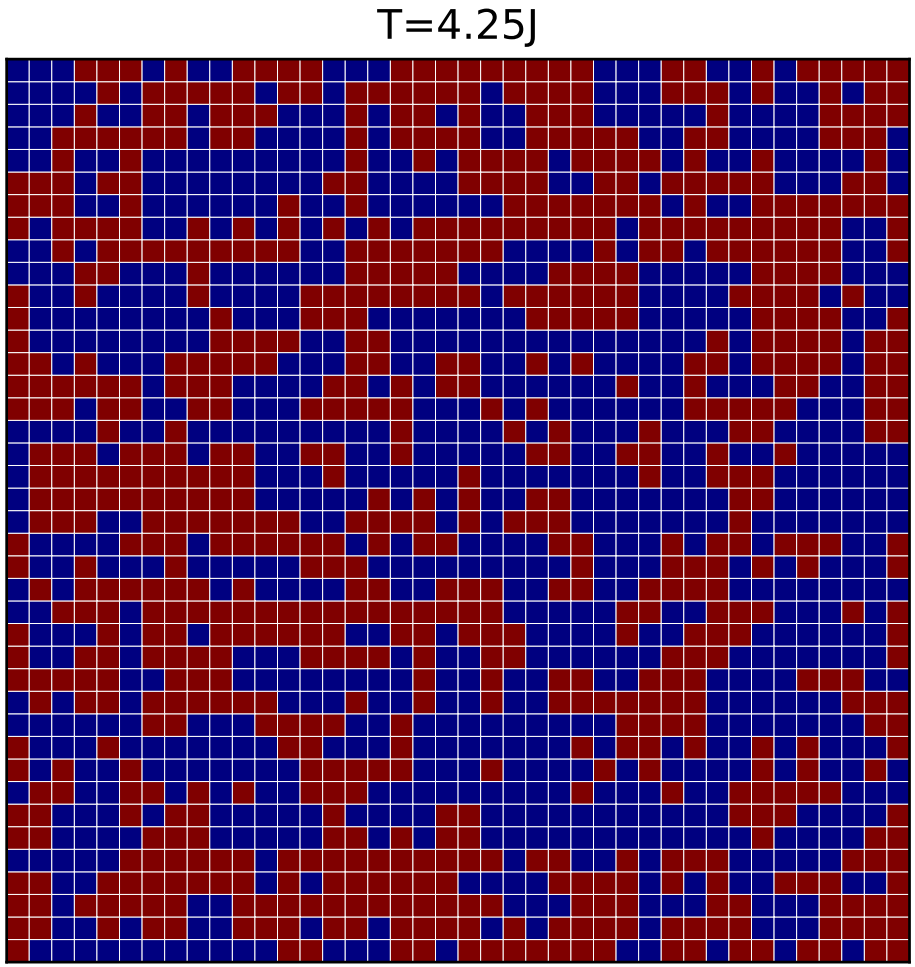
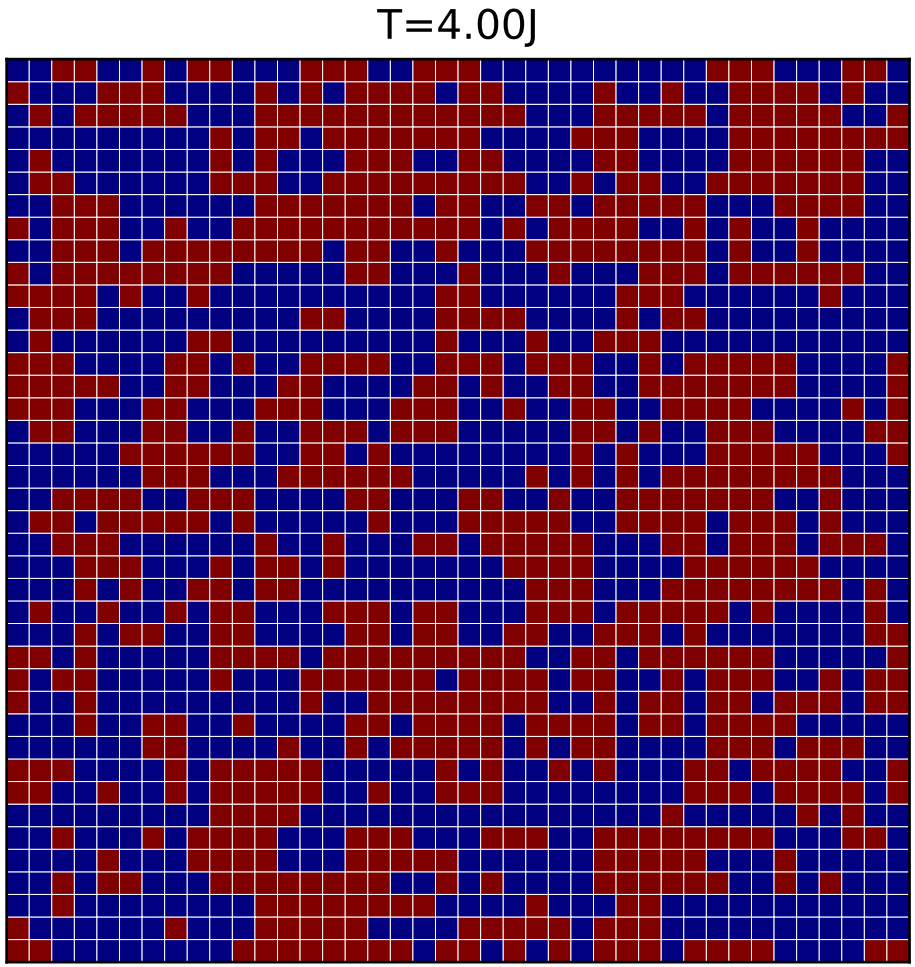


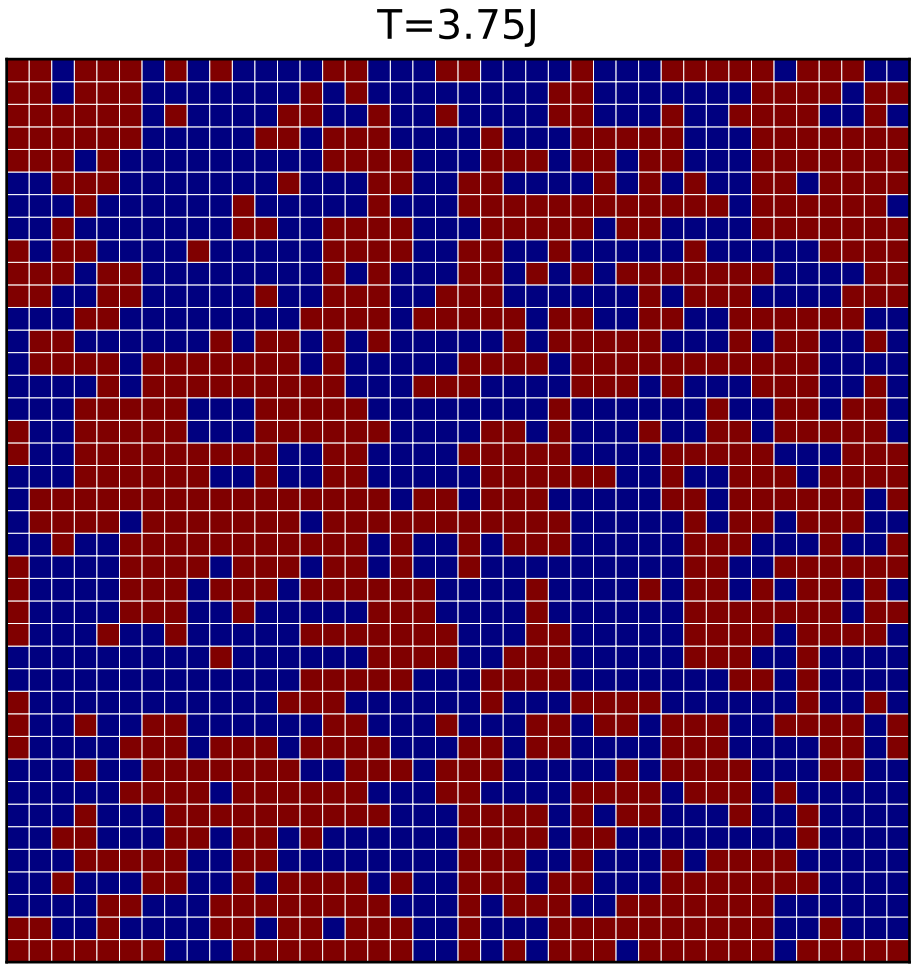
Simple example: Ising



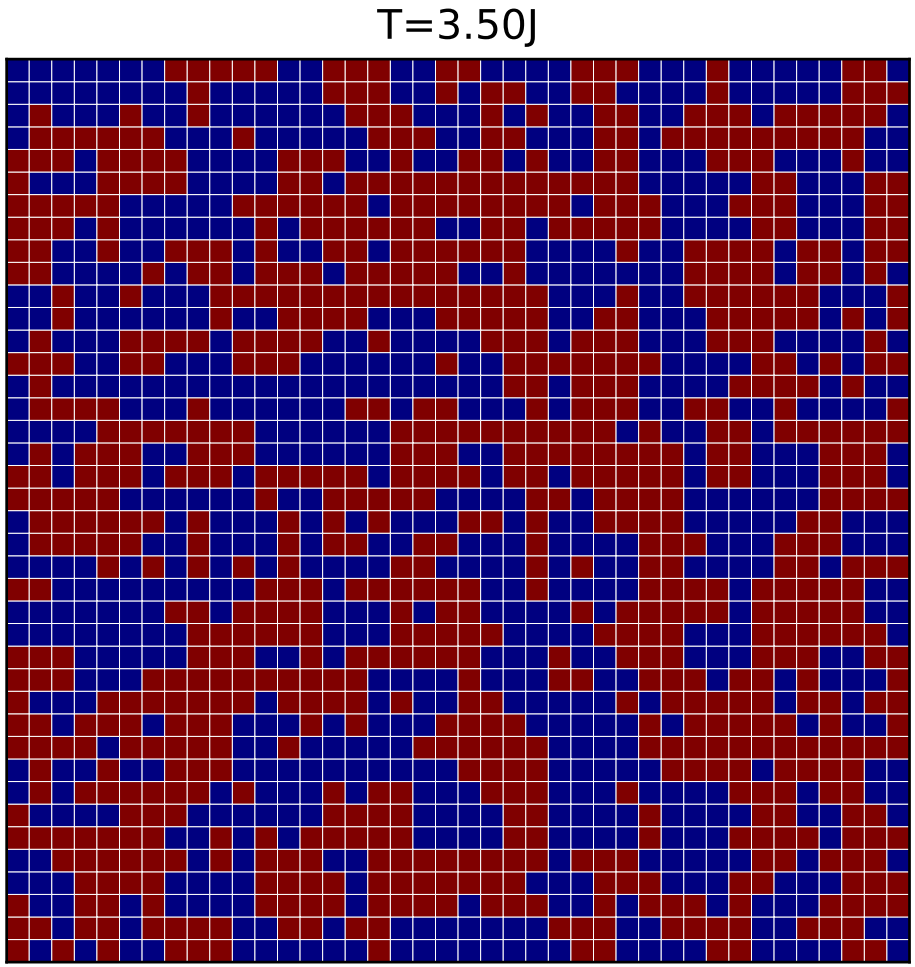
Simple example: Ising



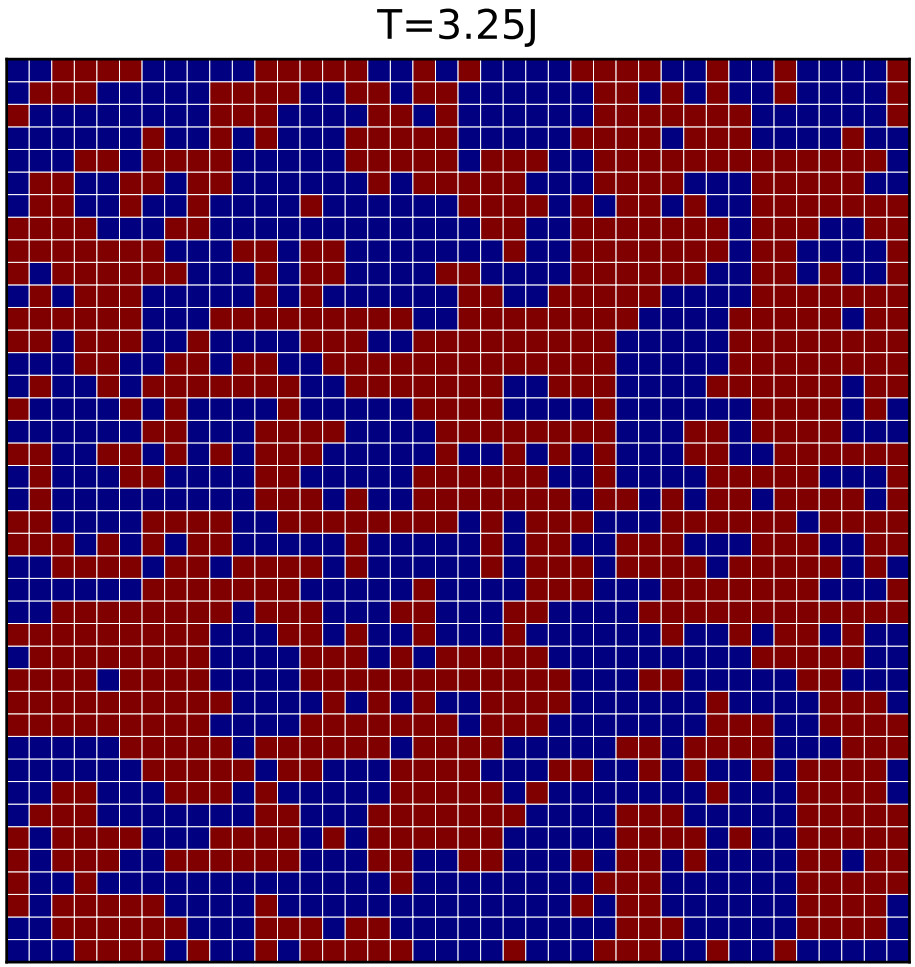
Simple example: Ising



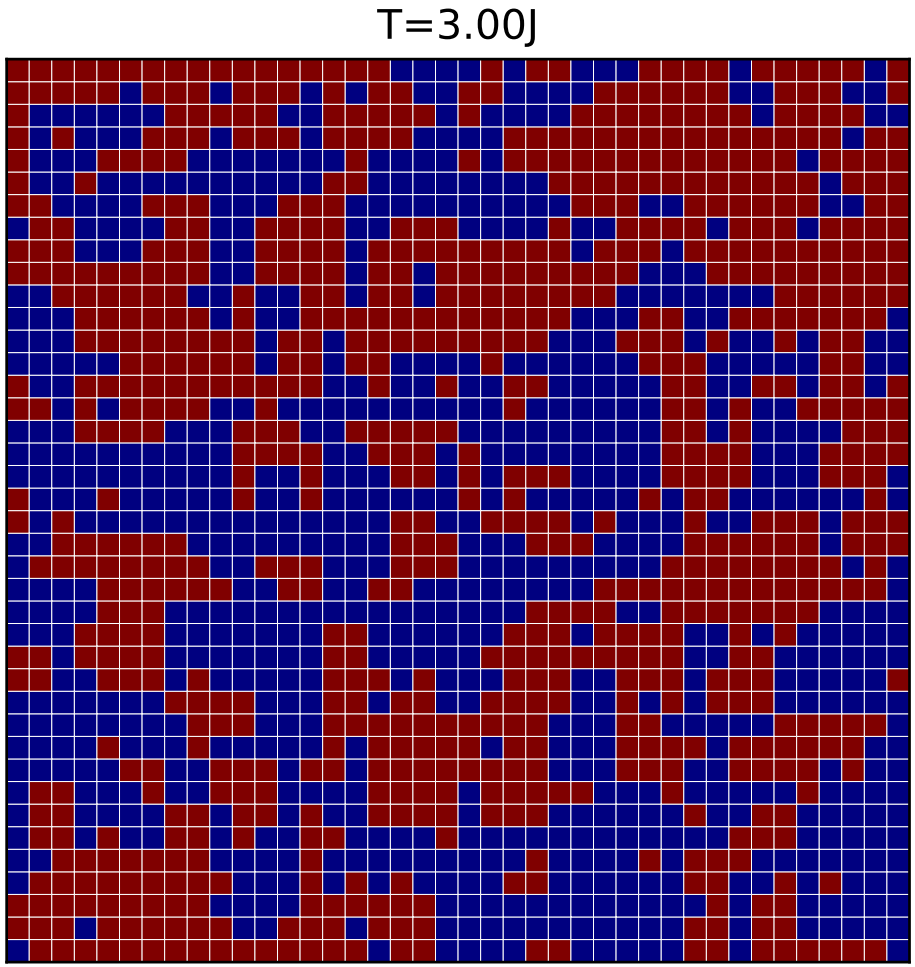
Simple example: Ising



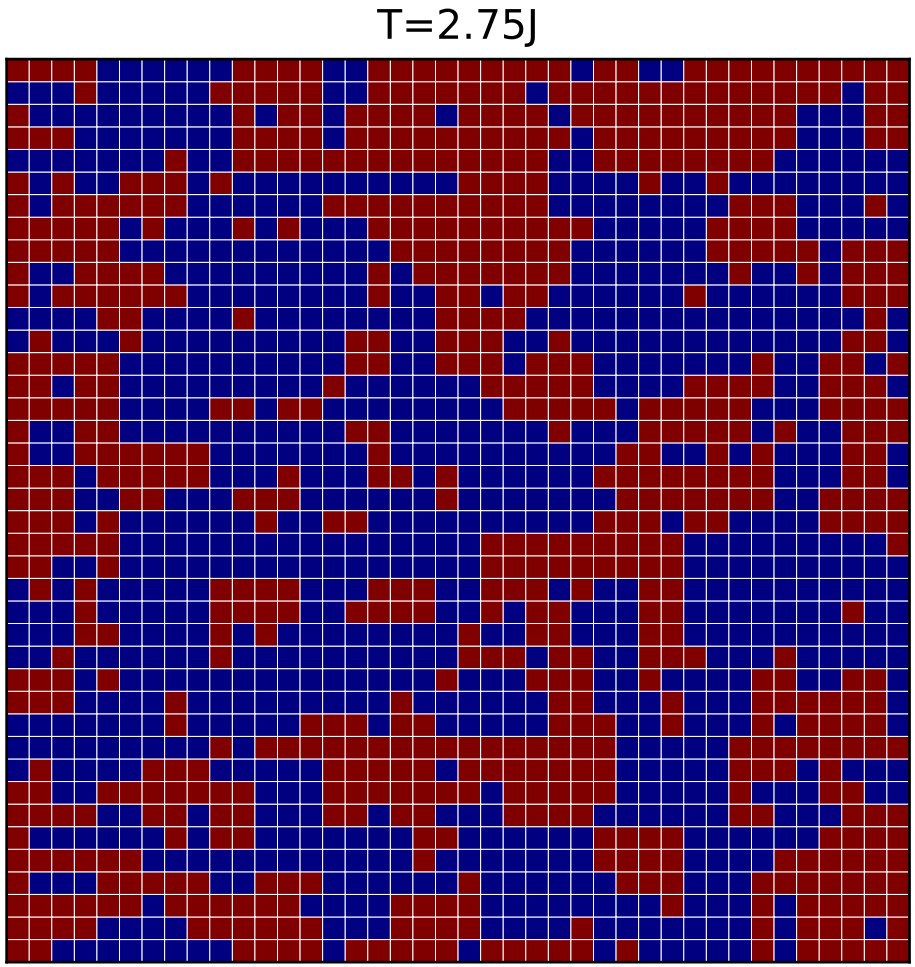
Simple example: Ising



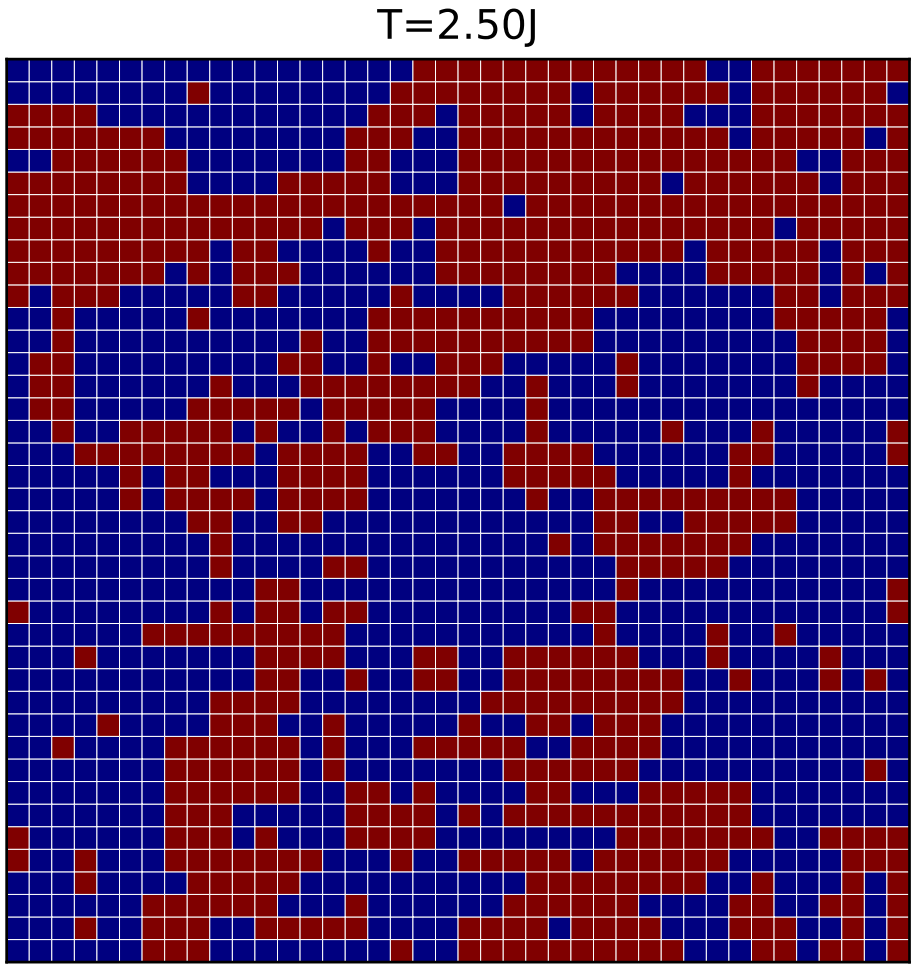
Simple example: Ising



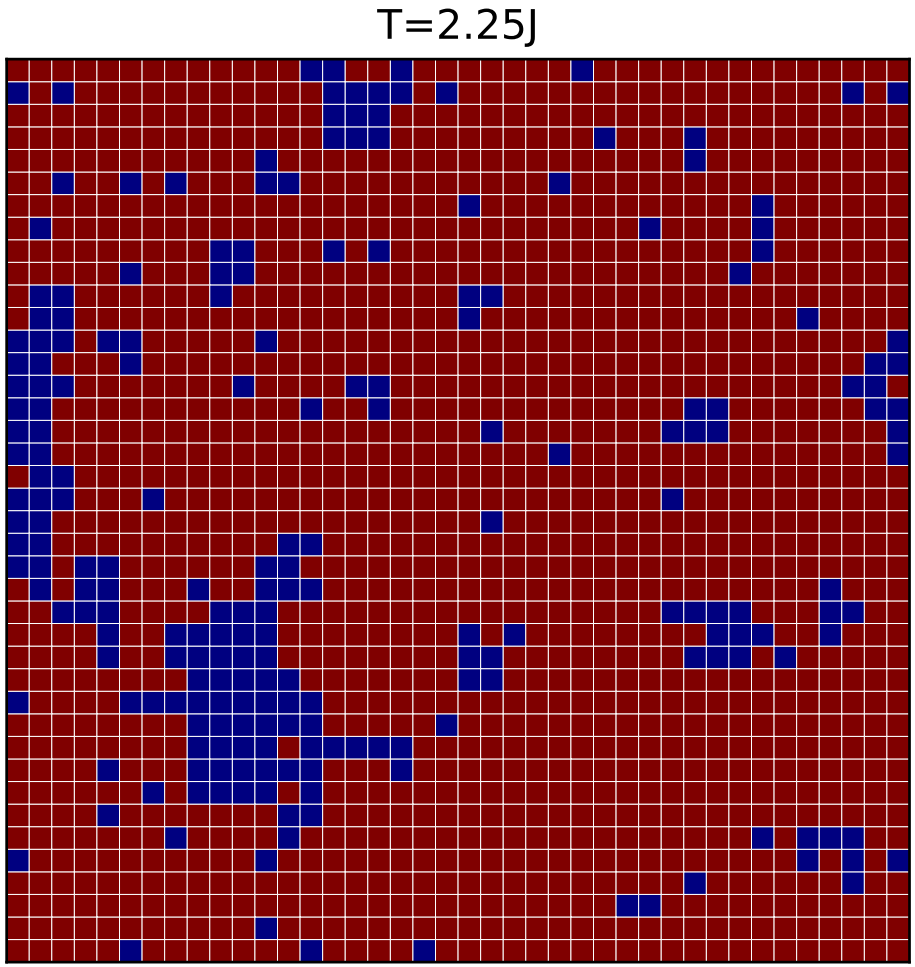
Simple example: Ising



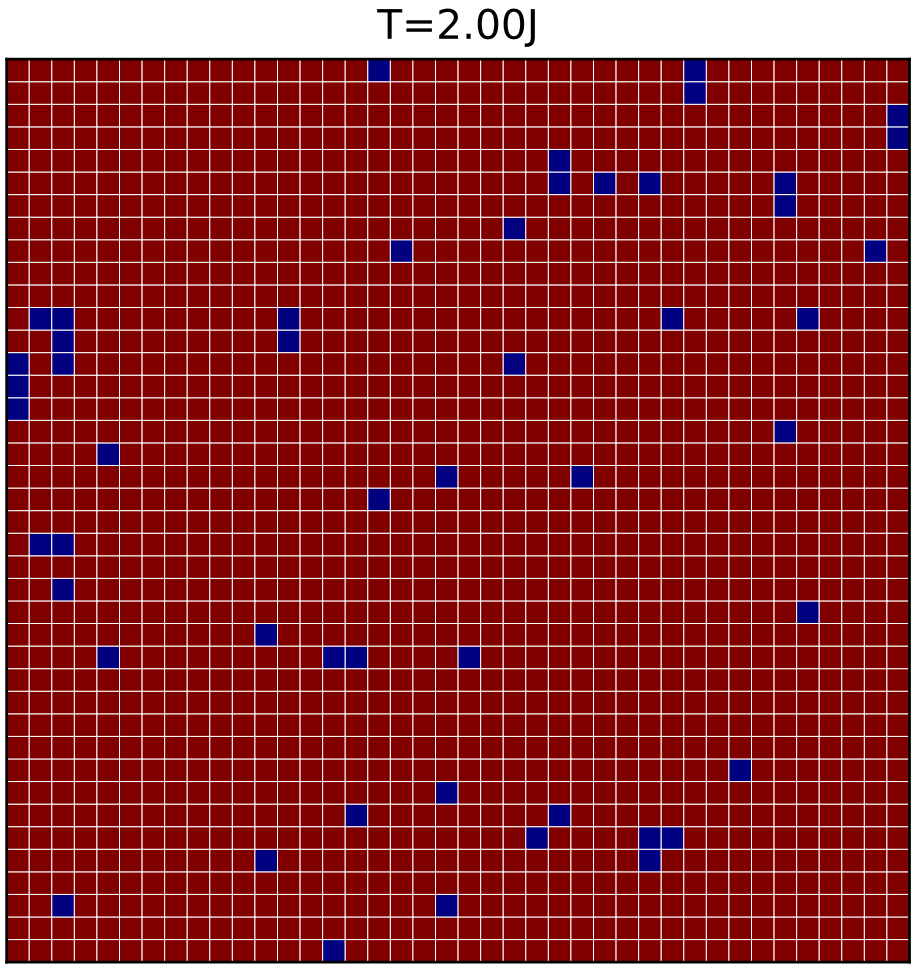
Simple example: Ising



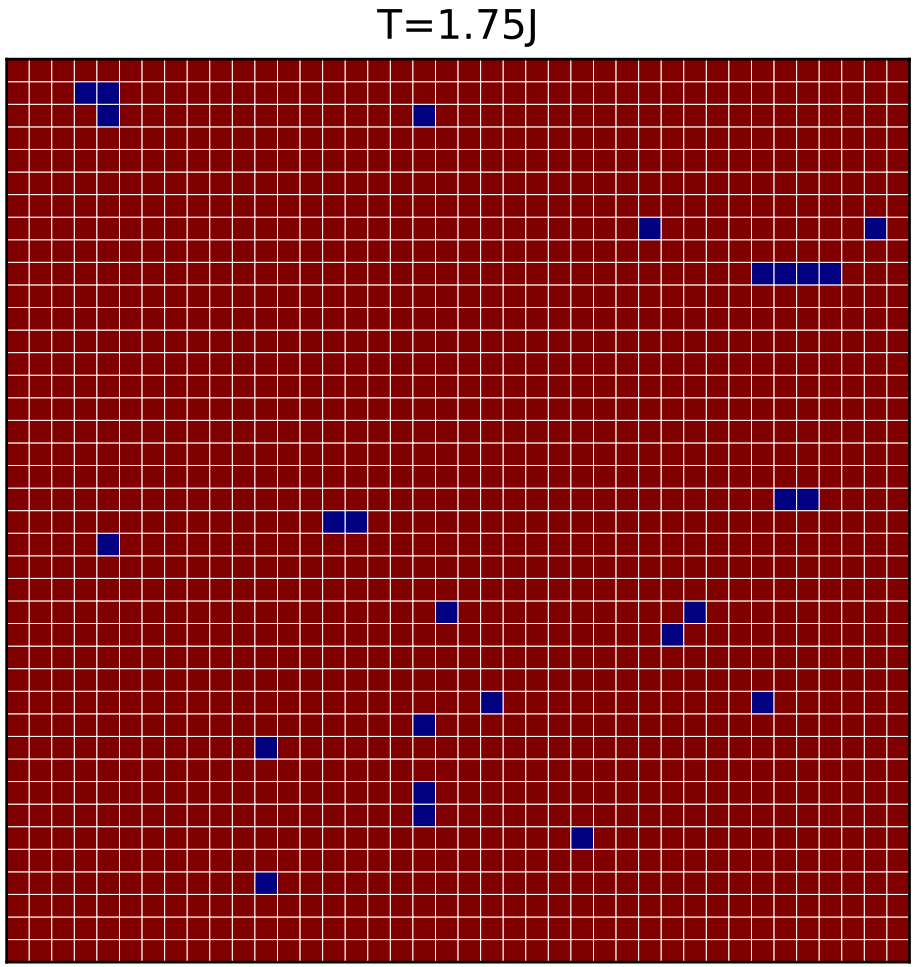
Simple example: Ising



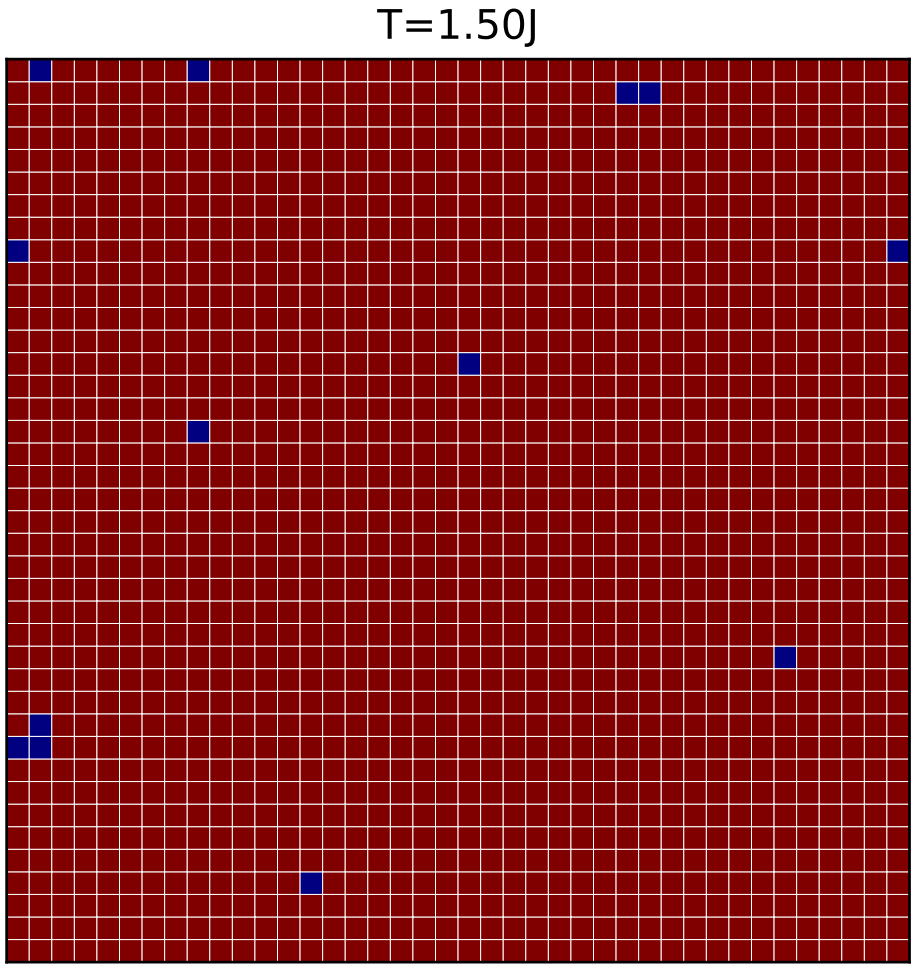
Simple example: Ising



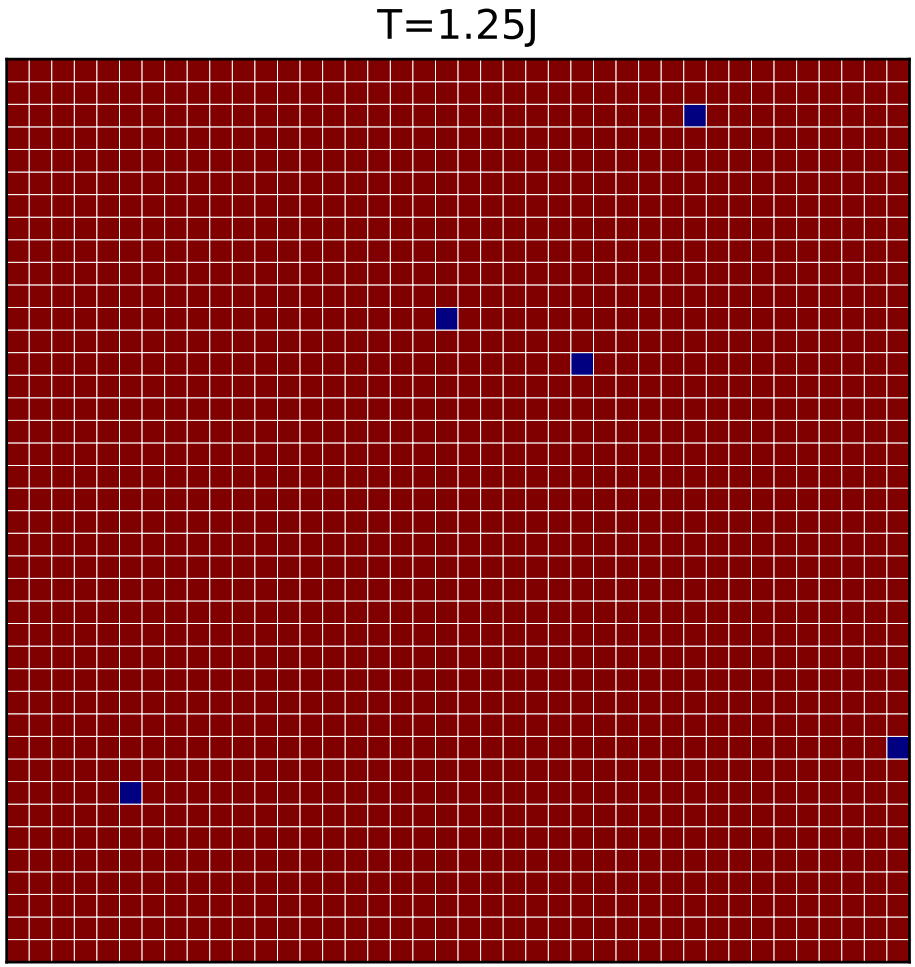
Simple example: Ising



Simple example: Ising

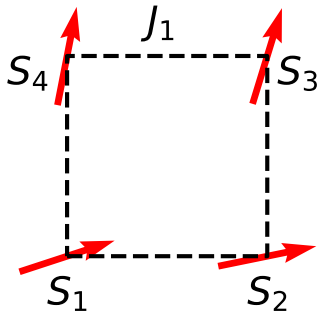


Simple example: Ising



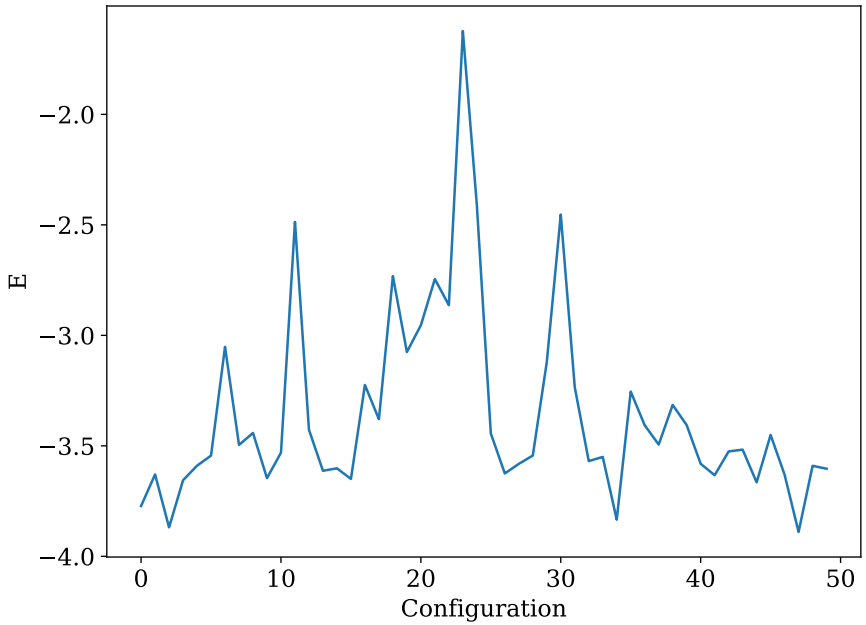
Parallel tempering (replica exchange)

Consider the following non-periodic spin system:



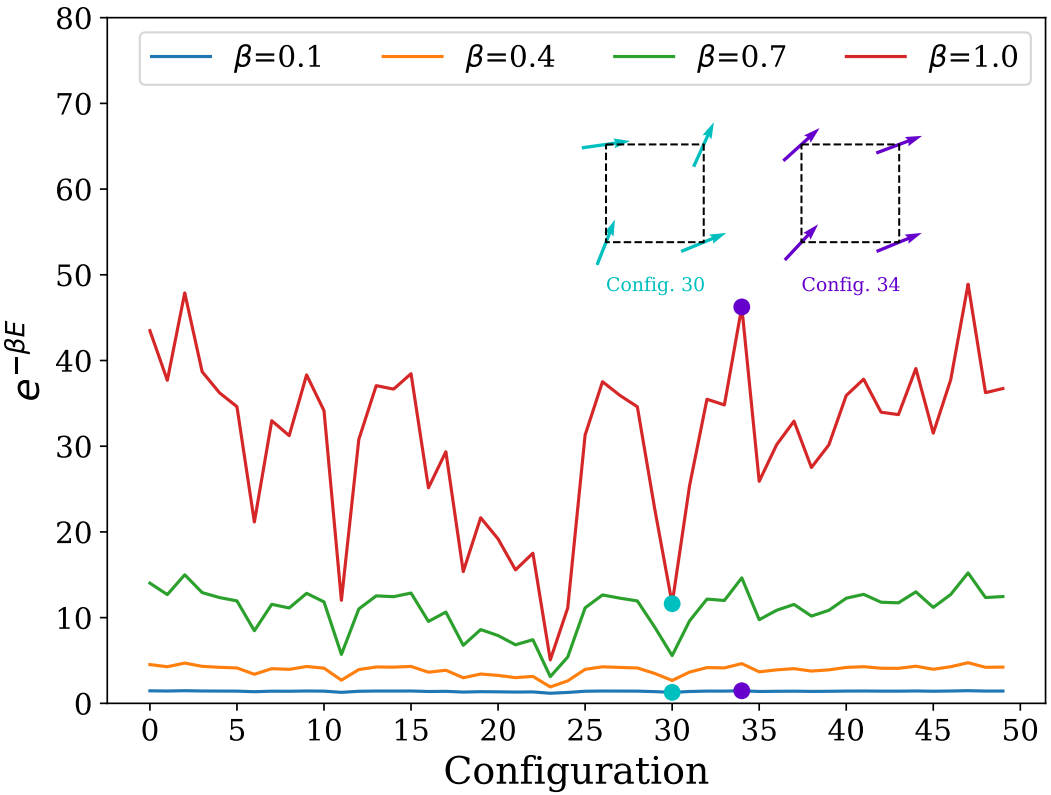
$$E = -J_1(S_1 \cdot S_2 + S_2 \cdot S_3 + S_3 \cdot S_4 + S_4 \cdot S_1)$$

Generating 50 spin configurations by random changing of the spin directions:



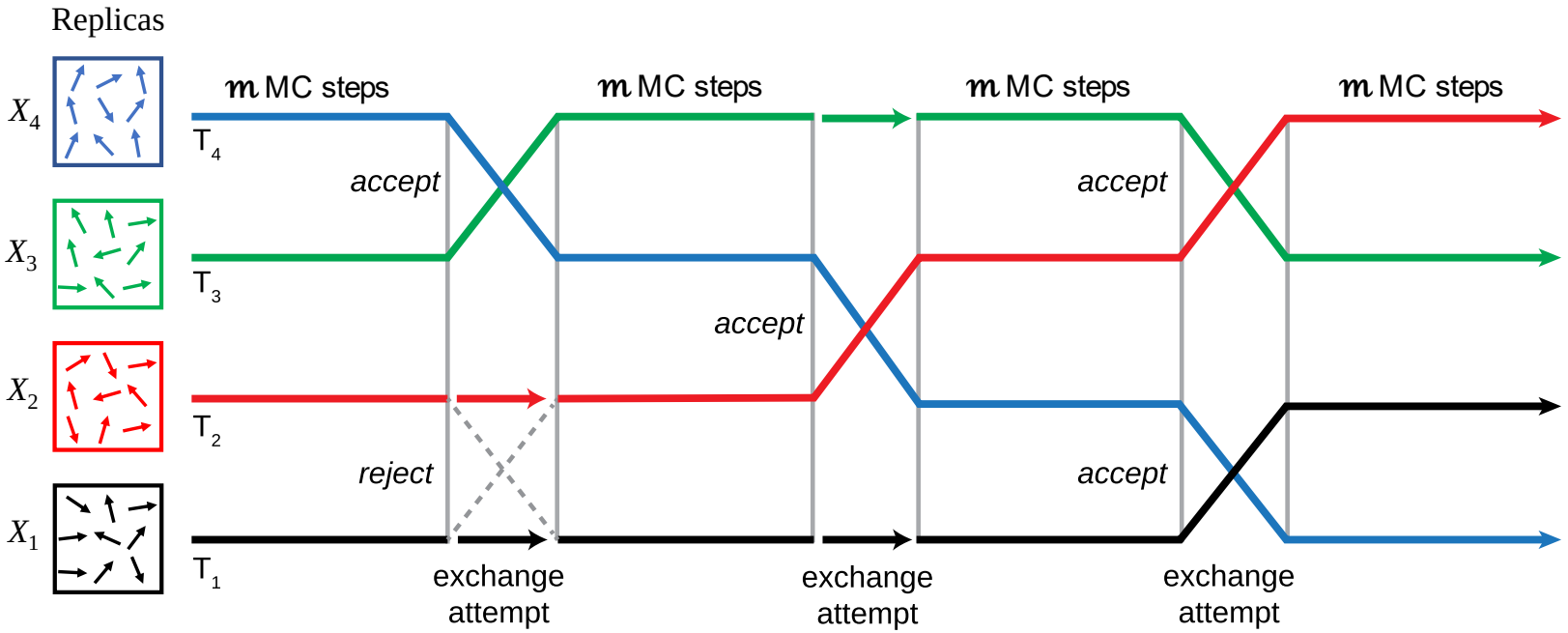
Parallel tempering (replica exchange)

Traversing in phase space can be done more quickly at higher temperatures using local updating:



Therefore we can use higher temperatures MC samplings for the lower temperatures.

Parallel tempering (replica exchange)



The swapping probability between two replicas is:

$$\mathcal{T}(\{\boldsymbol{X}\} \rightarrow \{\boldsymbol{X}'\}) = min\left[e^{\Delta\beta\Delta E}, 1\right]$$

where:

$$\begin{aligned} \{\boldsymbol{X}\} &= \{(X_1, \beta_1), \cdots, (X_i, \beta_i), (X_{i+1}, \beta_{i+1}), \cdots, (X_K, \beta_K)\} \\ \{\boldsymbol{X}'\} &= \{(X_1, \beta_1), \cdots, (X_{i+1}, \beta_i), (X_i, \beta_{i+1}), \cdots, (X_K, \beta_K)\} \end{aligned}$$

Download

```
git clone https://github.com/nafiserb/ESpinS.git
```

ESpinS directory tree:

```
ESpinS
├── config
├── examples
│   ├── example01
│   ├── example02
│   ├── example03
│   ├── example04
│   └── example05
├── src
├── user-guide
│   └── images
└── utility
    ├── mc-hist
    ├── optimize-temperatures
    └── visualize-spin
```

Edit make.sys

For parallel compilation using Intel Fortran Compiler (ifort):

```
#=============
# For Linux
#=============
F90 = ifort
COMMS=mpi
MPIF90=mpifort
FCOPTS=-O2
LDOPTS=-O2
#=========================================================
# Intel mkl libraries. Set LIBPATH if not in default path
#=========================================================

LIBDIR = /opt/intel/mkl/lib/intel64
LIBS   =  -L$(LIBDIR) -lmkl_core -lmkl_intel_lp64 -lmkl_sequential -lpthread
```

To compile, type:

```
make
```

After compilation, an executable file, named `mc.x` is created:

```
#ls
#config examples License.txt Makefile make.sys mc.x README.md src user-guide utility
```

Edit make.sys

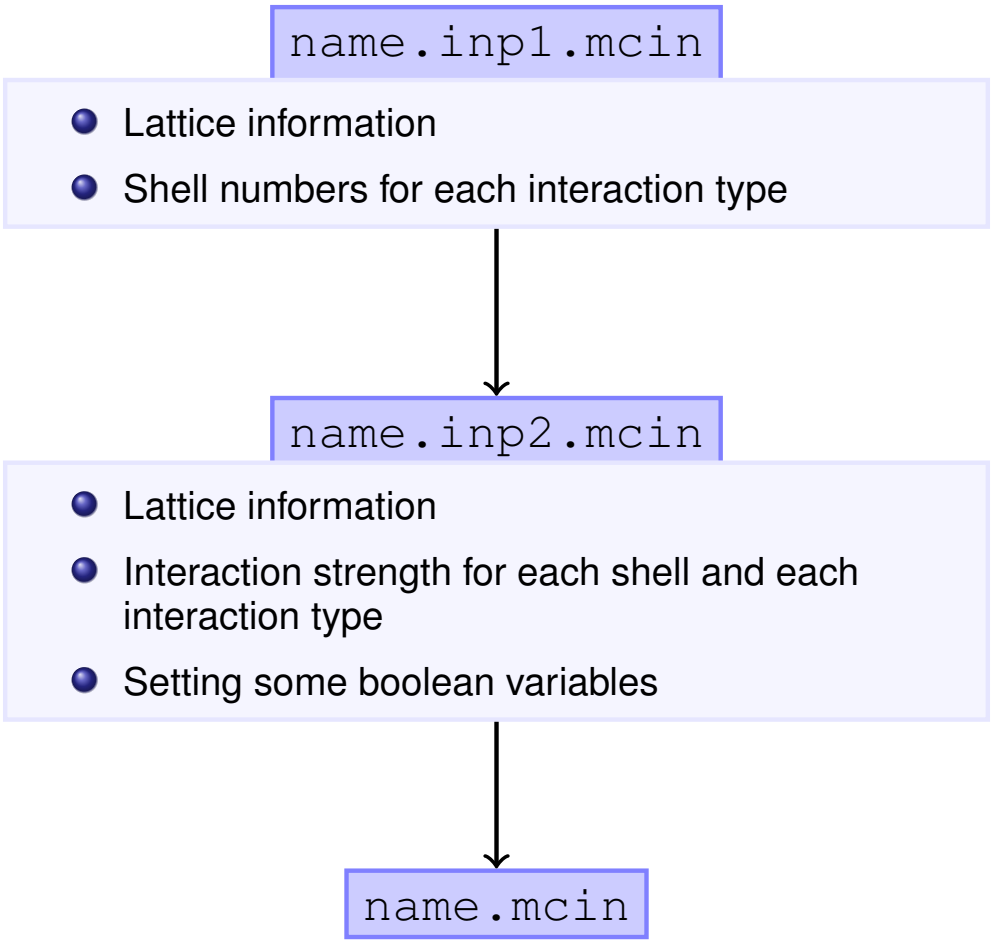
For serial compilation, comment `COMMS` with #:

```
#=============
# For Linux
#=============
F90 = ifort
#COMMS=mpi
MPIF90=mpifort
FCOPTS=-O2
LDOPTS=-O2
#=====================================================
# Intel mkl libraries. Set LIBPATH if not in default path
#=====================================================

LIBDIR = /opt/intel/mkl/lib/intel64
LIBS   =  -L$(LIBDIR) -lmkl_core -lmkl_intel_lp64 -lmkl_sequential -lpthread
```

The strategy to make main input file

EspinS has three input files: primary (`name.inp1.mcin`), secondary (`name.inp1.mcin`) and main (`name.mcin`) input files



Step 1, create `name.inp1.mcin`

Create a templete for `name.inp1.mcin`:

```
# cd ESpinS/utility
# bash inpfile.tem
```

```
Begin  Unit_Cell_Cart
 !Bohr
 A_1x        A_1y        A_1z
 A_2x        A_2y        A_2z
 A_3x        A_3y        A_3z
End Unit_Cell_Cart

Begin  Atoms_Frac
 atom_symbol  atom_pos_x  atom_pos_y  atom_pos_z  magnetic_moment
End  Atoms_Frac

Shells_jij      = 1
!! Spin_glass      = .True.
!! Ham_bij         = .True.
!! Shells_bij      = 1
!! Ham_dij         = .Ture.
!! Shells_dij      = 1

!! Length_unit     = Bohr
!! Parameter_unit  = Ryd
!! Coordinate      = Cart
```

- The file's name (i.e., `name`) is arbitrary, but the suffix should be `inp1.mcin`
- The exclamation mark (!) and Hash (#) used for comments

Step 1, create `name.inp1.mcin`

Create a templete for `name.inp1.mcin`:

```
# cd ESpinS/utility
# bash inpfile.tem
```

```
Begin  Unit_Cell_Cart
 !Bohr
 A_1x        A_1y        A_1z
 A_2x        A_2y        A_2z
 A_3x        A_3y        A_3z
End Unit_Cell_Cart

Begin  Atoms_Frac
 atom_symbol  atom_pos_x  atom_pos_y  atom_pos_z  magnetic_moment
End  Atoms_Frac

Shells_jij      = 1
!! Spin_glass      = .True.
!! Ham_bij         = .True.
!! Shells_bij      = 1
!! Ham_dij         = .Ture.
!! Shells_dij      = 1

!! Length_unit     = Bohr
!! Parameter_unit  = Ryd
!! Coordinate      = Cart
```

- The file's name (i.e., `name`) is arbitrary, but the suffix should be `inp1.mcin`
- The exclamation mark (!) and Hash (#) used for comments

Step 1, create `name.inp1.mcin`

Lattice vectors:

```
Begin  Unit_Cell_Cart
 !Bohr
 A_1x         A_1y         A_1z
 A_2x         A_2y         A_2z
 A_3x         A_3y         A_3z
End Unit_Cell_Cart
```

Lattice sites and magnetic moments ($\mathbf{S}_i$):

```
Begin  Atoms_Frac
 atom_symbol  atom_pos_x  atom_pos_y  atom_pos_z  magnetic_moment
End  Atoms_Frac
```

Shell numbers:

```
Shells_jij      = 1
```

step 1, create `name.inp1.mcin`

For example for a cubic lattice (e.g. `cubic.inp1.mcin`):

```
Begin unit_cell_cart
 Bohr
  10.000 0.000 0.000
  0.000 10.000 0.000
  0.000 0.000 10.000
End unit_cell_cart

Begin atoms_frac
  Mn 0.00   0.00   0.00  1.00
End atoms_frac

Shells_jij=1
```

step 2, create `name.inp2.mcin`

Typing following command creates secondary input file (`name.inp2.mcin`):

```
# mc.x  -inp1 cubic
```

The output files:

```
cubic.inp2.mcin  cubic.mcout  cubic.neigh  cubic.xsf
```

step 2, create `name.inp2.mcin`

`cubic.inp2.mcin:`

```
Begin Unit_Cell_Cart
    5.29177211   0.00000000   0.00000000
    0.00000000   5.29177211   0.00000000
    0.00000000   0.00000000   5.29177211
End Unit_Cell_Cart

Begin Atoms_Frac
 Mn       0.0000000   0.0000000   0.0000000    1.00
End Atoms_Frac

!! Order_parameter  = .True.
!! Sfactor          = .True.
!! Staggered_m      = .True.
!! Binning_error    = .True.
!! Spin_correlation = .True.
!! Energy_write     = .True.

## Hamiltonian
!! Boundary         =  Open
!! Ham_singleion    = .True.
!! Ham_field        = .True.
!! Spin_glass       = .True.   !Add the sigma parameters as sig=.. in Parameters_Jij Block

Begin Parameters_Jij
 t1=  1:t2=  1:sh= 1:Jij= ??????!:sig=?????!:d= 5.29177211
End Parameters_Jij
```

step 2, create `name.inp2.mcin`

Setting parameters such as exchange:

```
Begin Parameters_Jij
 t1=  1:t2=  1:sh= 1:Jij= ??????!:sig=?????!:d= 5.29177211
End Parameters_Jij
```

$J_1 = 0.00300$ eV:

```
Begin Parameters_Jij
 t1=  1:t2=  1:sh= 1:Jij= 0.00300!:sig=?????!:d= 5.29177211
End Parameters_Jij
```

main input file `name.mcin`

```
# mc.x  -inp2 cubic
```

Output files:

```
cubic.inp2.mcin  cubic.mcin  cubic.mcout  cubic.neigh  cubic.xsf
```

main input file `name.mcin`

`cubic.mcin:`

```
Begin Unit_Cell_Cart
    5.29177211   0.00000000   0.00000000
    0.00000000   5.29177211   0.00000000
    0.00000000   0.00000000   5.29177211
End Unit_Cell_Cart

Begin Atoms_Frac
 Mn       0.0000000   0.0000000   0.0000000    1.00
End Atoms_Frac

tem_start          =   5
tem_end            =   5
tems_num           =   1
!! tems_mode          = man
!! tems               = 5.00 10.00 15.00 20.00

!! Pt                = .True.
!! Pt_steps_swap      = 10

steps_warmup      =       100000
steps_mc          =       200000
steps_measure     =            2

initial_sconfig   =        ferro
mcarlo_mode       =       random

supercell_size    =      4     4     4

 ## Hamiltonian
Begin Jij_parameters
 f1=    0.000000,    0.000000,    0.000000:f2=    1.000000,    0.000000,    0.000000:jij=  0.00300000!:sh=  1!:t1=  1:t2=  1
 f1=    0.000000,    0.000000,    0.000000:f2=    0.000000,    1.000000,    0.000000:jij=  0.00300000!:sh=  1!:t1=  1:t2=  1
 f1=    0.000000,    0.000000,    0.000000:f2=    0.000000,    0.000000,    1.000000:jij=  0.00300000!:sh=  1!:t1=  1:t2=  1
 f1=    0.000000,    0.000000,    0.000000:f2=    0.000000,    0.000000,   -1.000000:jij=  0.00300000!:sh=  1!:t1=  1:t2=  1
 f1=    0.000000,    0.000000,    0.000000:f2=    0.000000,   -1.000000,    0.000000:jij=  0.00300000!:sh=  1!:t1=  1:t2=  1
 f1=    0.000000,    0.000000,    0.000000:f2=   -1.000000,    0.000000,    0.000000:jij=  0.00300000!:sh=  1!:t1=  1:t2=  1
End Jij_parameters
```

main input file `name.mcin`

Monte Carlo parameters:

```
tem_start           =   5
tem_end             =   5
tems_num            =   1
!! tems_mode           = man
!! tems               = 5.00 10.00 15.00 20.00

!! Pt                 = .True.
!! Pt_steps_swap      = 10

steps_warmup      =       100000
steps_mc          =       200000
steps_measure     =            2

initial_sconfig   =        ferro
mcarlo_mode       =       random

supercell_size    =      4     4     4
```

main input file `name.mcin`

Monte Carlo parameters, temperature setting:

```
tem_start              =   25
tem_end                =   75
tems_num               =   20
!! tems_mode              = man
!! tems                   = 5.00 10.00 15.00 20.00
```

$N = 20, T_0 = 25K, \quad T_N = 75K, \quad \Delta T = (T_N - T_0)/(N-1)$

List of temperatures:

```
25.0000
27.6316
30.2632
32.8947
35.5263
38.1579
40.7895
43.4211
46.0526
48.6842
51.3158
53.9474
56.5789
59.2105
61.8421
64.4737
67.1053
69.7368
72.3684
75.0000
```

main input file `name.mcin`

Setting the temperature manually:

```
!tem_start           =   25
!tem_end             =   75
tems_num           = 4
tems_mode          = man
tems               = 5.00 10.00 15.00 20.00
```

main input file `name.mcin`

Parallel tempering setting:

```
Pt                    = .True.
Pt_steps_swap         = 10
```

If `Pt= .True.`,
swapping the replicas occur after every `pt_steps_swap` Monte-Carlo steps.

main input file `name.mcin`

Monte Carlo parameters:

```
steps_warmup        =        100000
steps_mc            =        200000
steps_measure       =             2
```

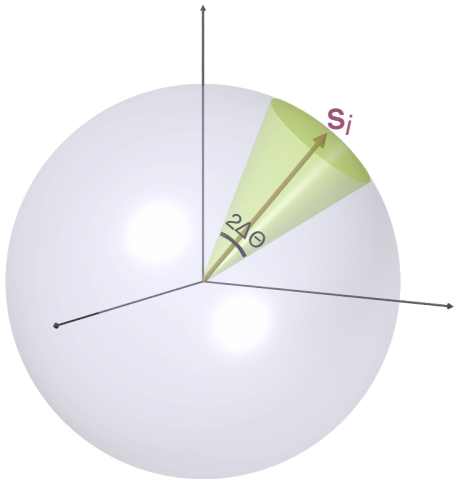
- `steps_warmup`: number of steps for warm-up
- `steps_mc`: number of steps for sampling
- `steps_measure`: number of steps between successive sampling
- Total number of MC steps is
  `steps_measure` × (`steps_warmup` + `steps_mc`)

main input file `name.mcin`

Monte Carlo parameters:

```
initial_sconfig    =         ferro
mcarlo_mode        =        random
```

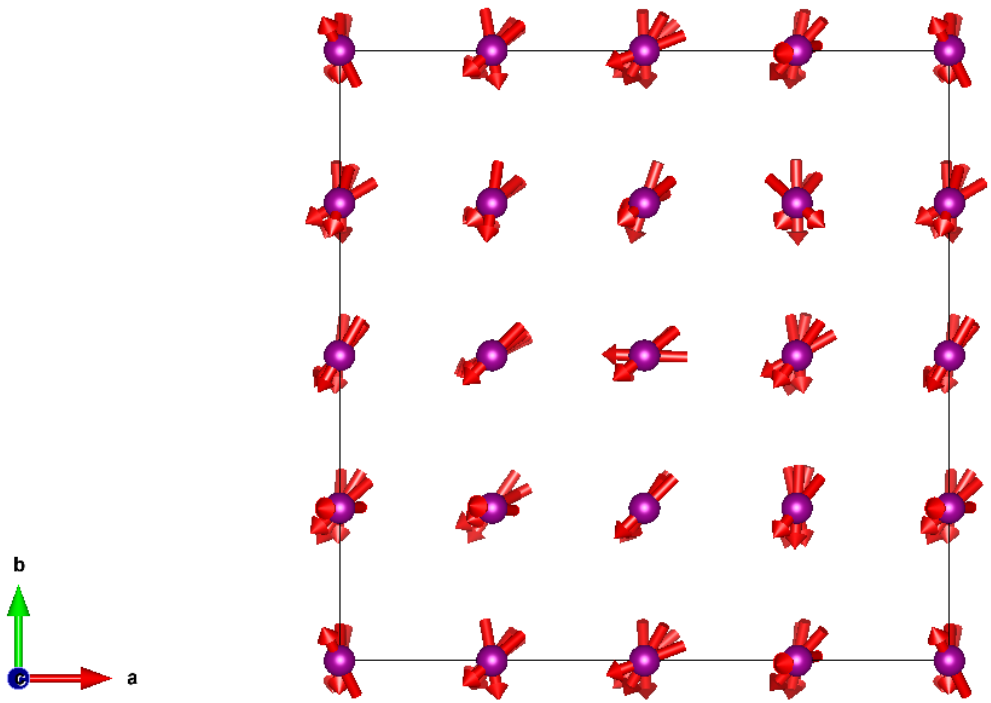
- `initial_sconfig`:
  - `ferro`
  - `rand`
  - `file`: Spin configuration is read from `name_sconfig.dat` file.
- `mcarlo_mode`:
  - `rand` or `random` (default)
  - `const` or `constraint`:
    The new direction of spin is chosen randomly inside a cone. The cone axis is the previous direction of the spin and the apex angle of cone ($2\Delta\Theta$) can be specified by `tilt_angles_max` keyword.



main input file `name.mcin`

Monte Carlo parameters: supercell

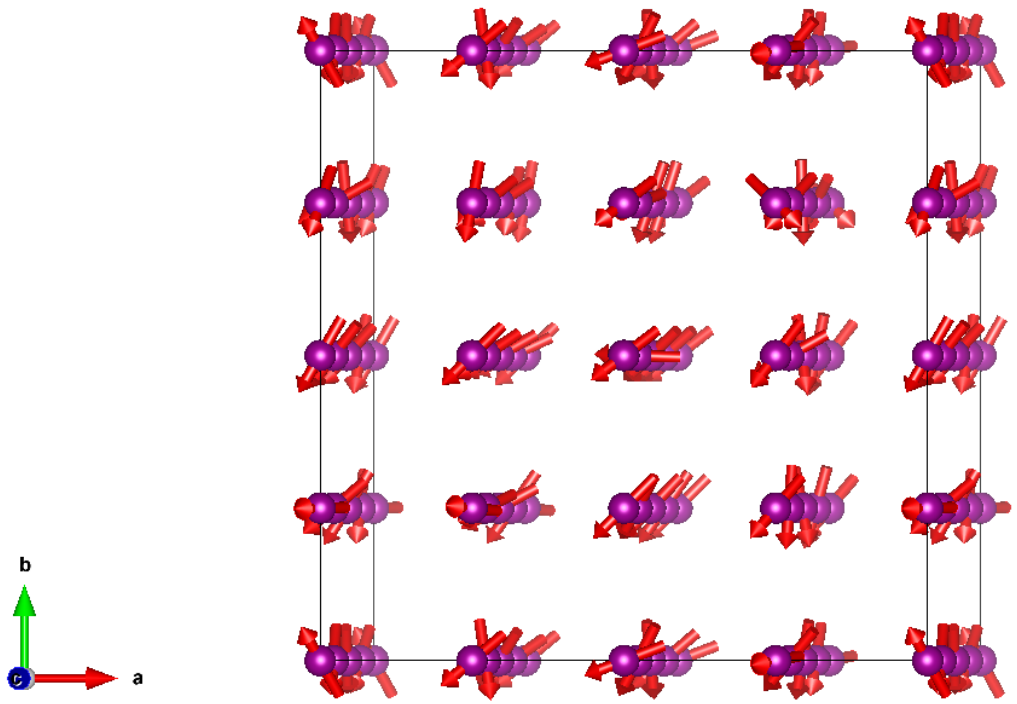
```
supercell_size     =        4       4       4
```



main input file `name.mcin`

Monte Carlo parameters: supercell

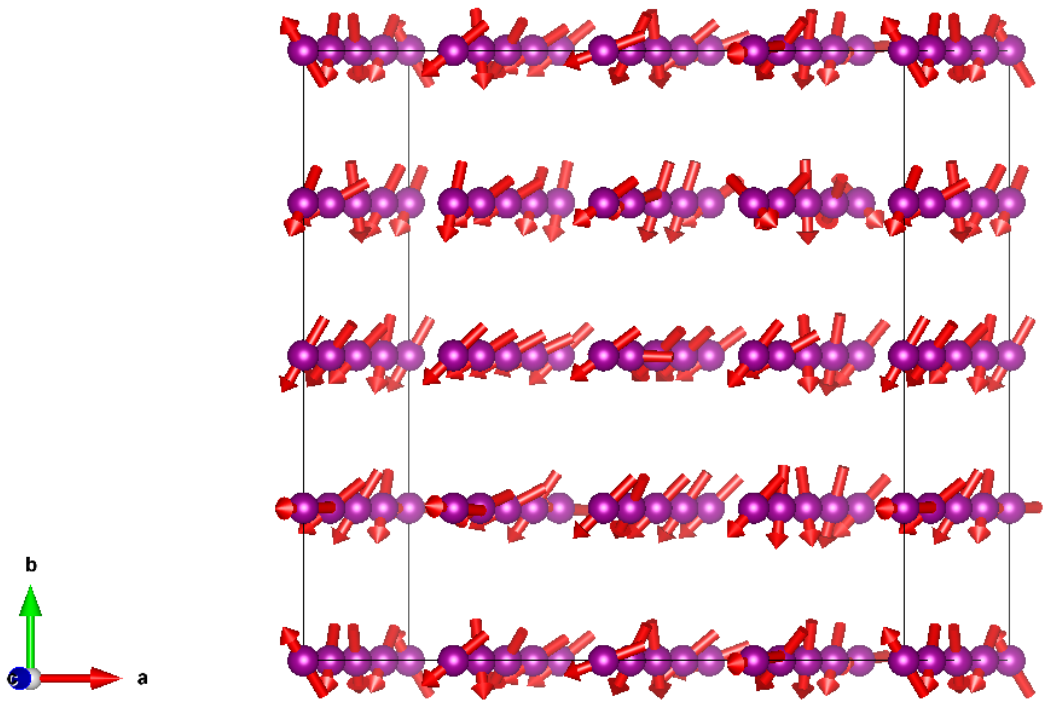
```
supercell_size     =        4       4       4
```



main input file `name.mcin`

Monte Carlo parameters: supercell

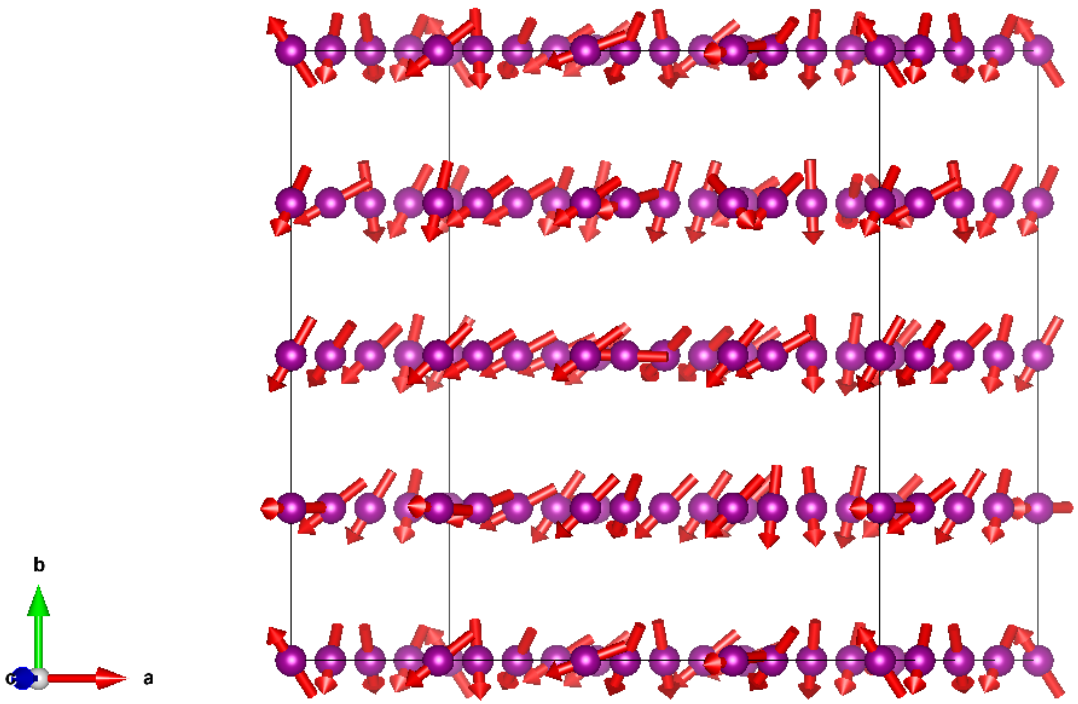
```
supercell_size     =        4       4       4
```



main input file `name.mcin`

Monte Carlo parameters: supercell

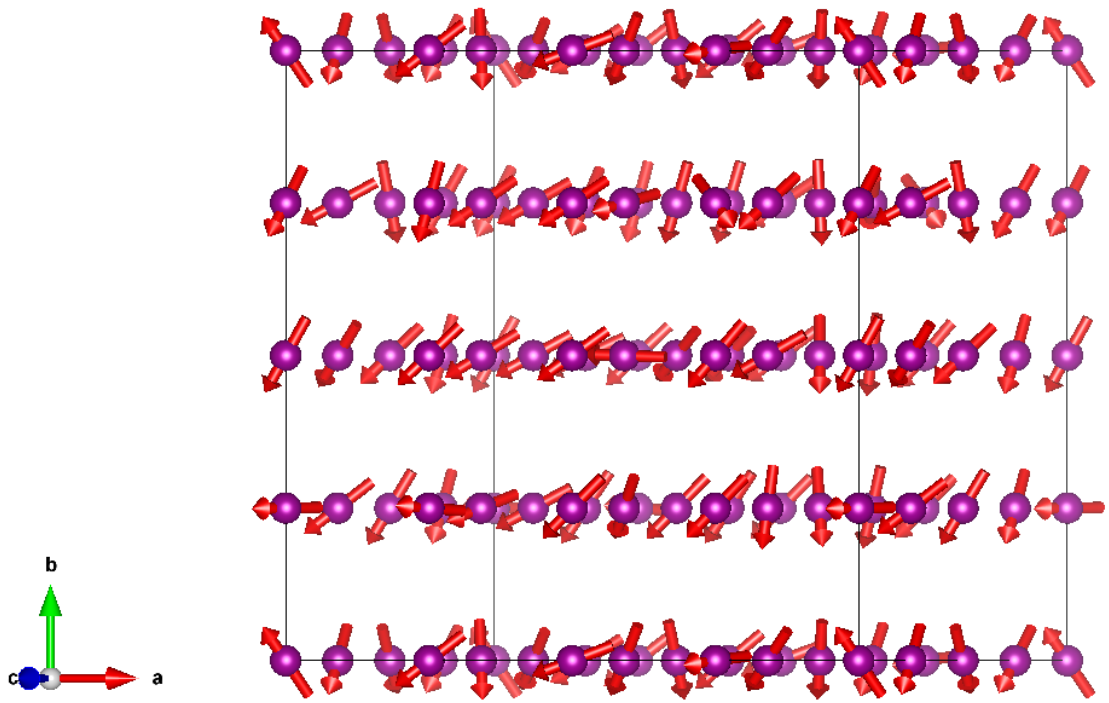
```
supercell_size     =       4       4       4
```



main input file `name.mcin`

Monte Carlo parameters: supercell

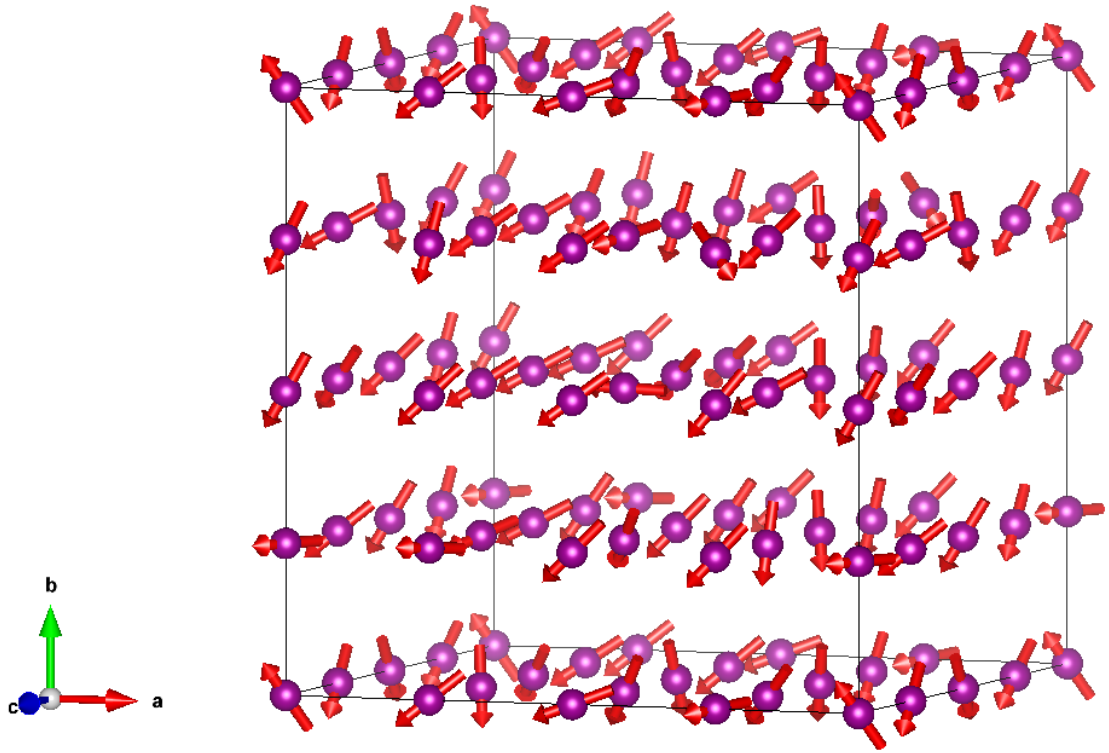
```
supercell_size     =        4       4       4
```



main input file `name.mcin`

Monte Carlo parameters: supercell

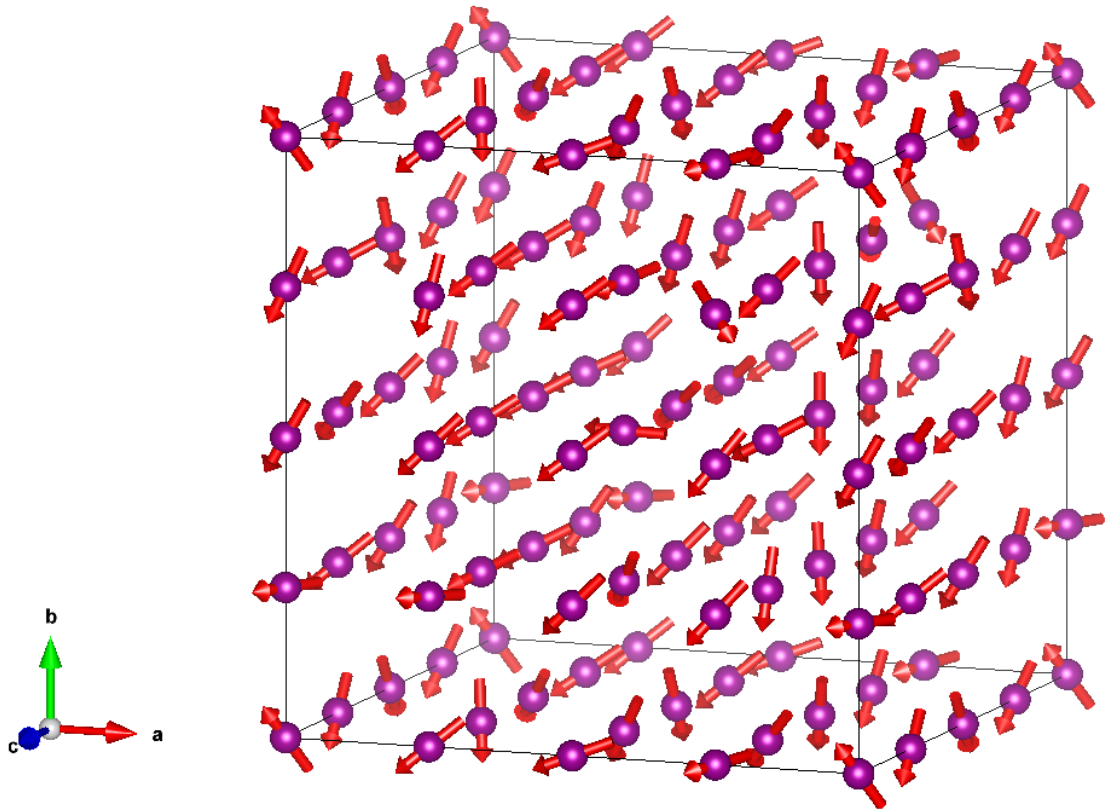
```
supercell_size     =       4       4       4
```



main input file `name.mcin`

Monte Carlo parameters: supercell

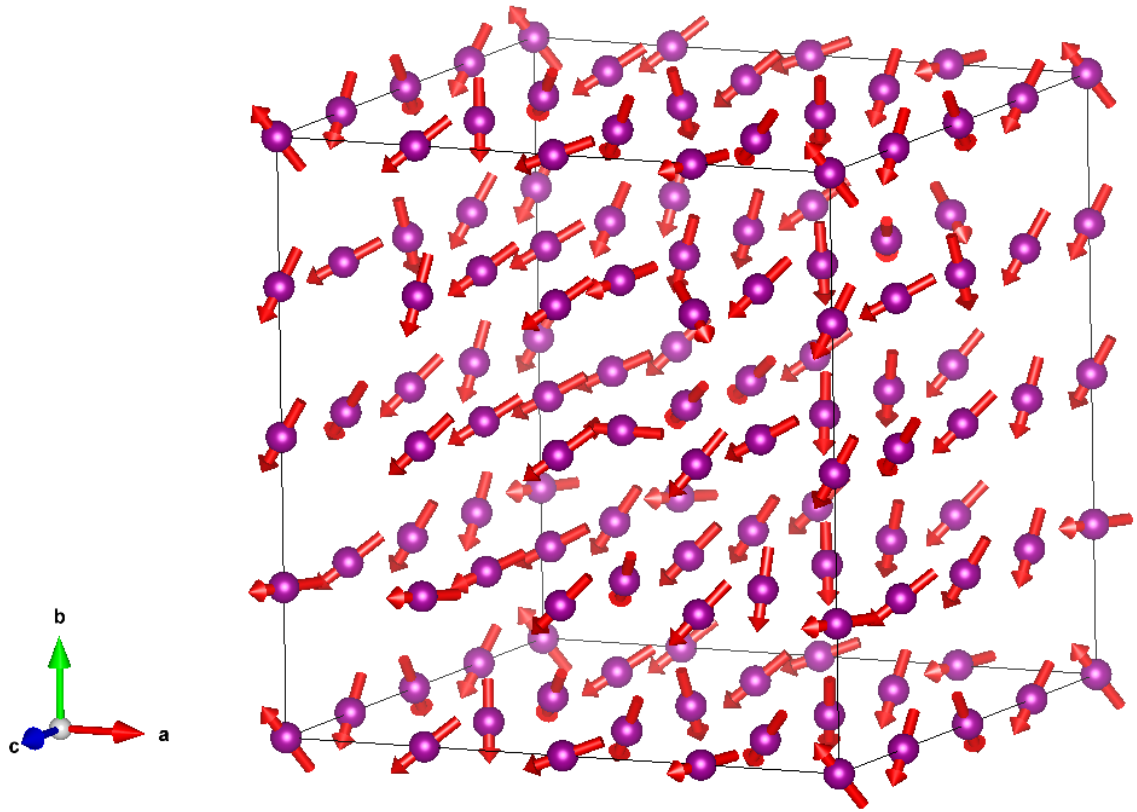
```
supercell_size     =        4       4       4
```



main input file `name.mcin`

Monte Carlo parameters: supercell

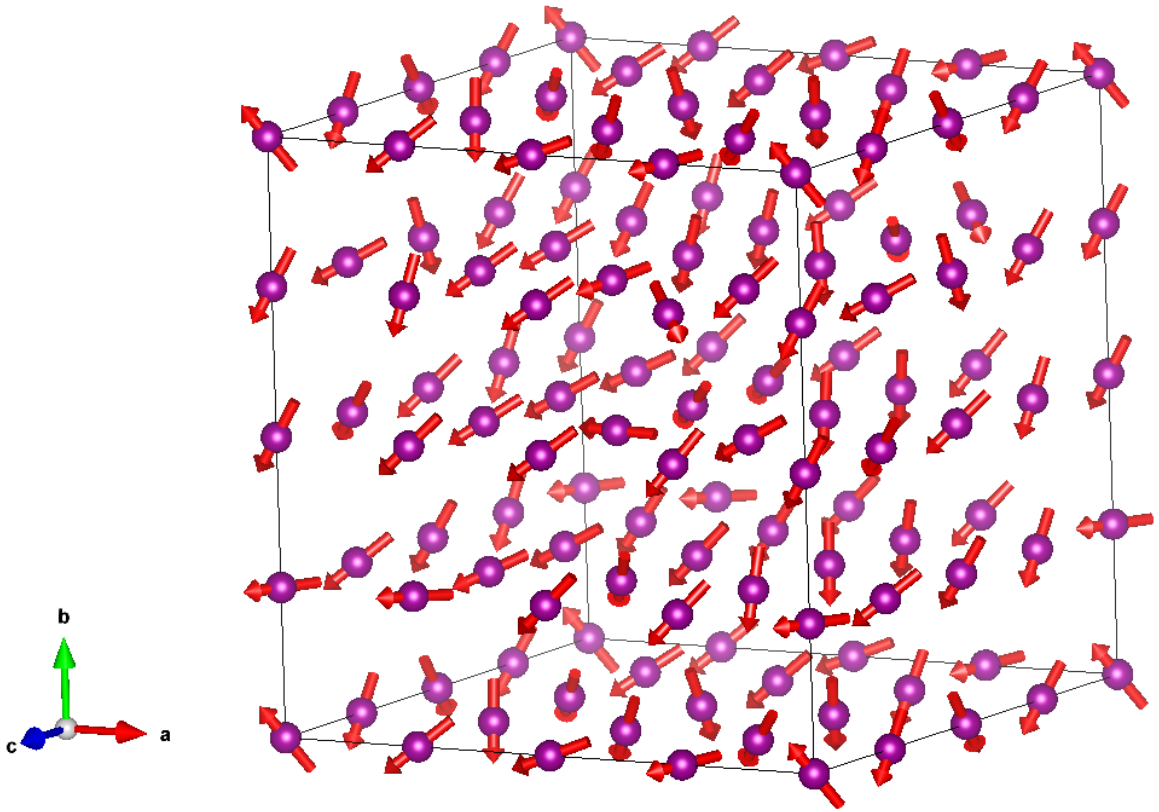
```
supercell_size     =        4       4       4
```



main input file `name.mcin`

Monte Carlo parameters: supercell

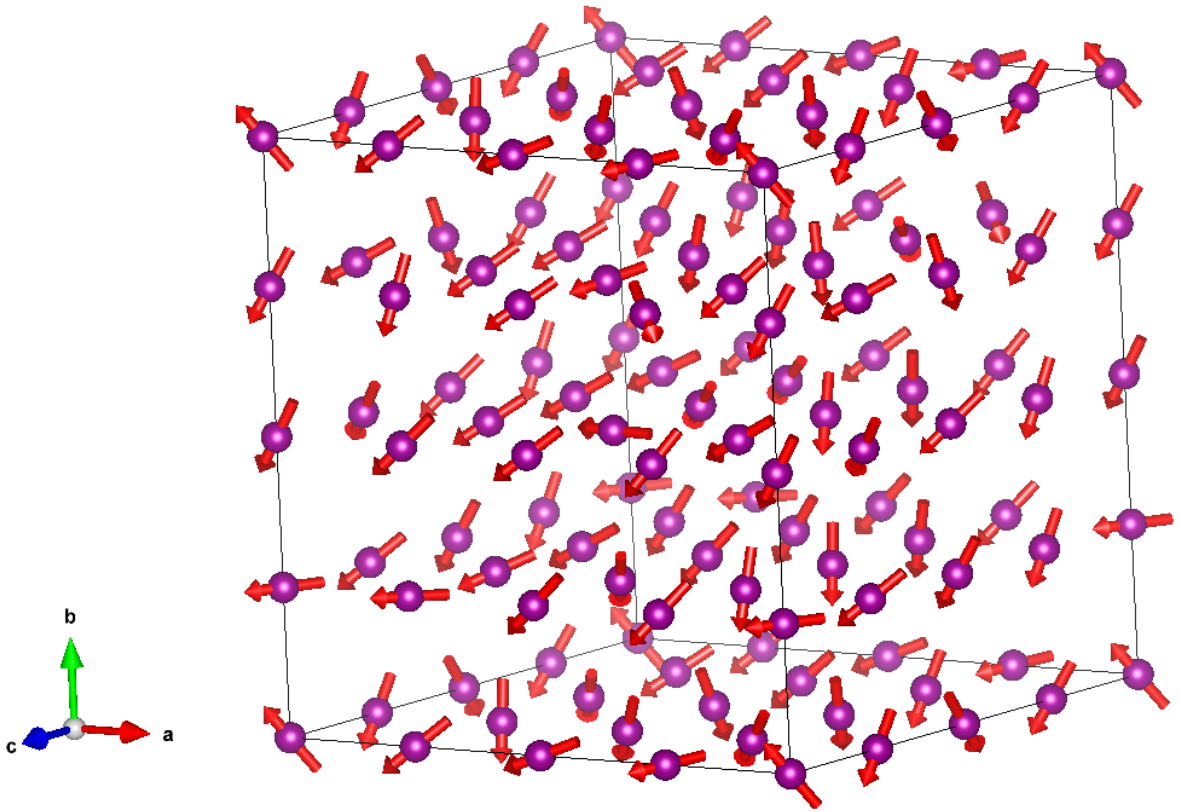
```
supercell_size     =        4       4       4
```



main input file `name.mcin`

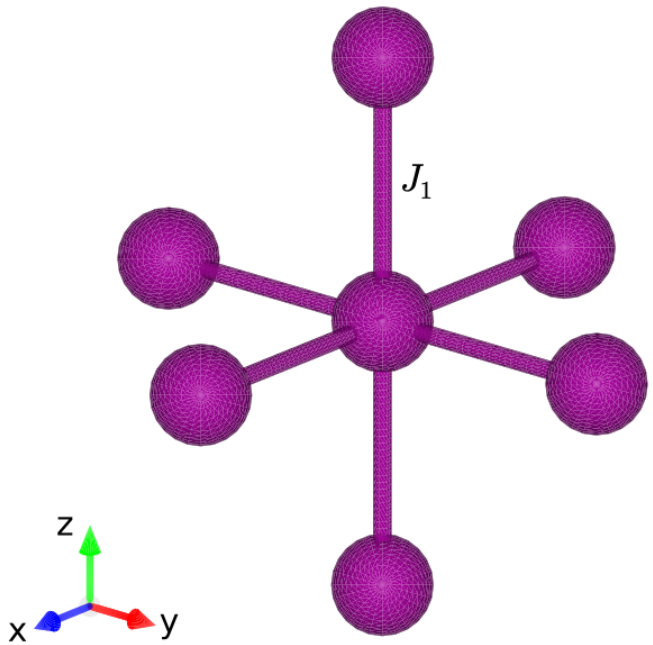
Monte Carlo parameters: supercell

```
supercell_size     =        4       4       4
```



main input file `name.mcin`

```
Begin Jij_parameters
 f1=   0.000000,   0.000000,   0.000000:f2=   1.000000,   0.000000,   0.000000:jij=  0.00300000
 f1=   0.000000,   0.000000,   0.000000:f2=   0.000000,   1.000000,   0.000000:jij=  0.00300000
 f1=   0.000000,   0.000000,   0.000000:f2=   0.000000,   0.000000,   1.000000:jij=  0.00300000
 f1=   0.000000,   0.000000,   0.000000:f2=   0.000000,   0.000000,  -1.000000:jij=  0.00300000
 f1=   0.000000,   0.000000,   0.000000:f2=   0.000000,  -1.000000,   0.000000:jij=  0.00300000
 f1=   0.000000,   0.000000,   0.000000:f2=  -1.000000,   0.000000,   0.000000:jij=  0.00300000
End Jij_parameters
```



Run MC simulation

Parallel:

```
mpiexec -np 4 mc.x cubic
```

Serial:

```
mc.x cubic
```

Output:

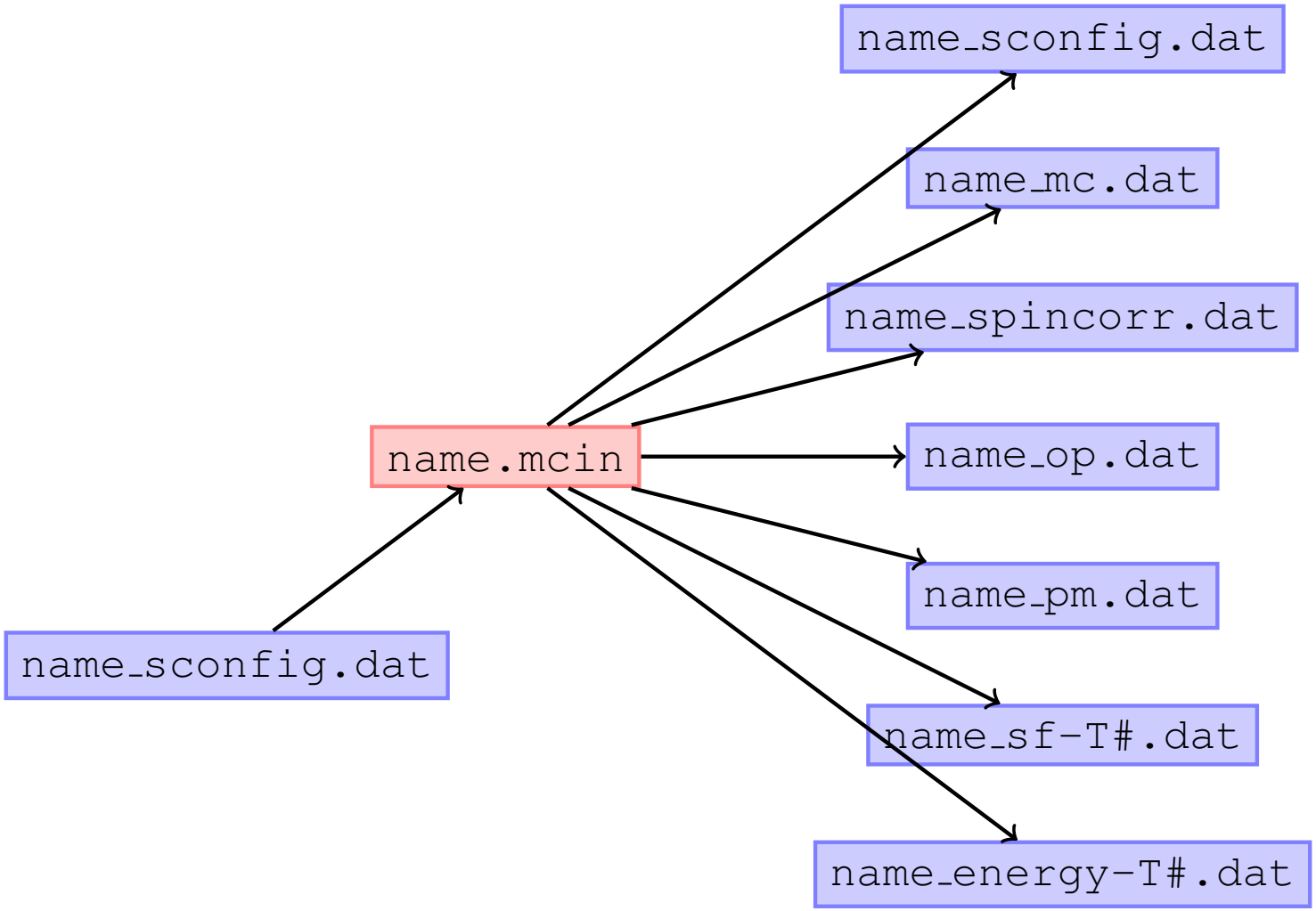
```
cubic_mc.dat   cubic.mcout   cubic_pm.dat   cubic_sconfig.dat
```

name_mc.dat

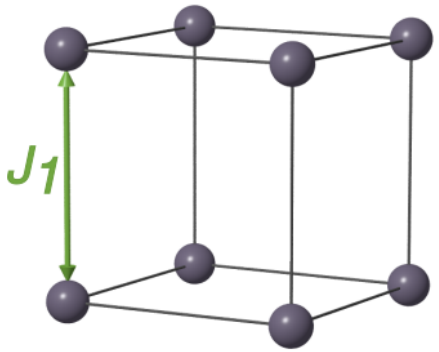
```
#written on  1Dec2019 at 16:53:37
#------------------------------------------------ MONTECARLO -------------------------------------------------#
# Temp      Magnetization     Energy_ave          C_M               Sus               U_E               U_M       #
#-------------------------------------------------------------------------------------------------------------#
 25.0000   0.83550519E+00  -0.77911542E+02   0.11757710E+01   0.16684575E-02   0.66418132E+00   0.66544024E+00
 27.6316   0.81393559E+00  -0.74764204E+02   0.12126343E+01   0.20123090E-02   0.66327460E+00   0.66495005E+00
 30.2632   0.79058810E+00  -0.71440867E+02   0.12718923E+01   0.24192441E-02   0.66201498E+00   0.66428286E+00
 32.8947   0.76625592E+00  -0.68084127E+02   0.13335515E+01   0.29341298E-02   0.66034539E+00   0.66334182E+00
 35.5263   0.73942613E+00  -0.64521905E+02   0.14043495E+01   0.35938322E-02   0.65808589E+00   0.66198791E+00
 38.1579   0.70985858E+00  -0.60734904E+02   0.14676085E+01   0.44110459E-02   0.65508426E+00   0.66007139E+00
 40.7895   0.67678794E+00  -0.56742752E+02   0.15649544E+01   0.55834312E-02   0.65065686E+00   0.65703480E+00
 43.4211   0.64038864E+00  -0.52588368E+02   0.16389253E+01   0.71311003E-02   0.64484445E+00   0.65248126E+00
 46.0526   0.59837624E+00  -0.48191253E+02   0.17123289E+01   0.93554612E-02   0.63638172E+00   0.64489868E+00
 48.6842   0.55166880E+00  -0.43668941E+02   0.17216844E+01   0.11913054E-01   0.62544914E+00   0.63360306E+00
 51.3158   0.50029902E+00  -0.39133828E+02   0.16418236E+01   0.14407892E-01   0.61204399E+00   0.61705462E+00
 53.9474   0.45335246E+00  -0.35189936E+02   0.14704517E+01   0.15697680E-01   0.59901097E+00   0.59832671E+00
 56.5789   0.40700519E+00  -0.31561116E+02   0.12375110E+01   0.15757752E-01   0.58724204E+00   0.57704497E+00
 59.2105   0.36899114E+00  -0.28622562E+02   0.10168323E+01   0.14786537E-01   0.57809401E+00   0.55805479E+00
 61.8421   0.33690216E+00  -0.26188301E+02   0.84029002E+00   0.13521563E-01   0.57020988E+00   0.53990337E+00
 64.4737   0.31021013E+00  -0.24172414E+02   0.68930003E+00   0.12182116E-01   0.56560115E+00   0.52439617E+00
 67.1053   0.28936051E+00  -0.22544486E+02   0.57927296E+00   0.10850404E-01   0.56078673E+00   0.51278915E+00
 69.7368   0.27114428E+00  -0.21107750E+02   0.49294400E+00   0.96330006E-02   0.55593184E+00   0.50228022E+00
 72.3684   0.25623871E+00  -0.19886224E+02   0.42248414E+00   0.86722238E-02   0.55209468E+00   0.49345021E+00
 75.0000   0.24452098E+00  -0.18862684E+02   0.36897650E+00   0.77449026E-02   0.54846263E+00   0.48934378E+00
```

name_sconfig.dat

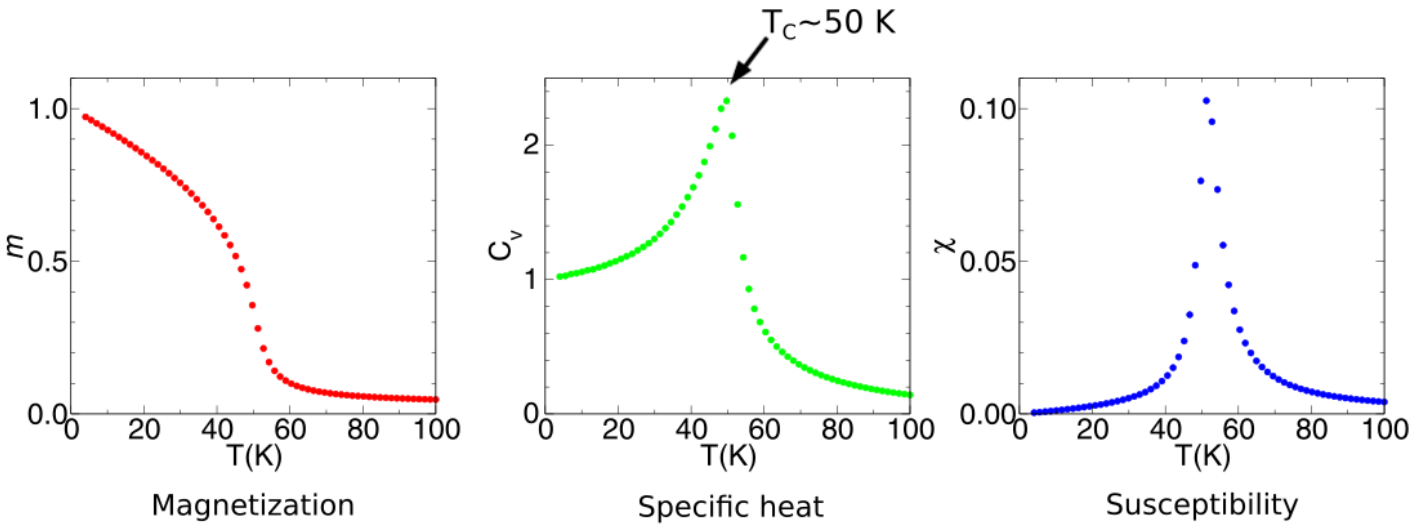
```
Created on 22Nov2021 at 12:46:34
    4     4     4
   64    20
  25.000000
  -0.525217   -0.234175    0.818113
  -0.328709    0.076391    0.941337
  -0.026791   -0.102281    0.994395
   0.104865   -0.160278    0.981486
   0.161734    0.300896    0.939843
  -0.030702   -0.156163    0.987254
  -0.055924    0.068898    0.996055
  -0.848830    0.294029    0.439356
   0.312755   -0.272783    0.909821
  -0.326866   -0.040888    0.944186
   0.143095    0.605099    0.783185
   0.030236   -0.277578    0.960227
  -0.236380   -0.508757    0.827823
  -0.134752   -0.813143    0.566251
  -0.077080    0.029248    0.996596
   0.304981    0.279298    0.910483
   0.222067   -0.370653    0.901833
   0.403009   -0.335567    0.851457
   0.782504    0.562700    0.266563
   0.449205    0.349361    0.822291
   0.801018    0.472643    0.367395
   0.629960   -0.416410    0.655556
   0.261368   -0.327883    0.907843
```


name_sconfig.dat
name_mc.dat
name_spincorr.dat
name.mcin
name_op.dat
name_pm.dat
name_sconfig.dat
name_sf-T#.dat
name_energy-T#.dat

Cubic with ferromagnetic first nearest neighbor interaction

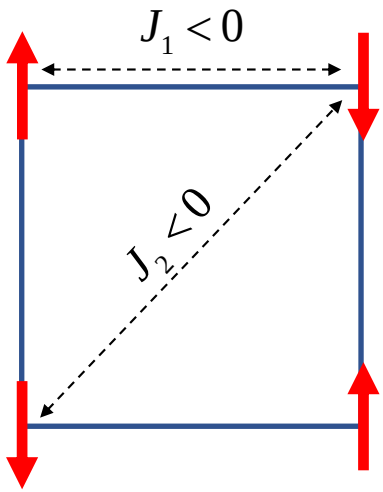


J_1=0.003 eV= 34.8 K

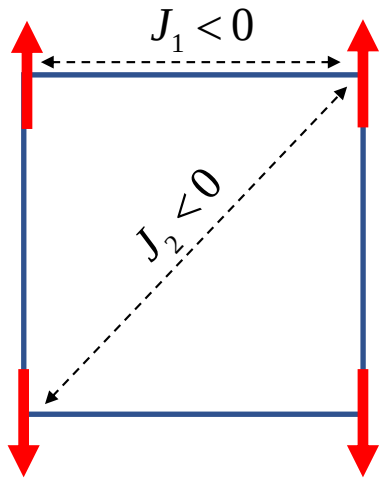


The result is compatibale with $J_1/k_BT_C = 0.6929$
(PRB 43, 6087 (1991))

Antiferromagnetic simple cubic with $J_1 = 0.26J_2$



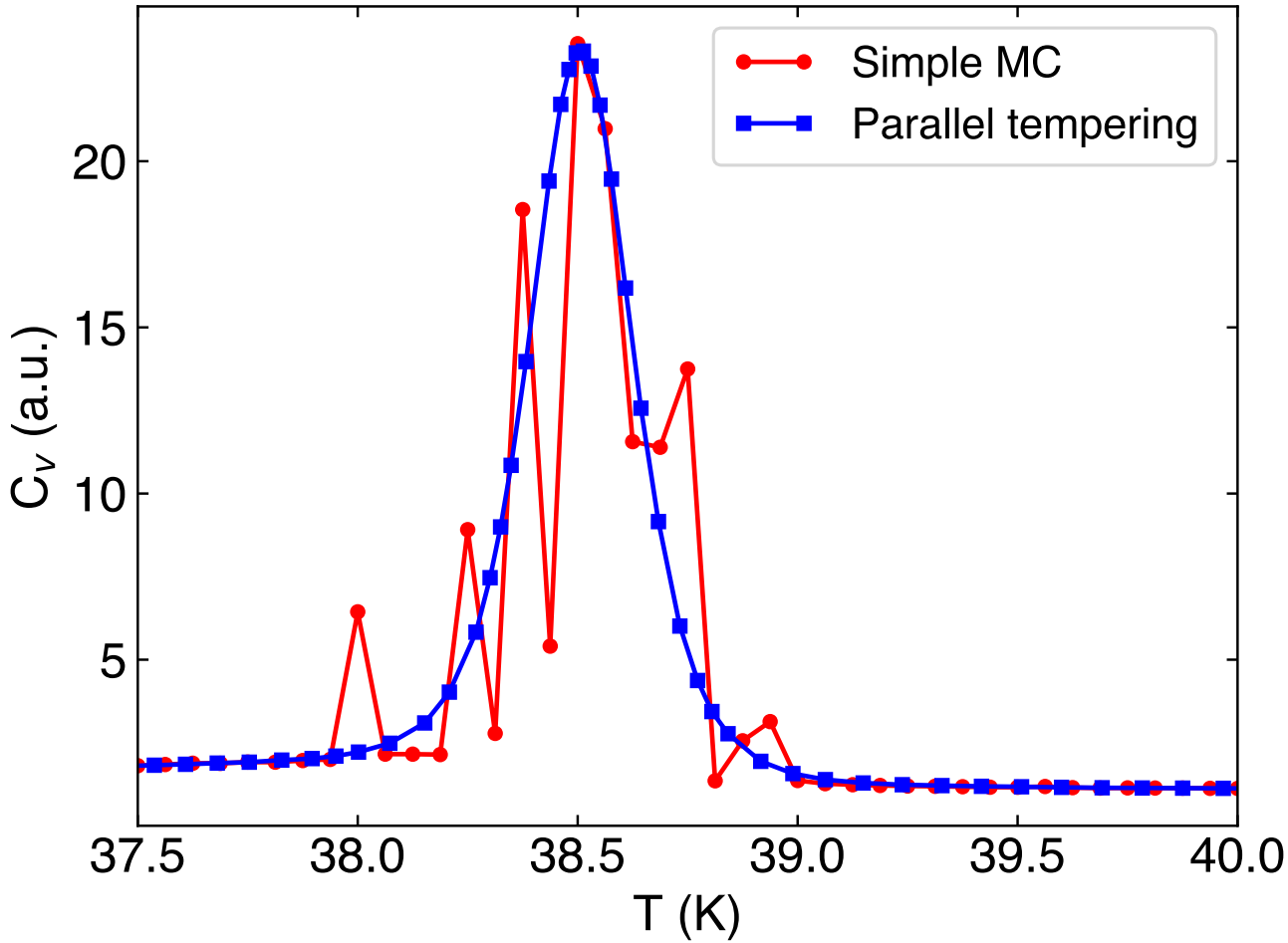
This configuration is preferred by $J_1 < 0$



This configuration is preferred by $J_2 < 0$

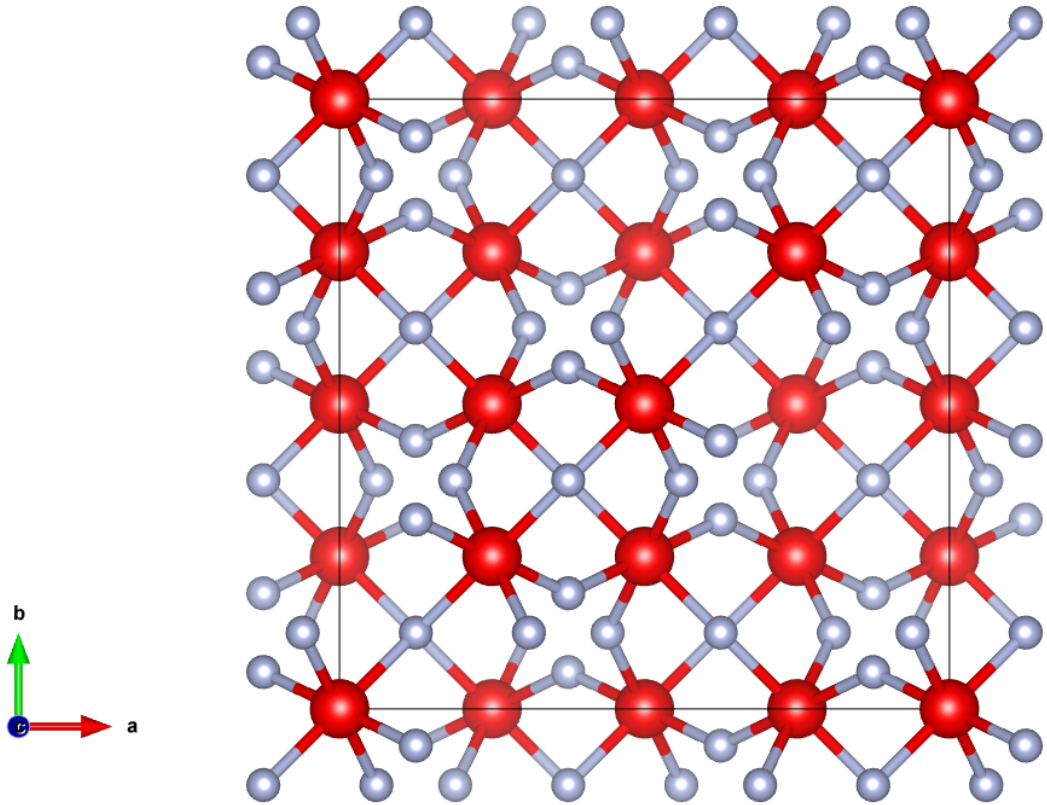
The frustration causes reaching into the equilibrium difficult.

Antiferromagnetic simple cubic with $J_1 = 0.26J_2$

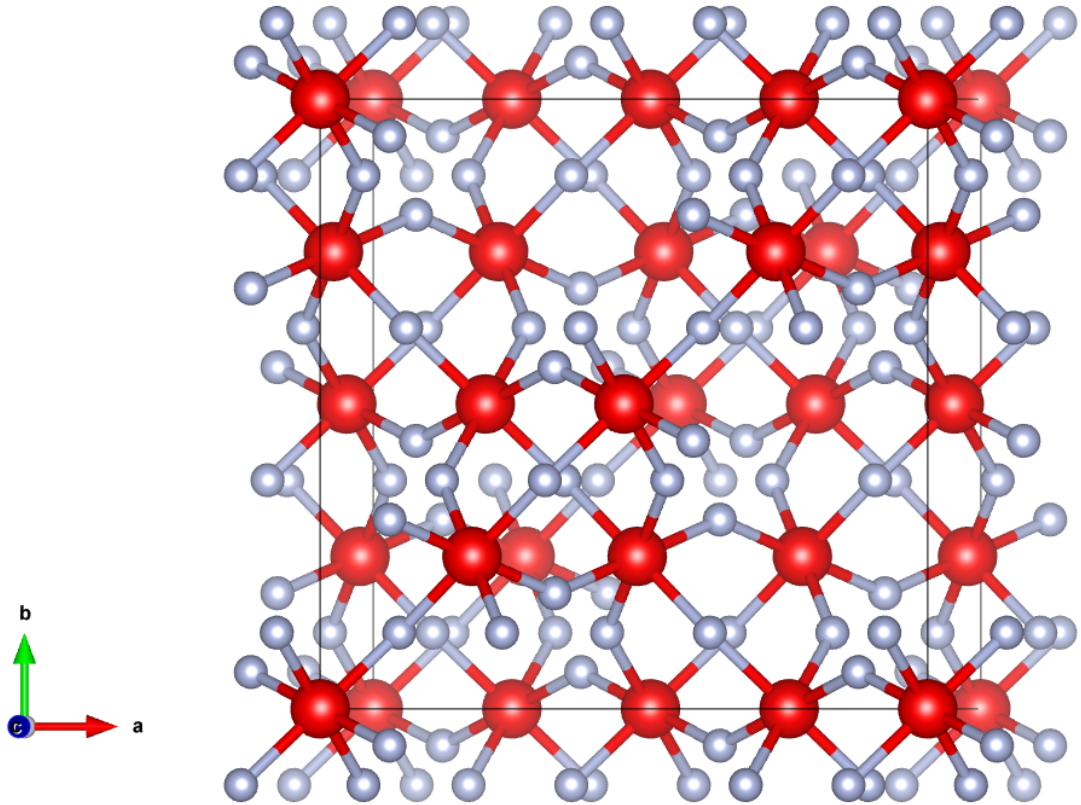


N. Rezaei, M. Alaei, H. Akbarzadeh, Computational Materials Science, 202, 110947 (2022)

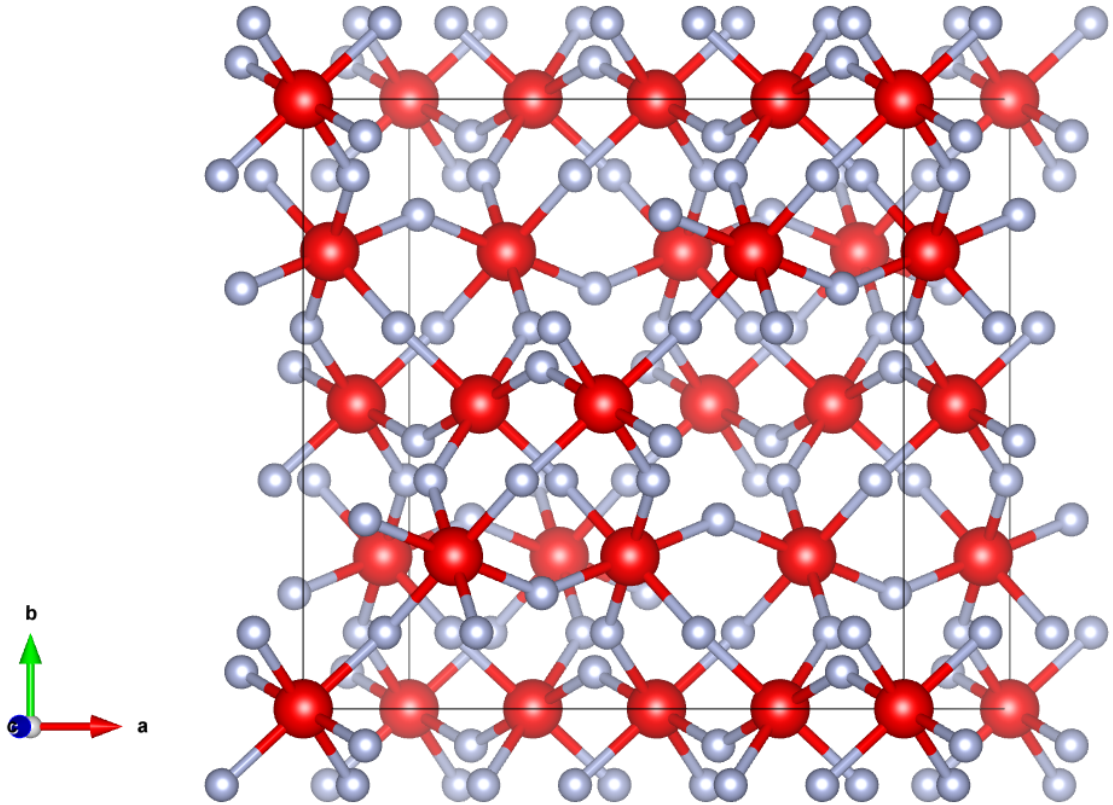
Pyrochlore FeF_3: A geometrical frustrated system



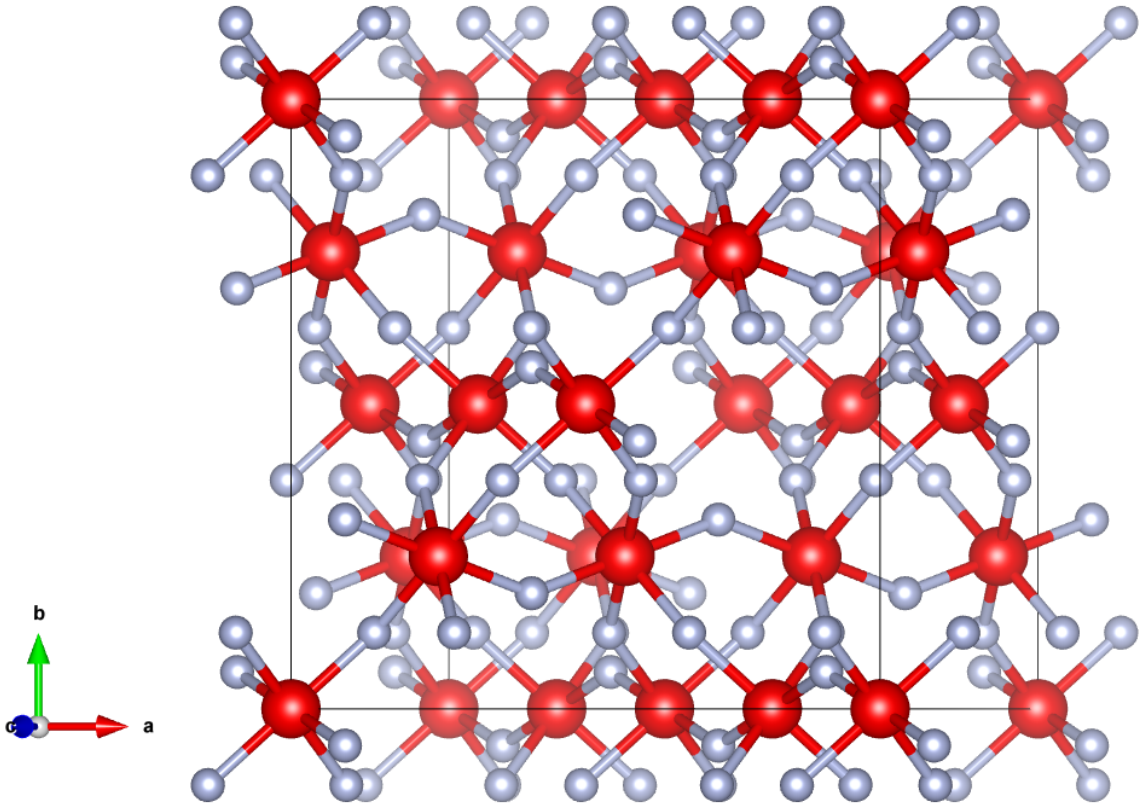
Pyrochlore FeF_3: A geometrical frustrated system



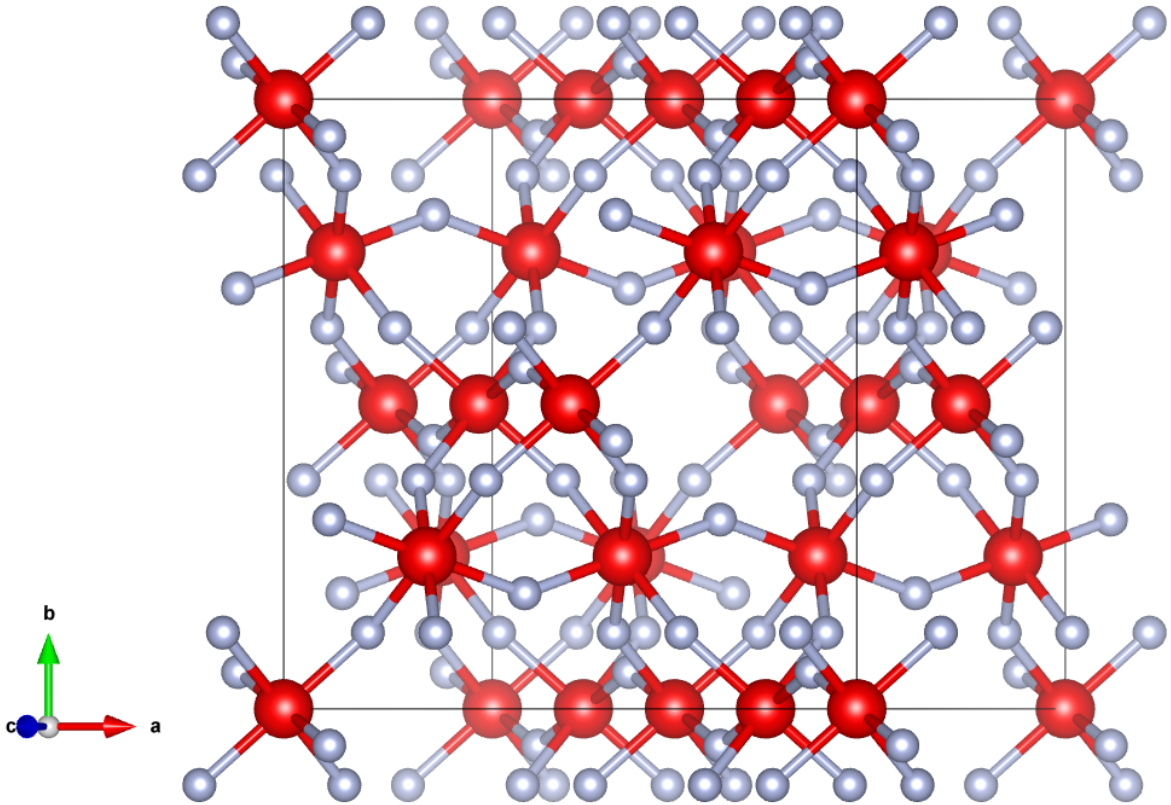
Pyrochlore FeF_3: A geometrical frustrated system



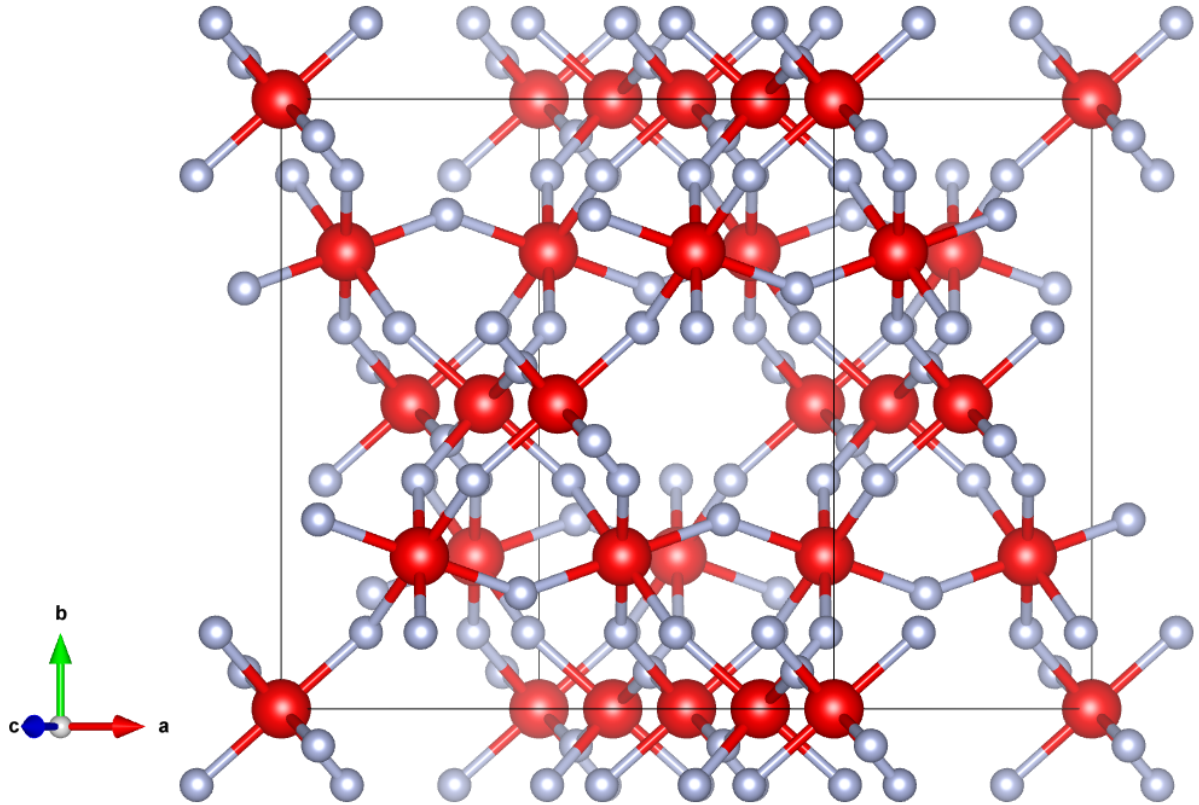
Pyrochlore FeF_3: A geometrical frustrated system



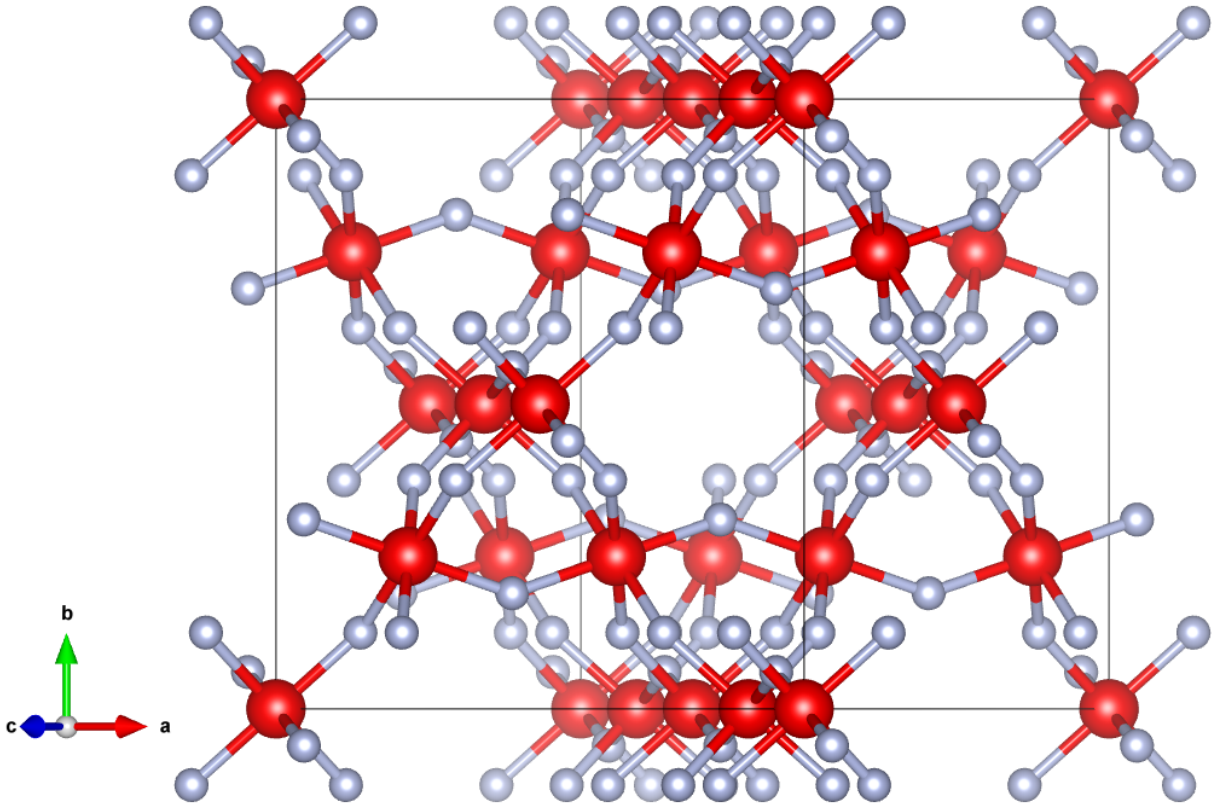
Pyrochlore FeF_3: A geometrical frustrated system



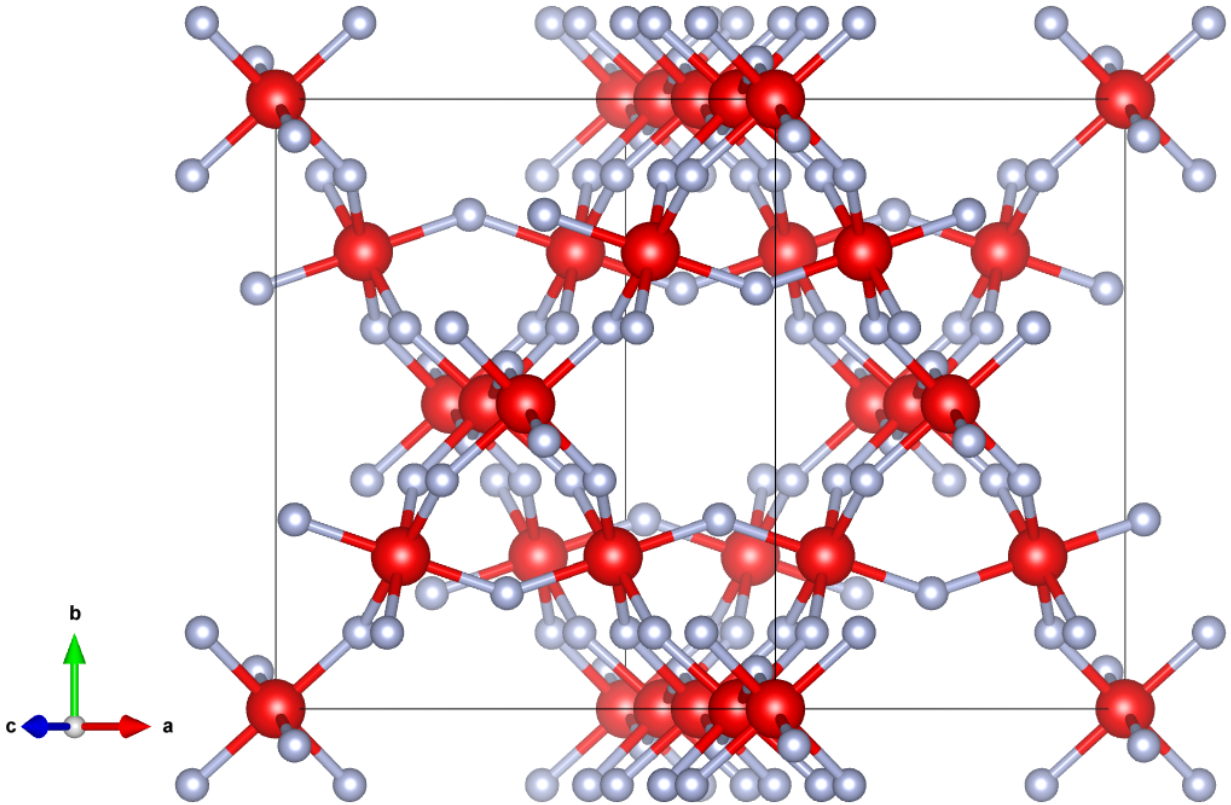
Pyrochlore FeF_3: A geometrical frustrated system



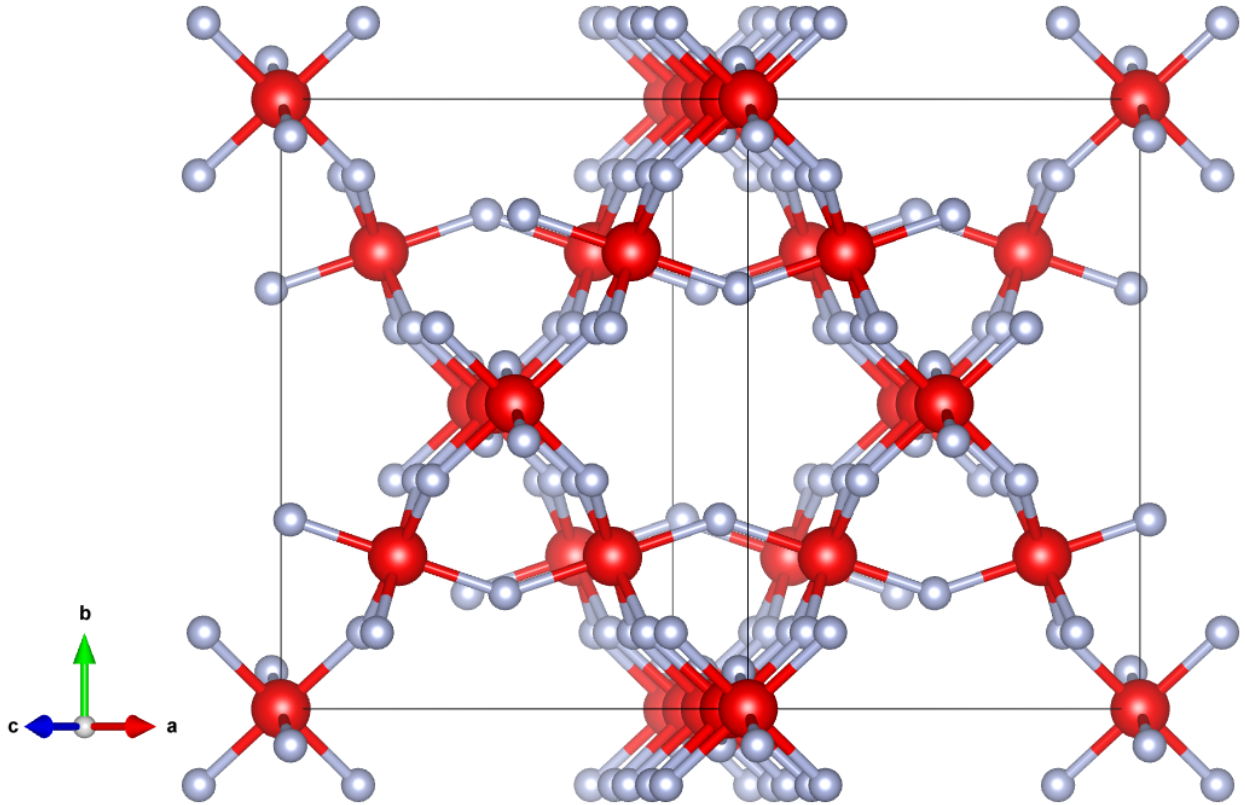
Pyrochlore FeF_3: A geometrical frustrated system



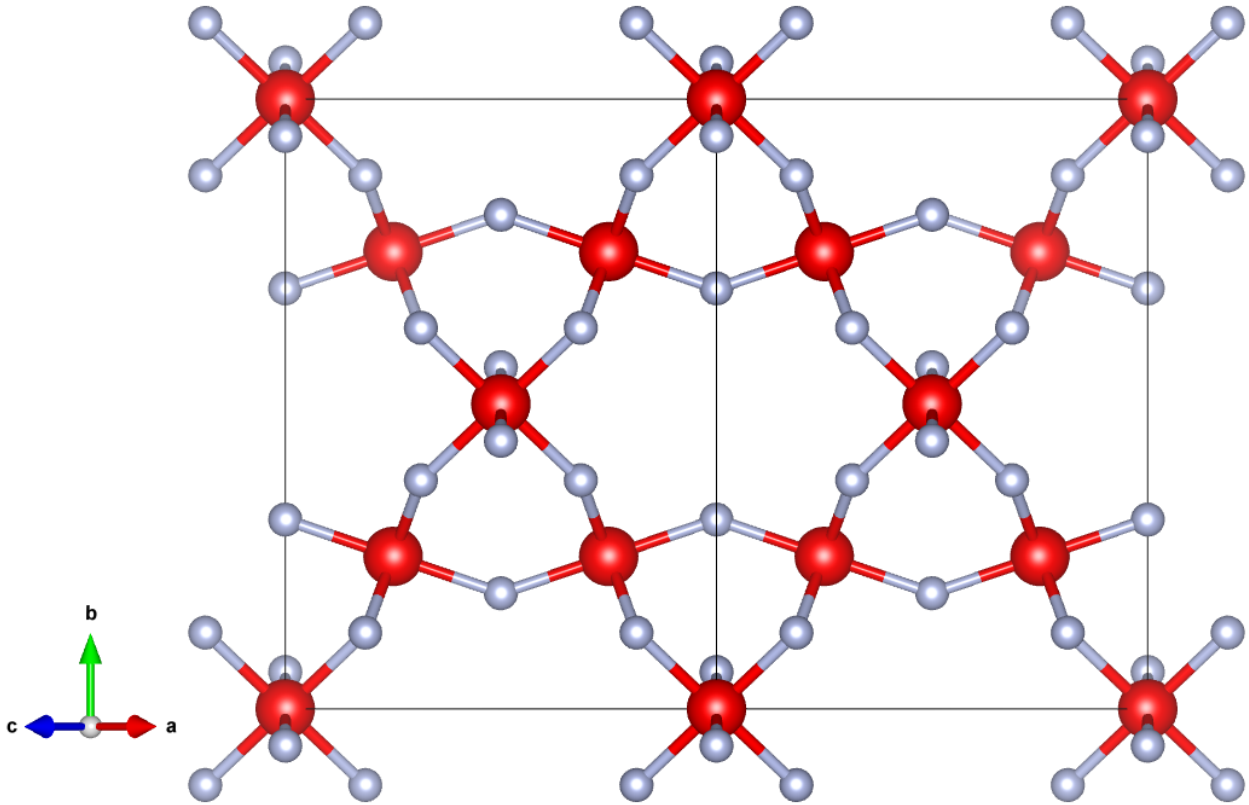
Pyrochlore FeF_3: A geometrical frustrated system



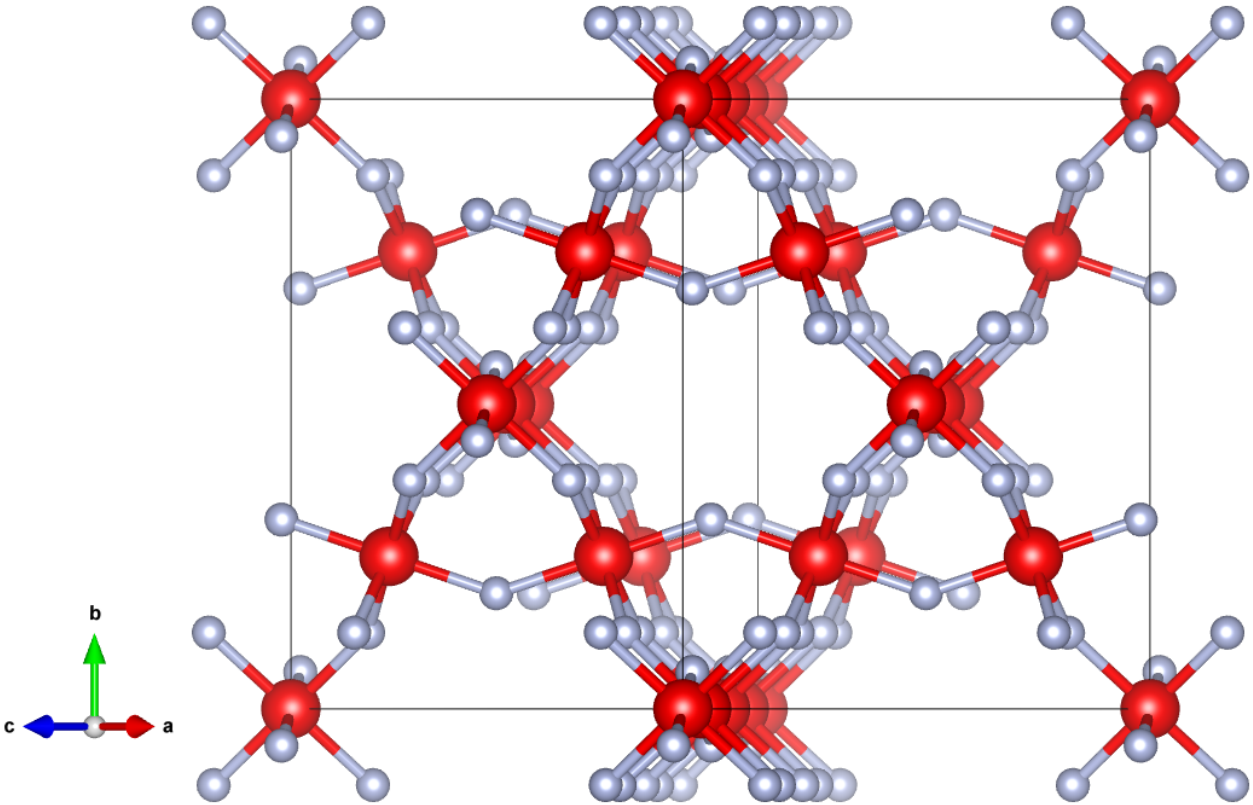
Pyrochlore FeF_3: A geometrical frustrated system



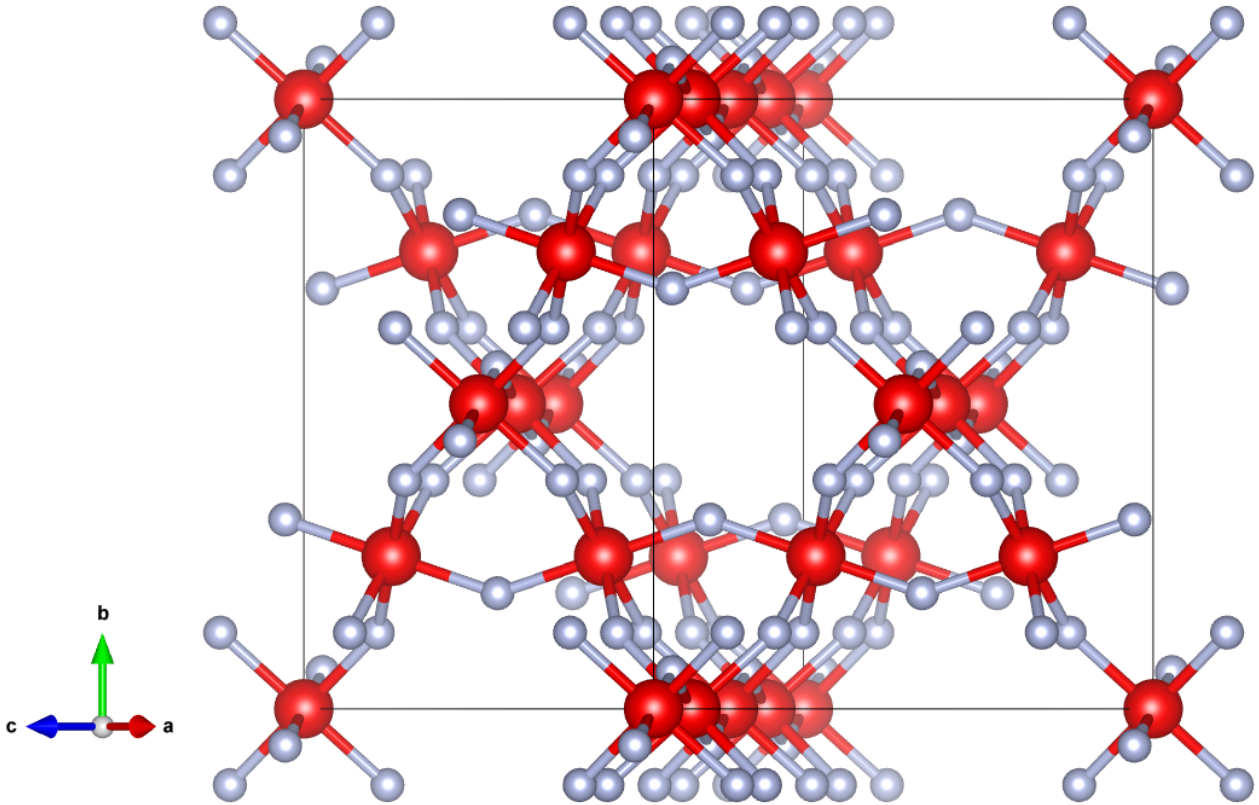
Pyrochlore FeF_3: A geometrical frustrated system



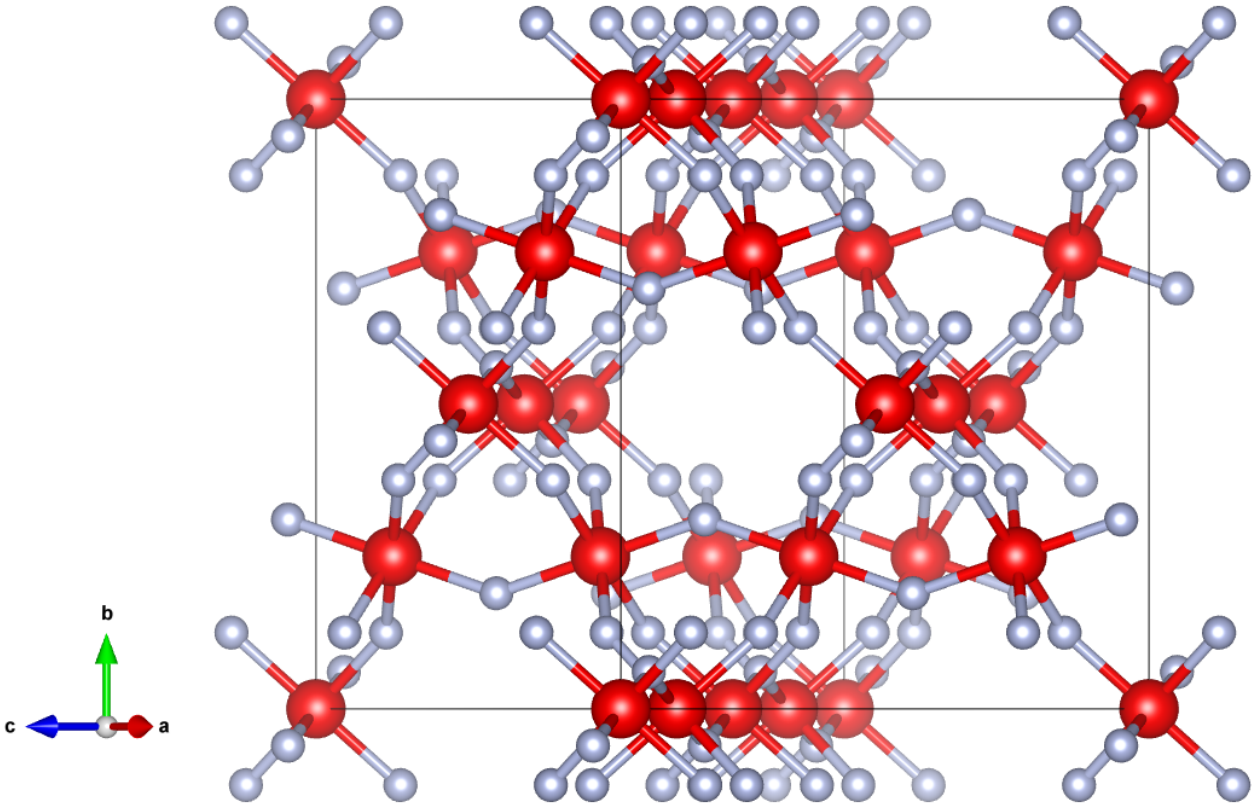
Pyrochlore FeF_3: A geometrical frustrated system



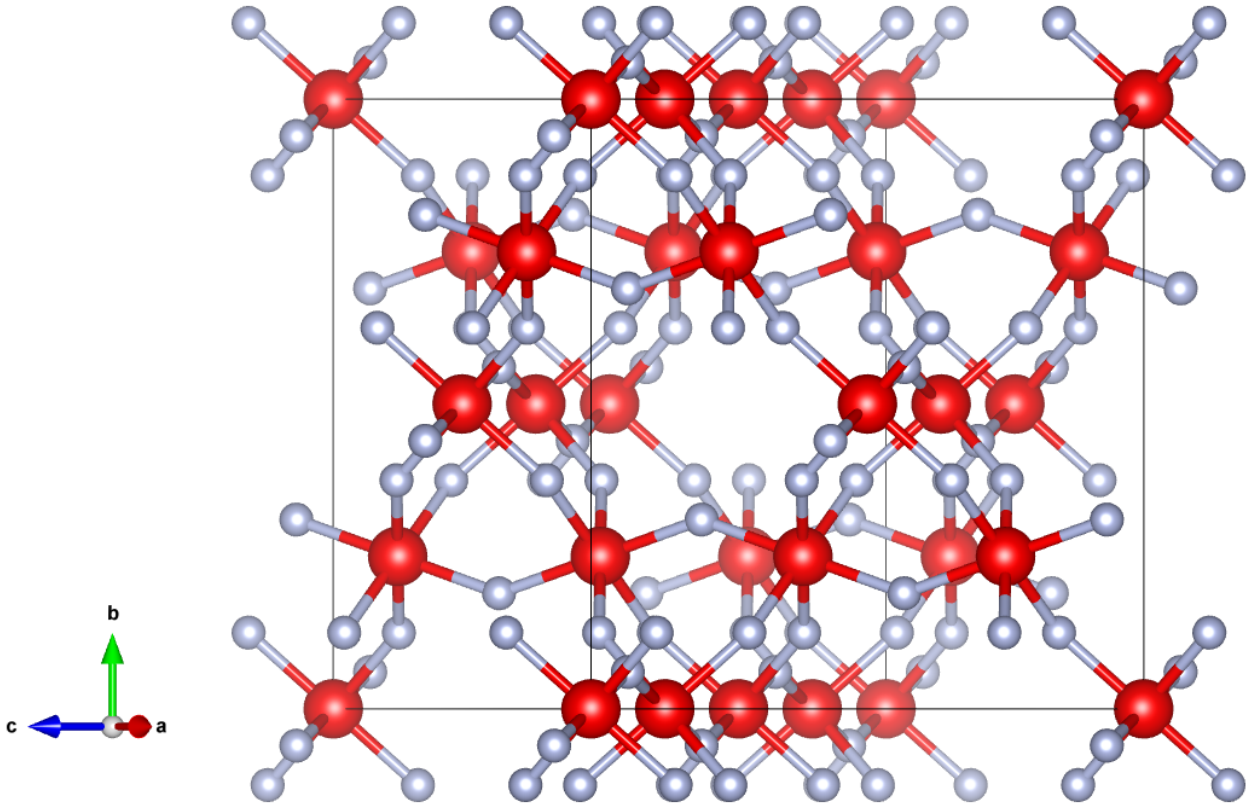
Pyrochlore FeF_3: A geometrical frustrated system



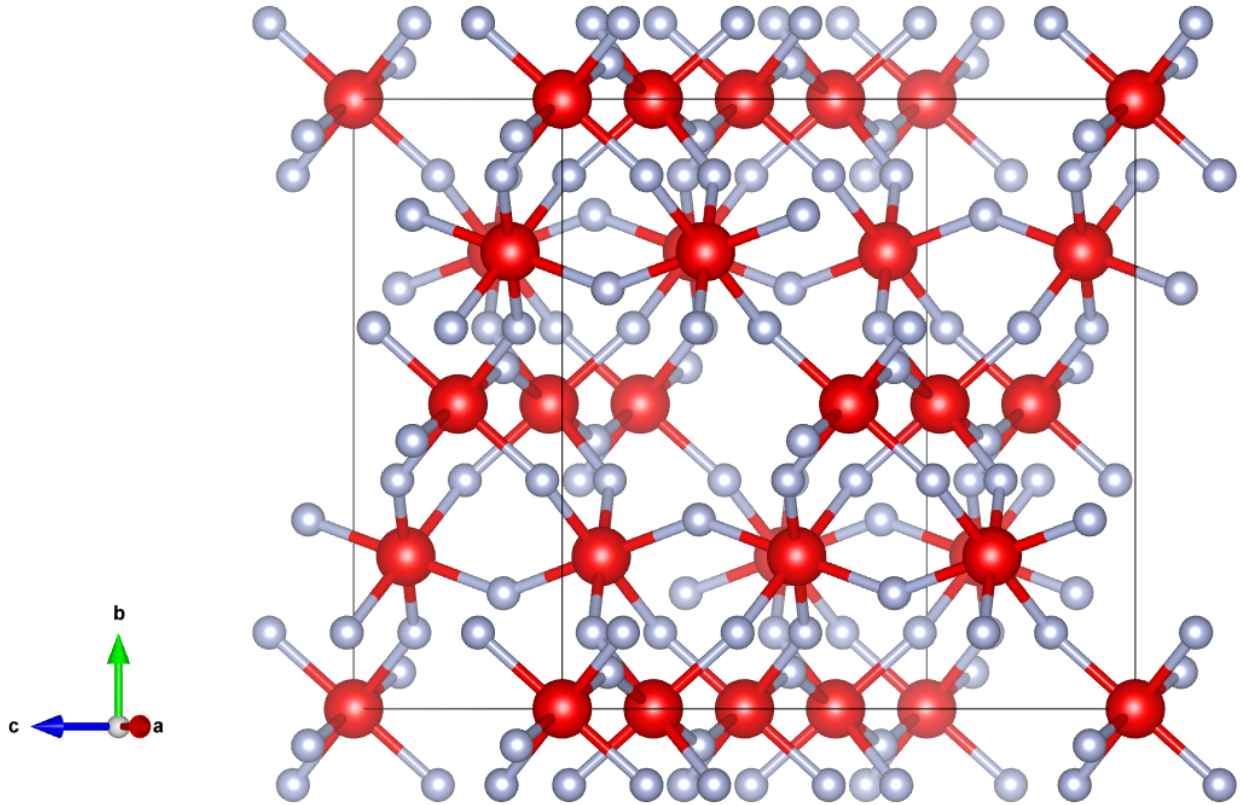
Pyrochlore FeF_3: A geometrical frustrated system



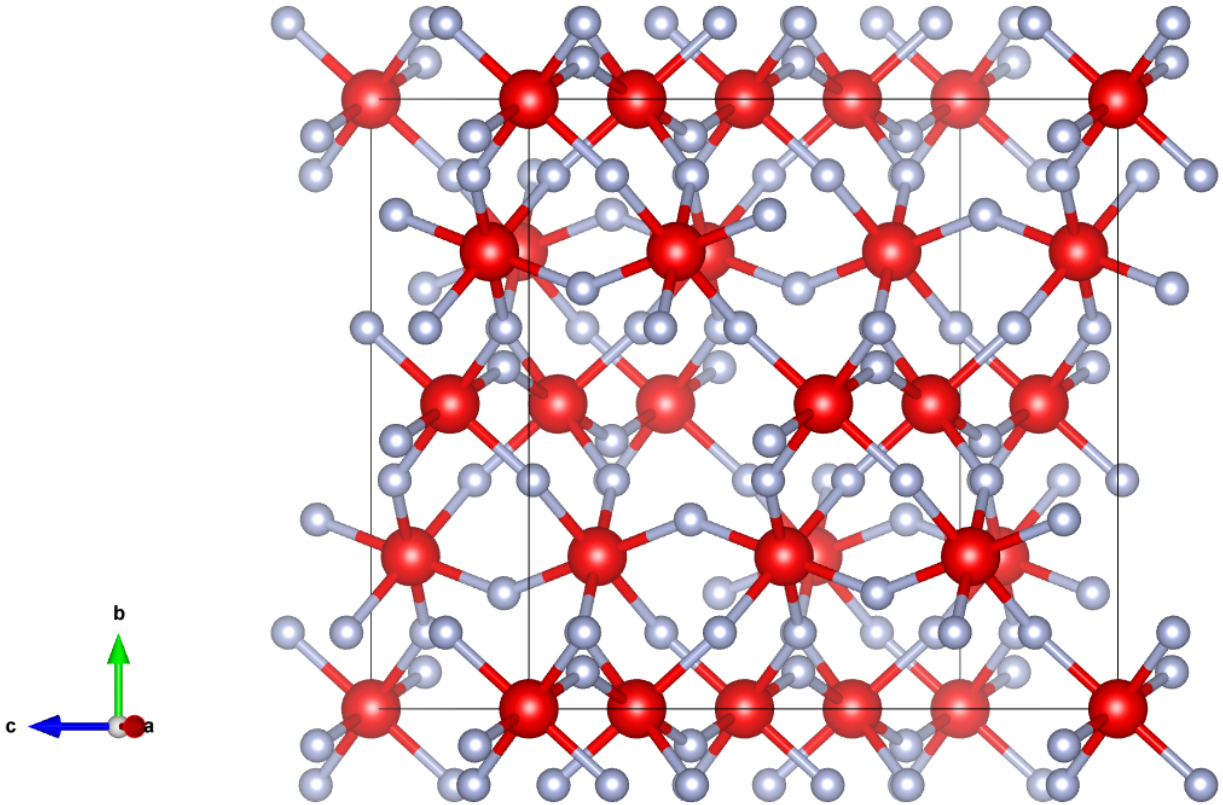
Pyrochlore FeF_3: A geometrical frustrated system



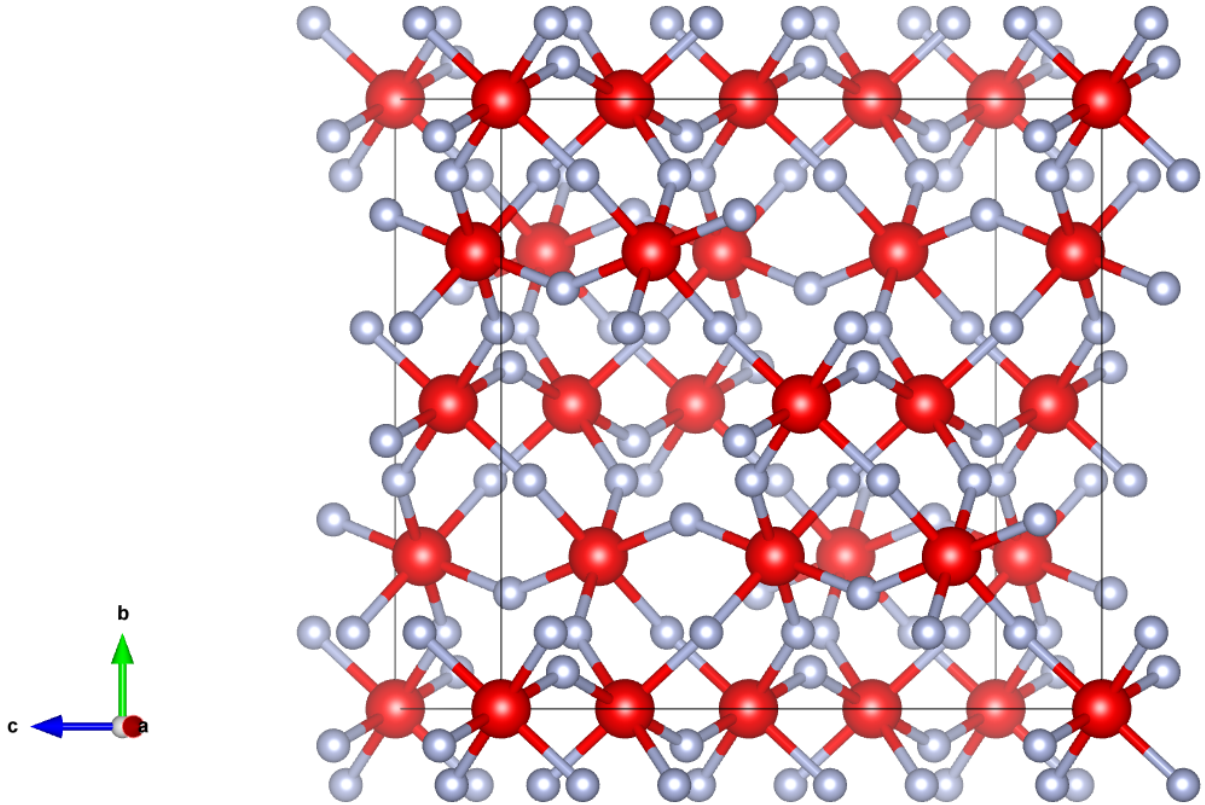
Pyrochlore FeF_3: A geometrical frustrated system



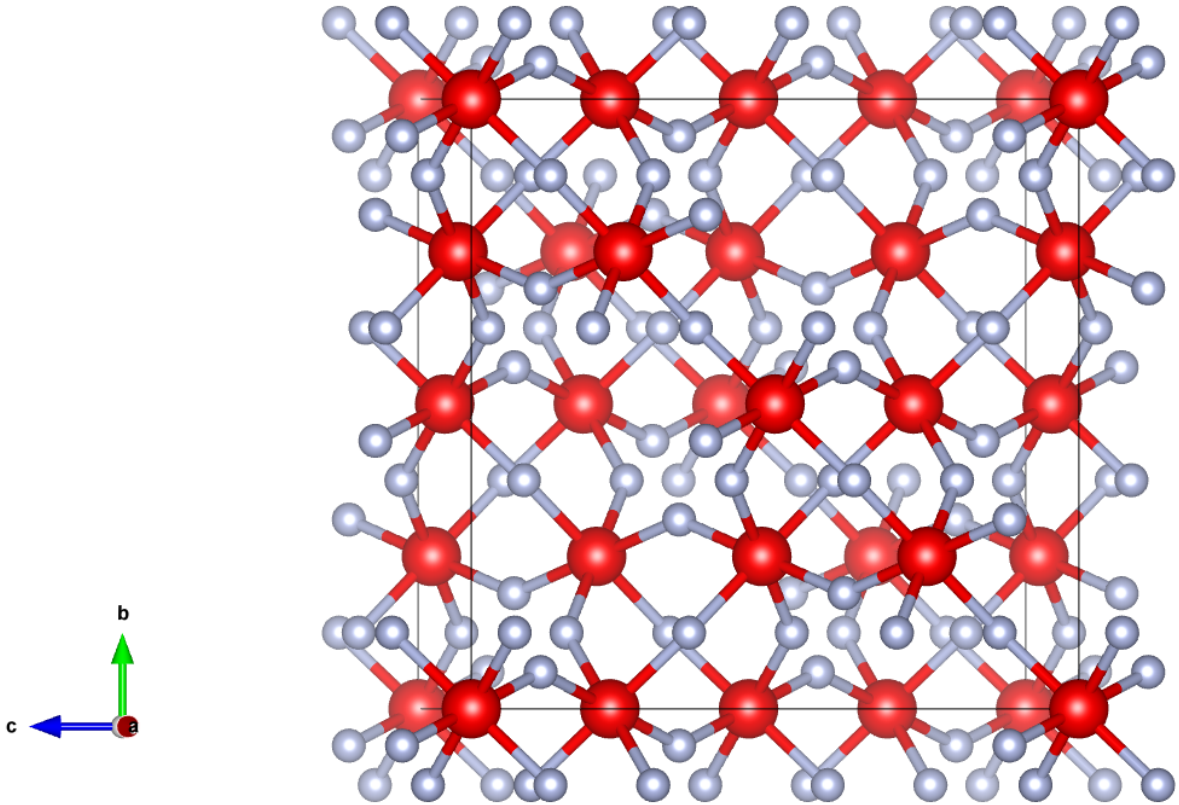
Pyrochlore FeF_3: A geometrical frustrated system



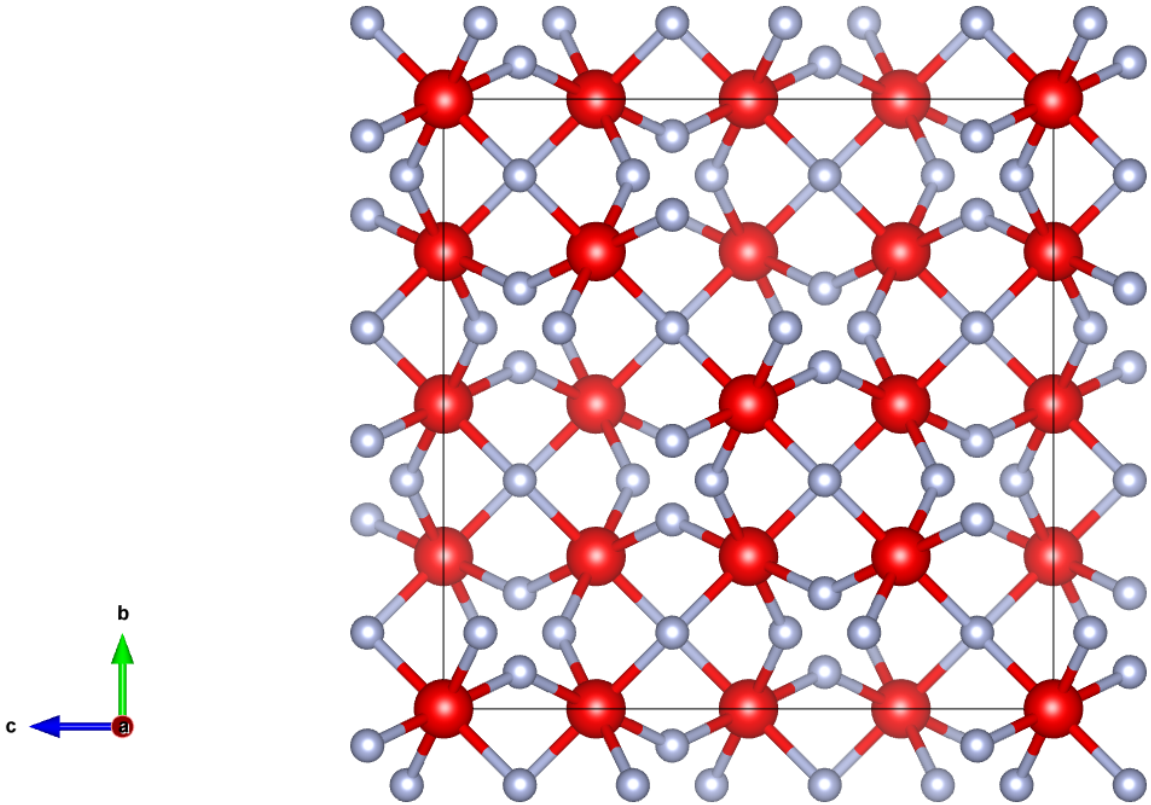
Pyrochlore FeF_3: A geometrical frustrated system



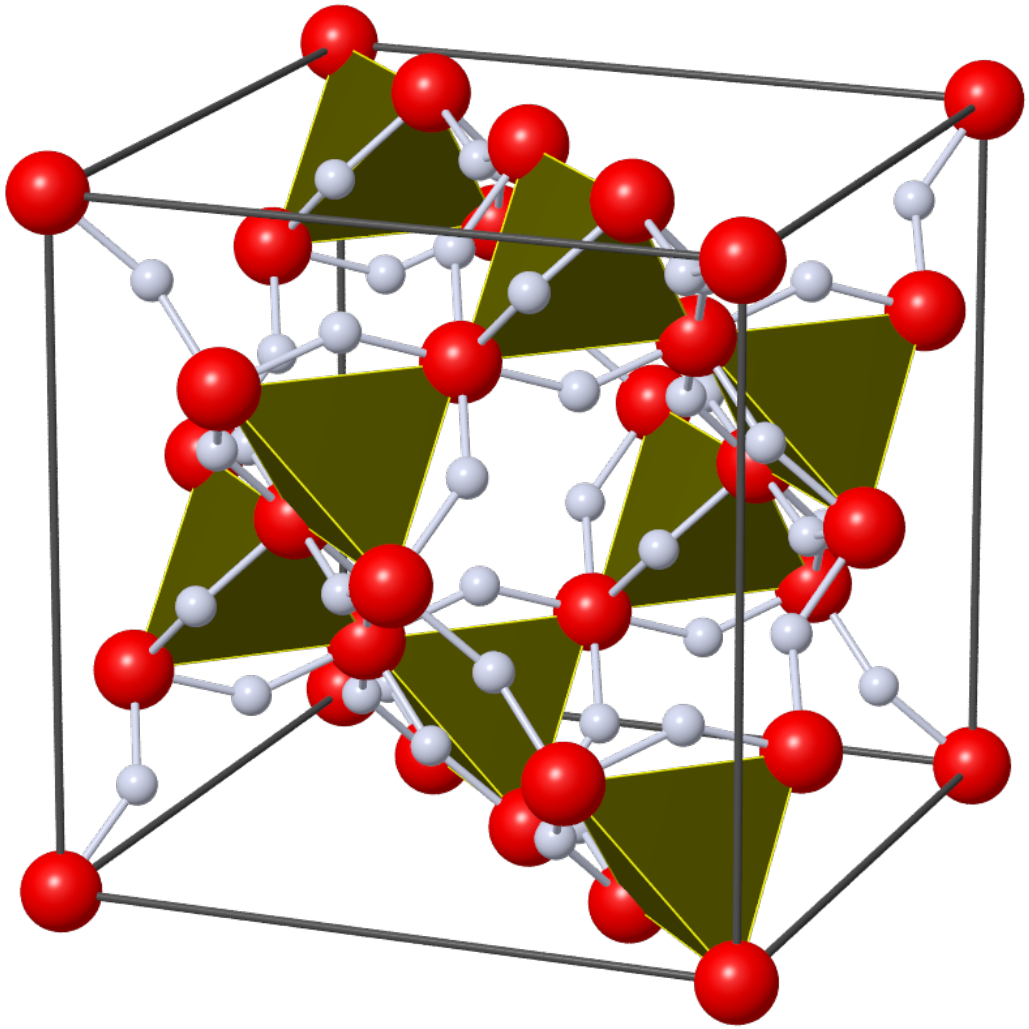
Pyrochlore FeF_3: A geometrical frustrated system



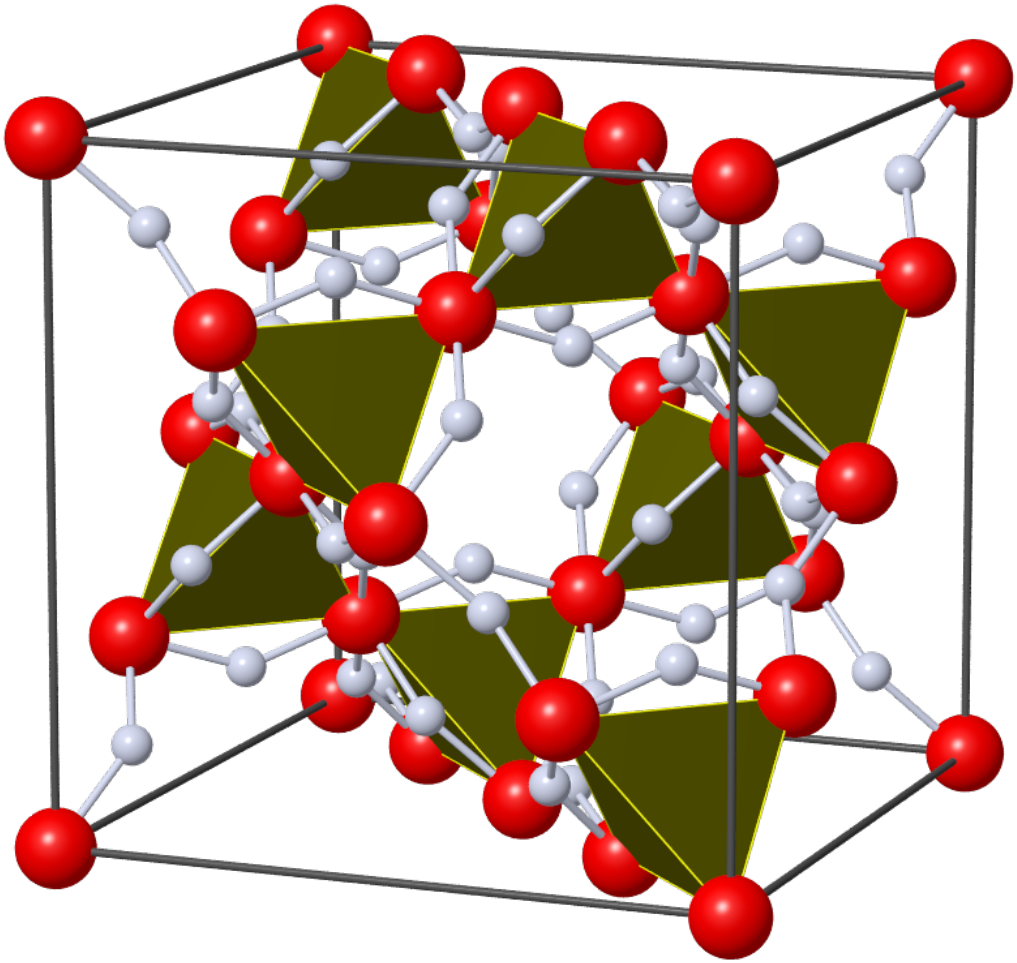
Pyrochlore FeF_3: A geometrical frustrated system



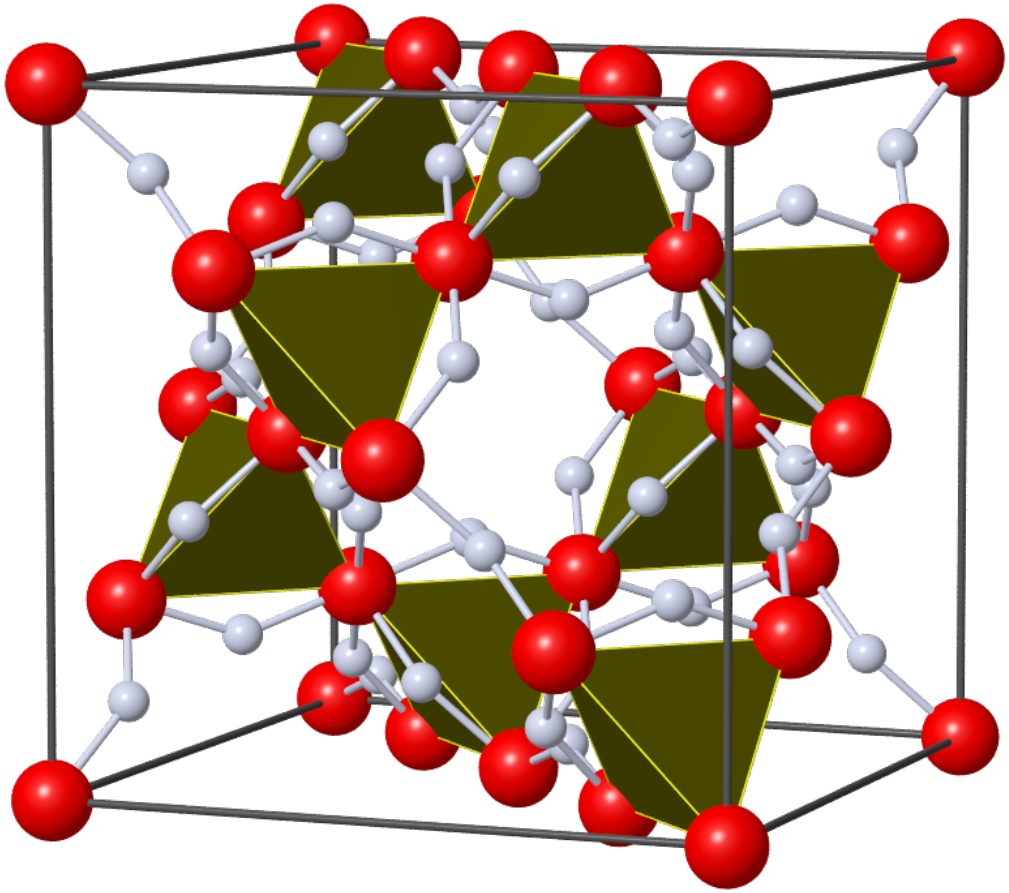
Pyrochlore FeF_3: A geometrical frustrated system



Pyrochlore FeF_3: A geometrical frustrated system



Pyrochlore FeF_3: A geometrical frustrated system



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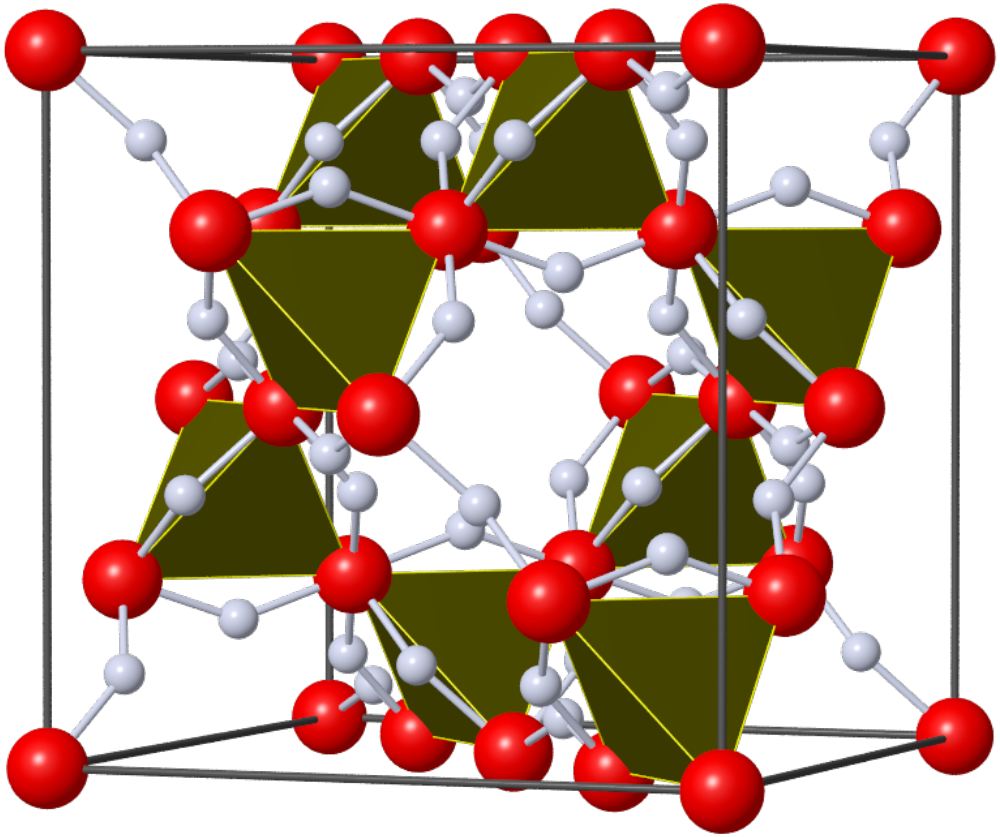

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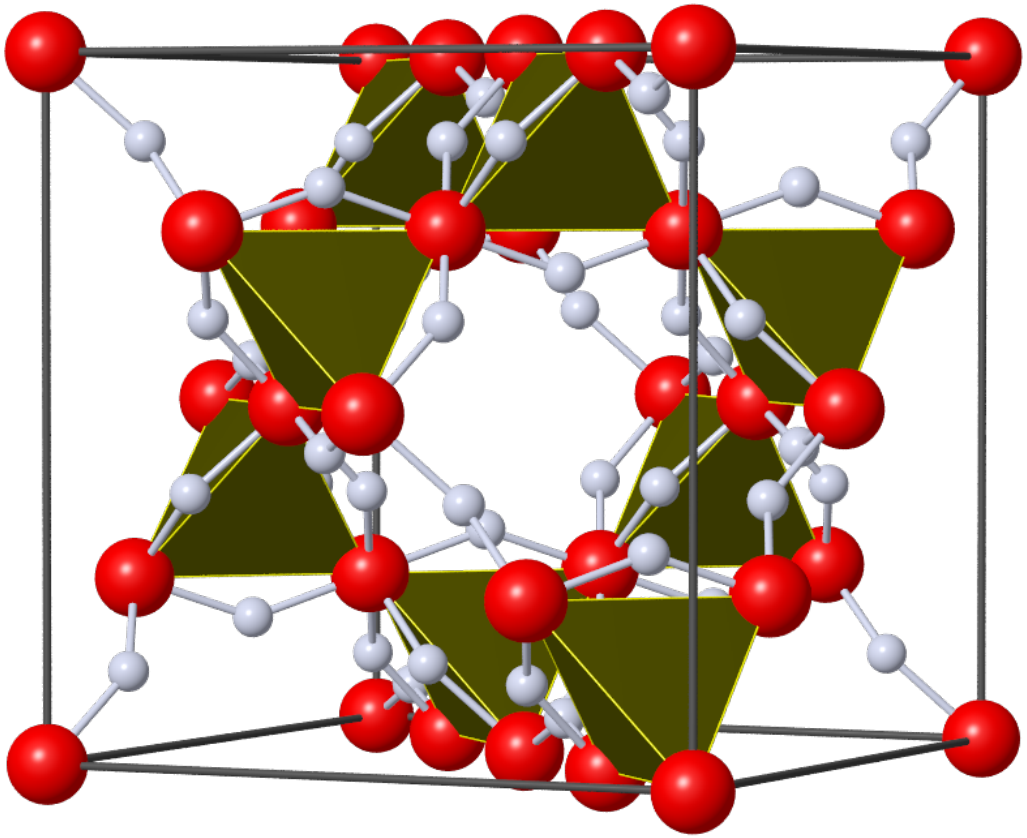

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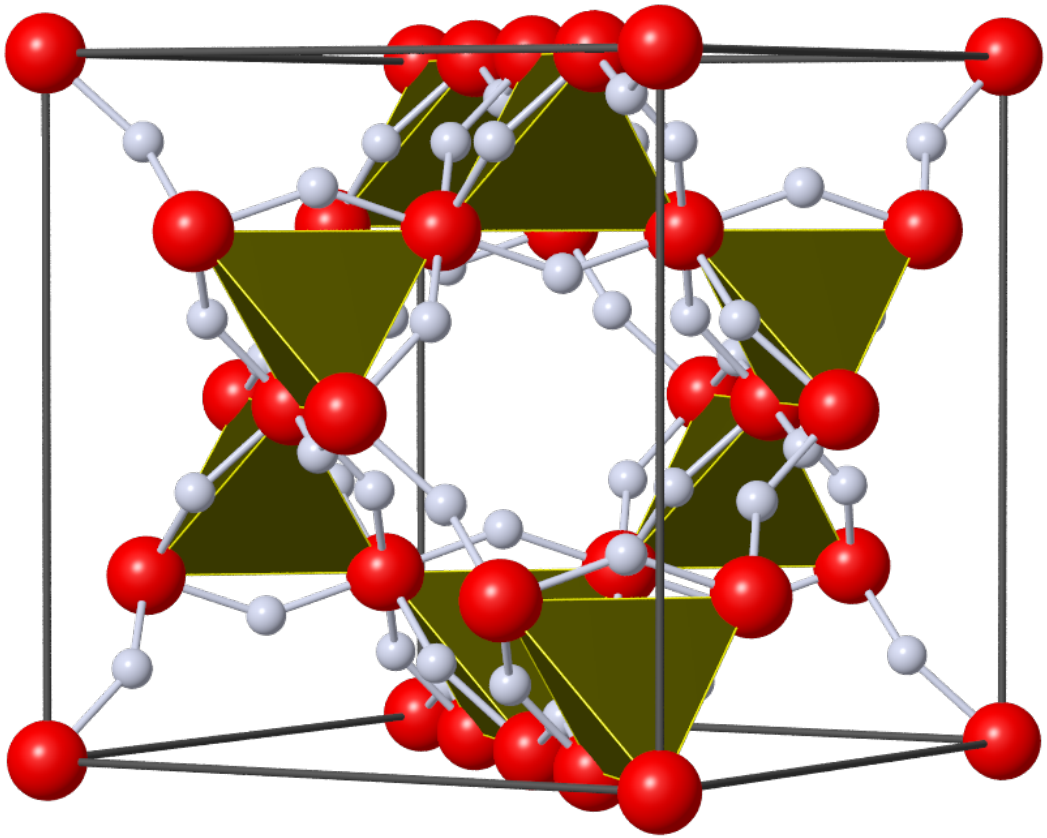

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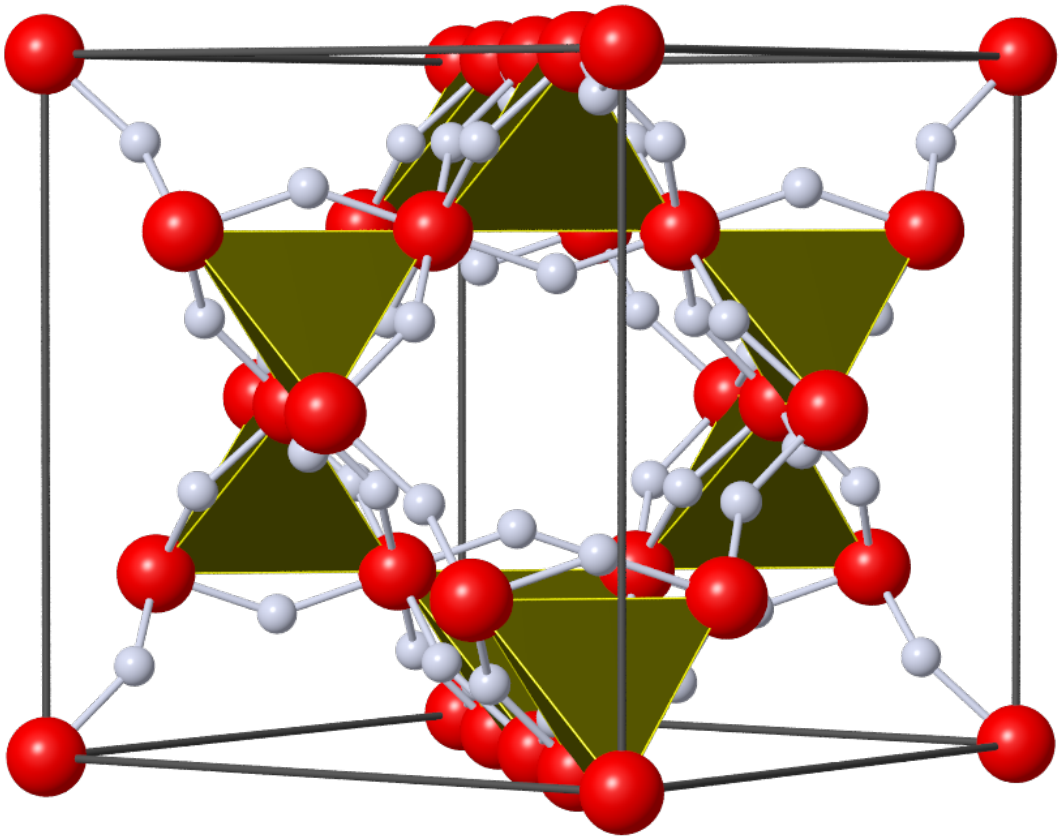

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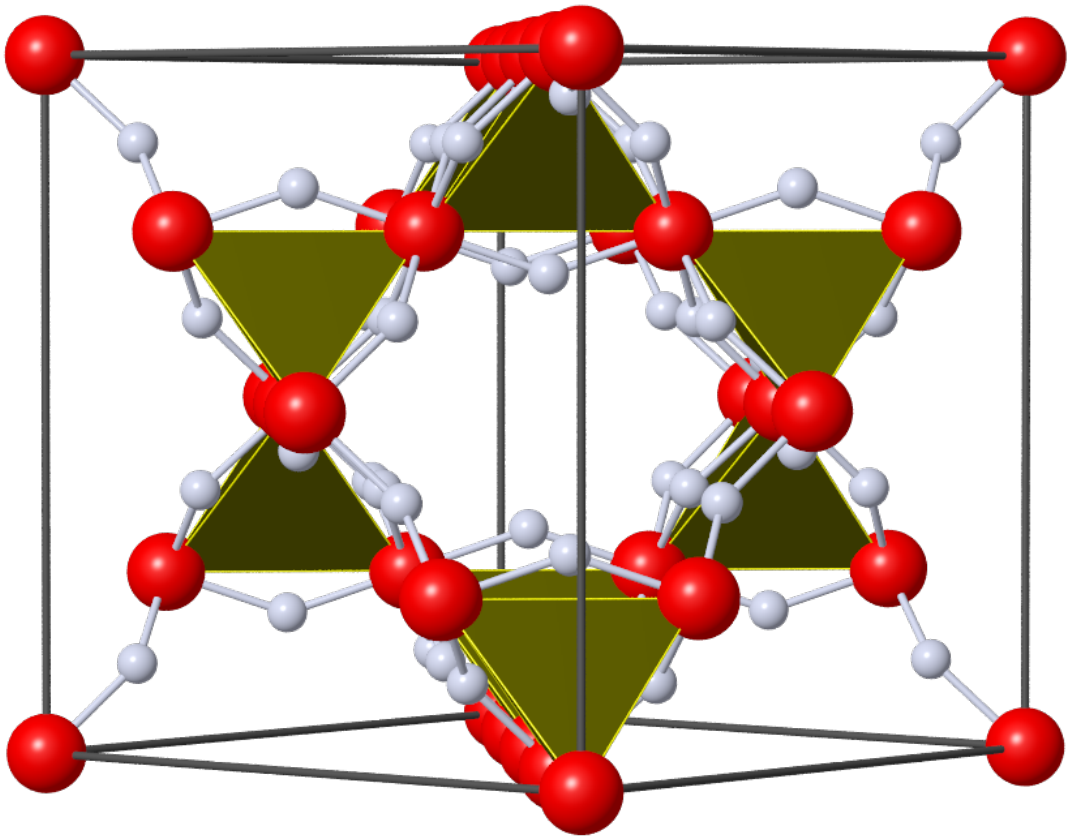

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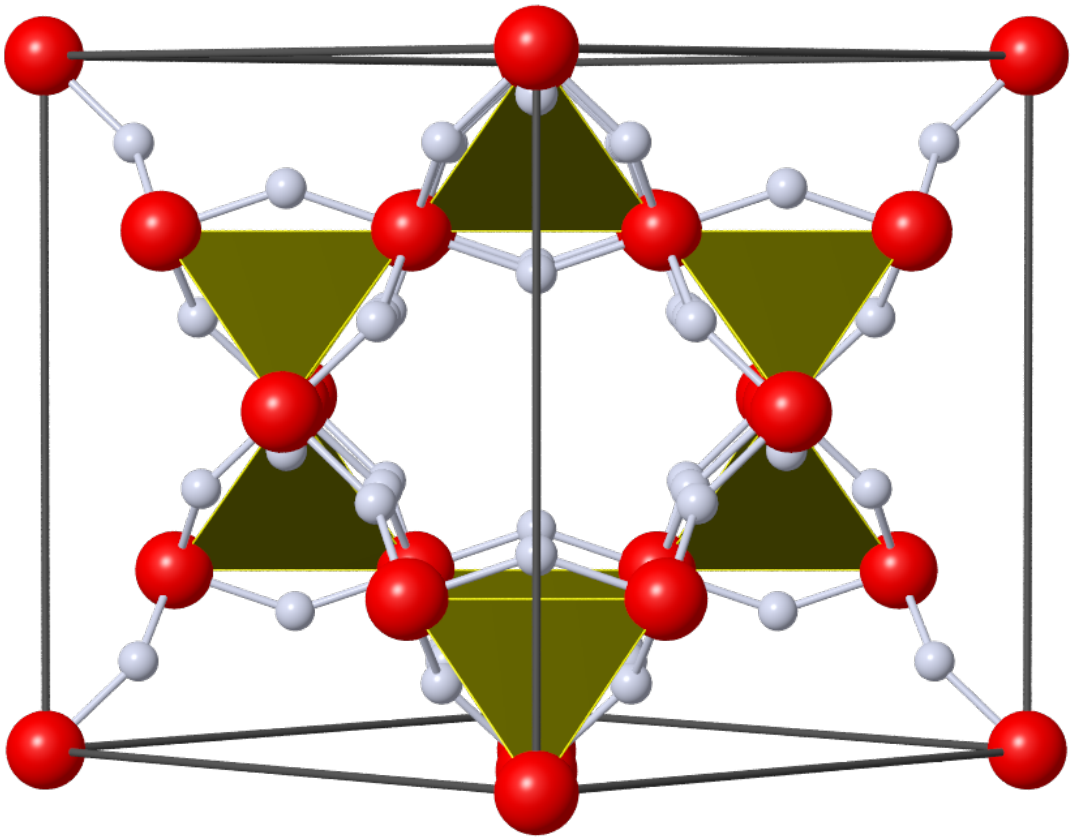

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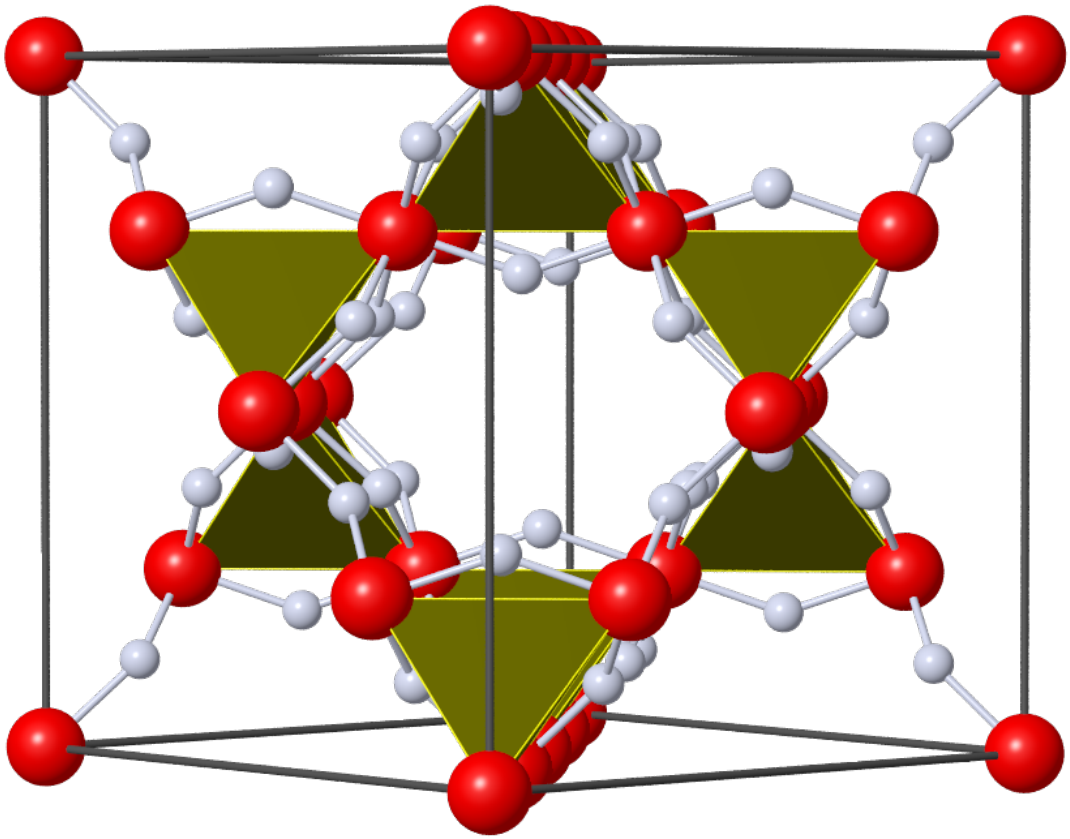

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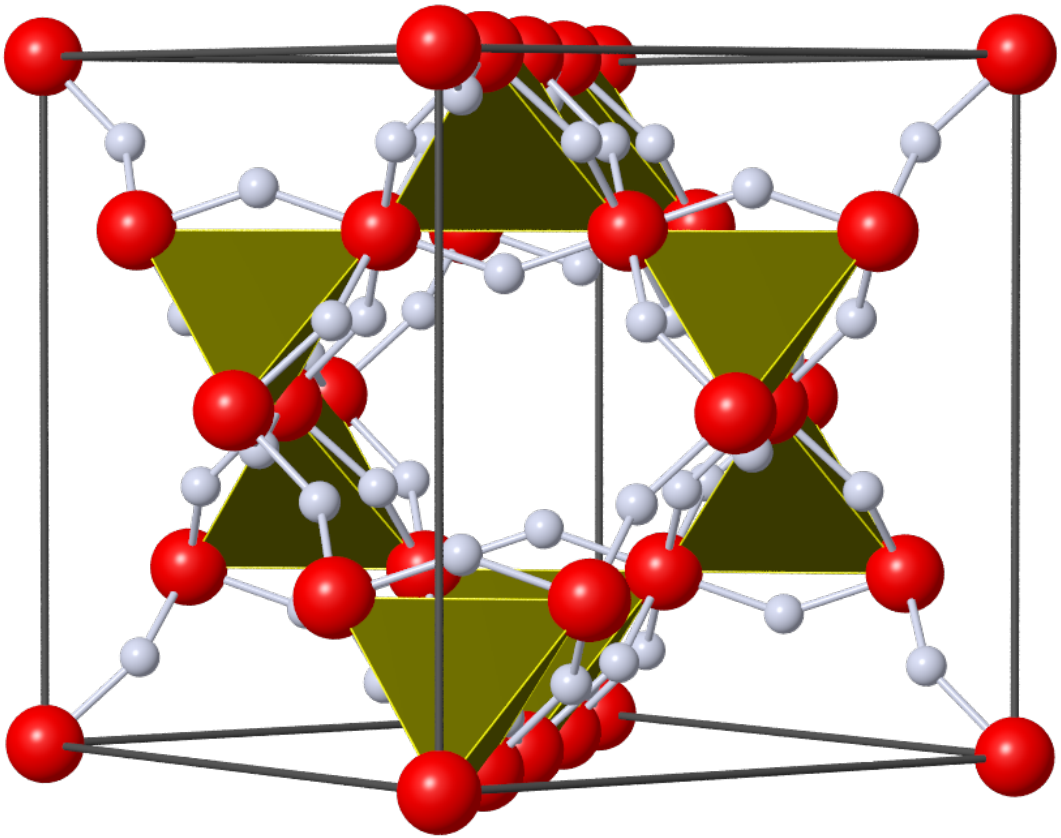

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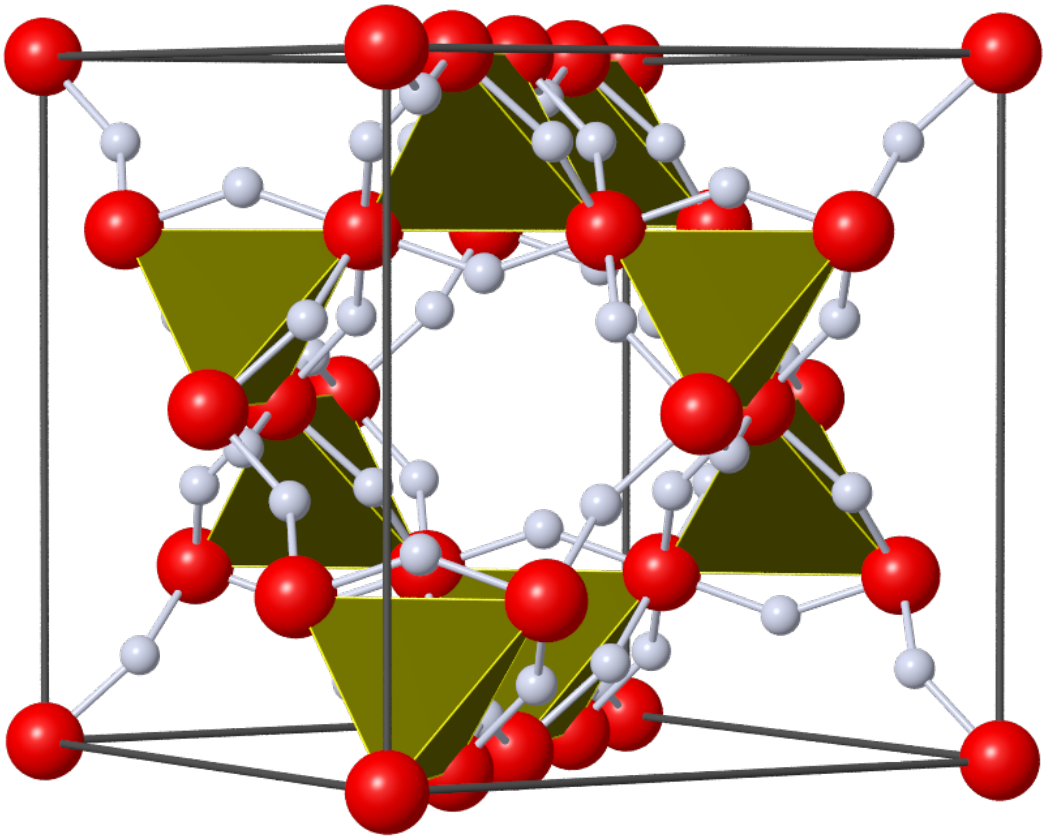

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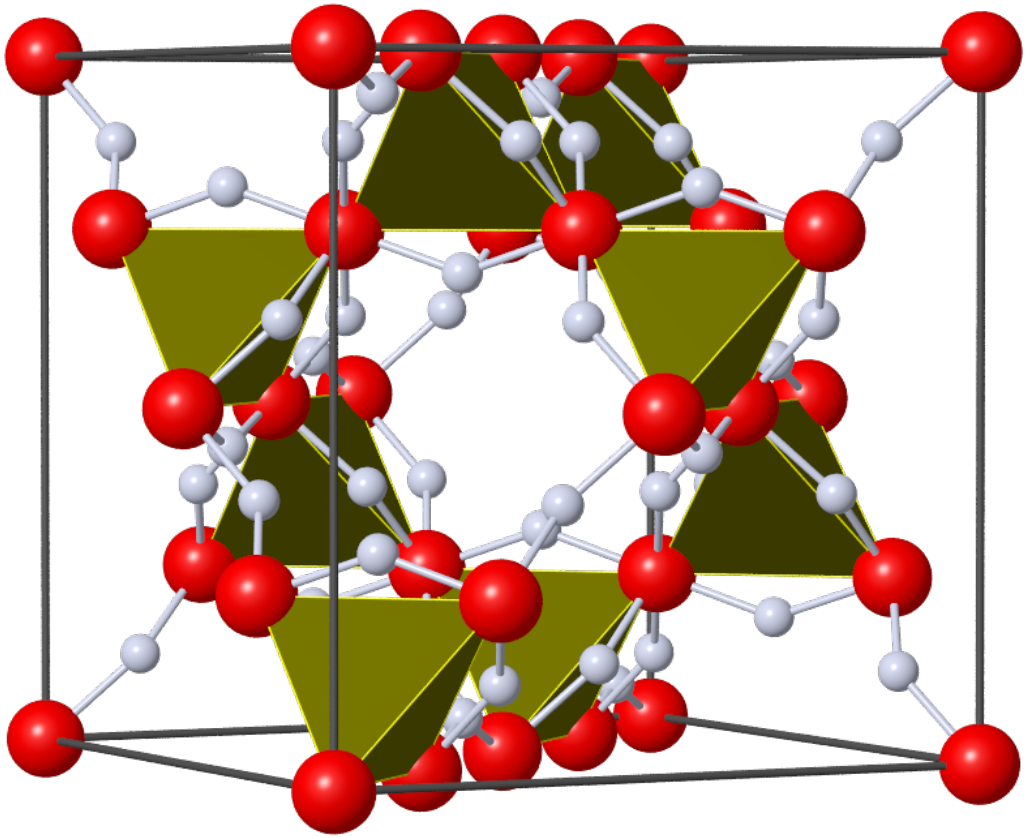

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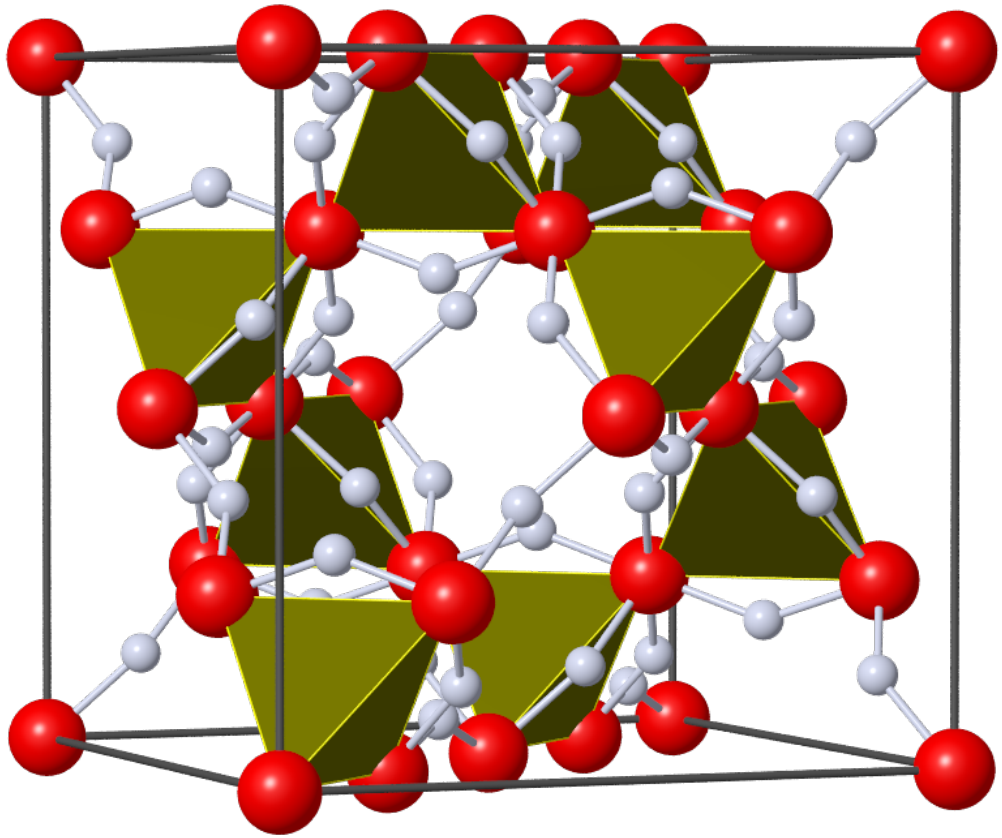

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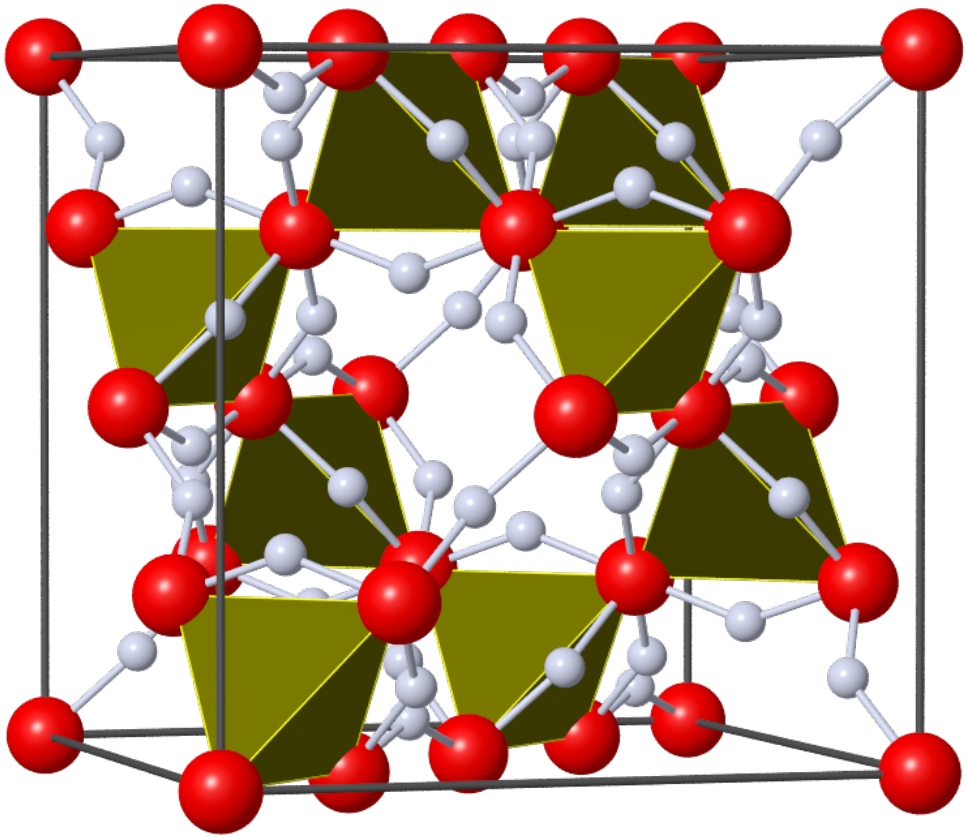

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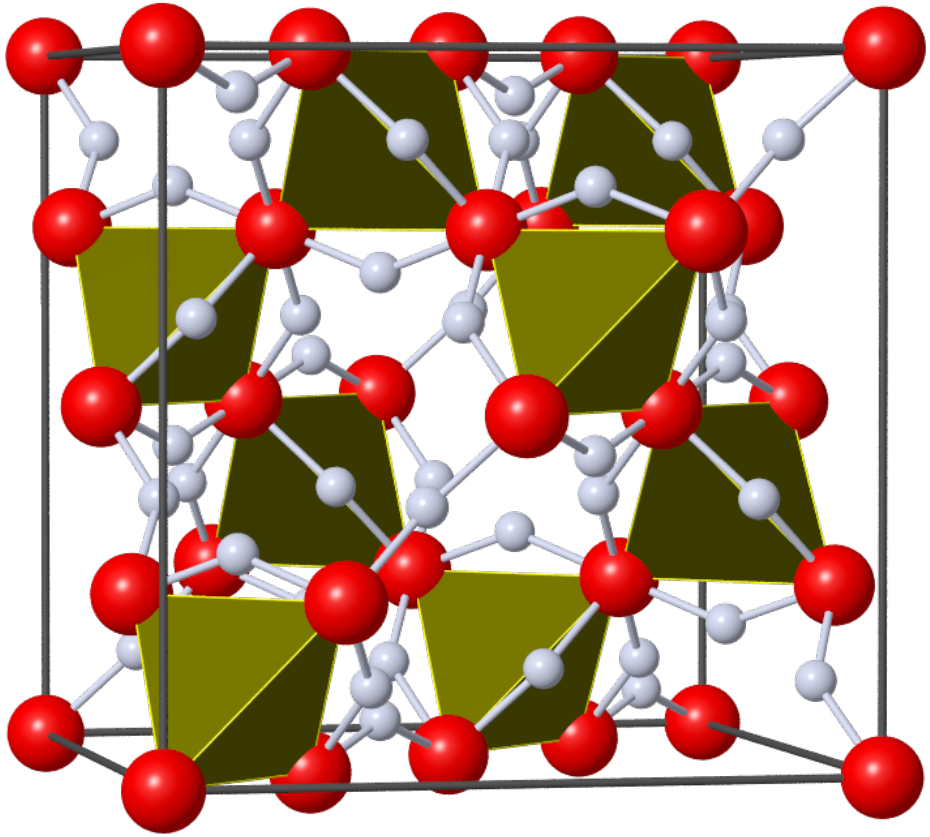

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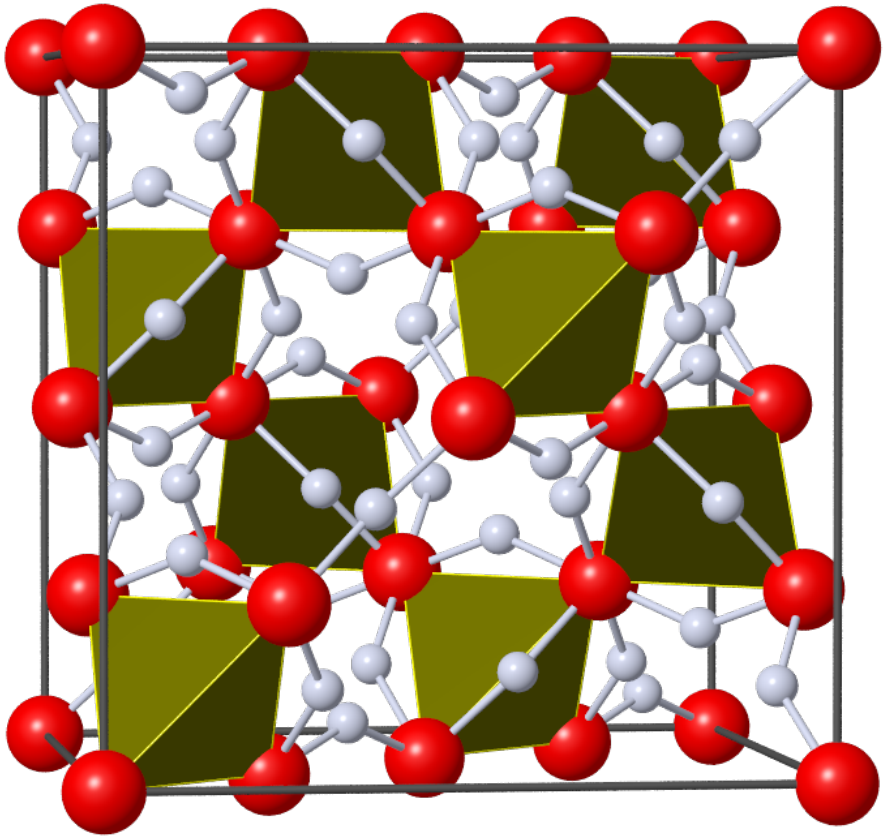

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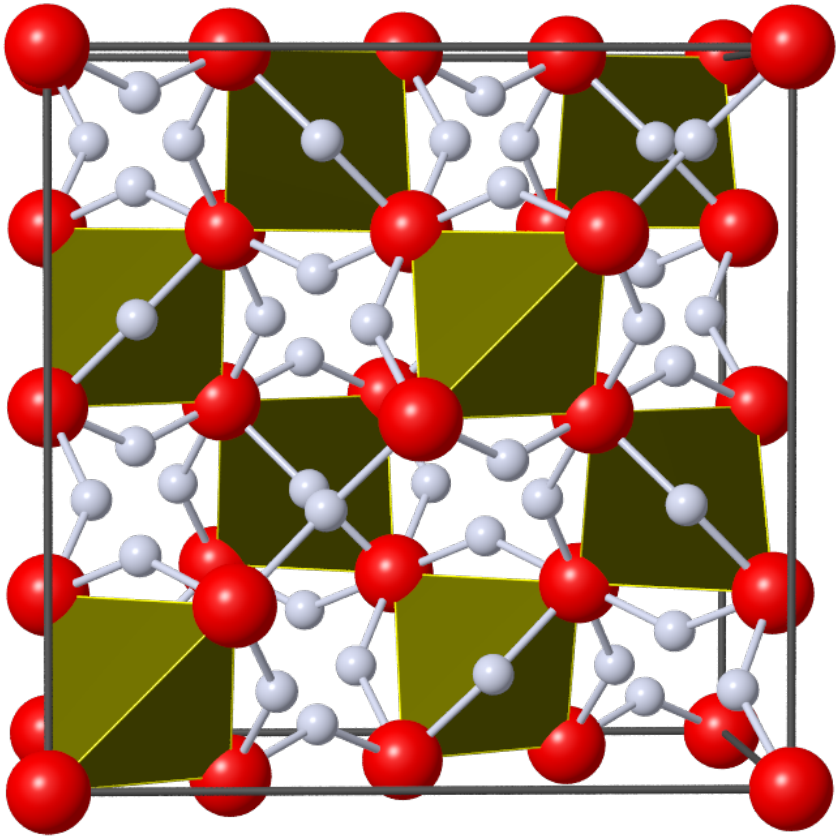
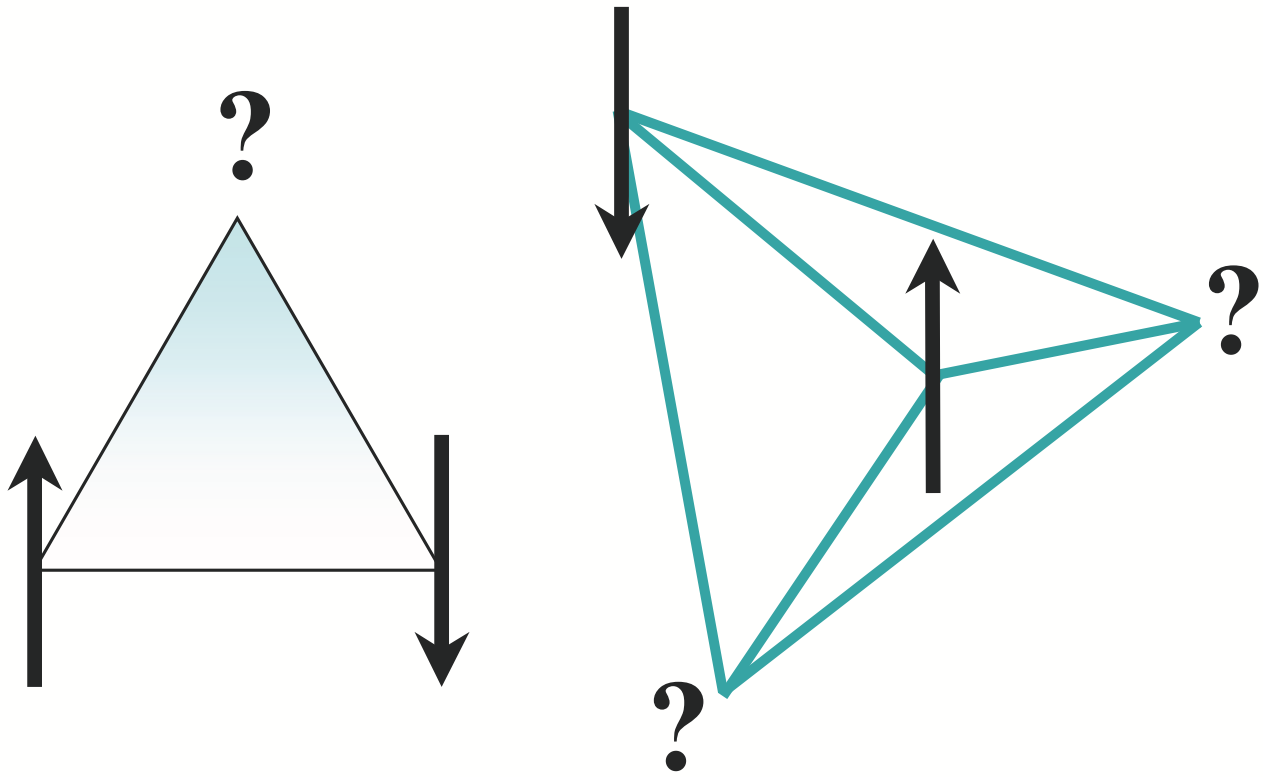


Pyrochlore FeF_3: A geometrical frustrated system

Geometrical frustration?



J. S. Gardner, M. J. P. Gingras, and J. E. Greedan Rev. Mod. Phys. 82, 53 (2010)

Pyrochlore FeF_3: A geometrical frustrated system

There is no long-range order with $J_1 < 0$

PHYSICAL REVIEW B VOLUME 45, NUMBER 13 1 APRIL 1992-I

Absence of long-range order in a three-dimensional geometrically frustrated antiferromagnet

J. N. Reimers*
Institute for Materials Research, McMaster University, Hamilton, Ontario, Canada L8S 4M1
(Received 15 May 1991; revised manuscript received 26 August 1991)

Classical Heisenberg spins on a lattice of *corner*-sharing tetrahedra with nearest-neighbor antiferromagnetic interactions are investigated with Monte Carlo (MC) techniques. The system is highly frustrated with an infinitely degenerate ground state. Mean-field theory predicts no long-range order (LRO) at any temperature. The MC calculations are consistent with this result, thus providing evidence that thermal fluctuations beyond the mean-field approximation do not stabilize LRO. The possibility of incommensurate and spin nematic order is considered. The temperature dependence of some spin-glass order parameters, such as the Edwards-Anderson order parameter and the single-spin autocorrelation function, are also investigated. The results show that no spin freezing occurs at nonzero temperatures.

But FeF_3 indicates an antiferromagnetic transition around 22K!

Pyrochlore FeF_3: A geometrical frustrated system

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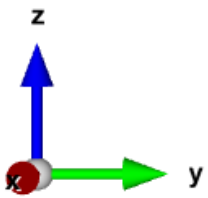

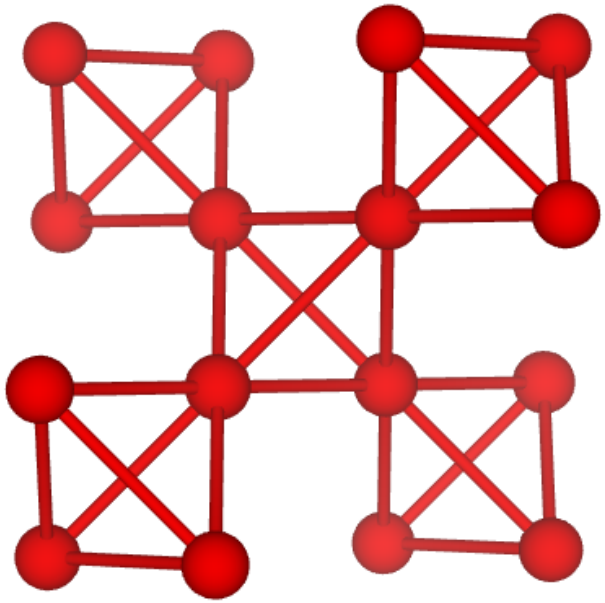

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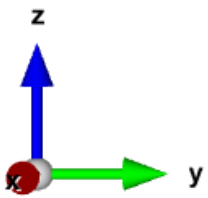

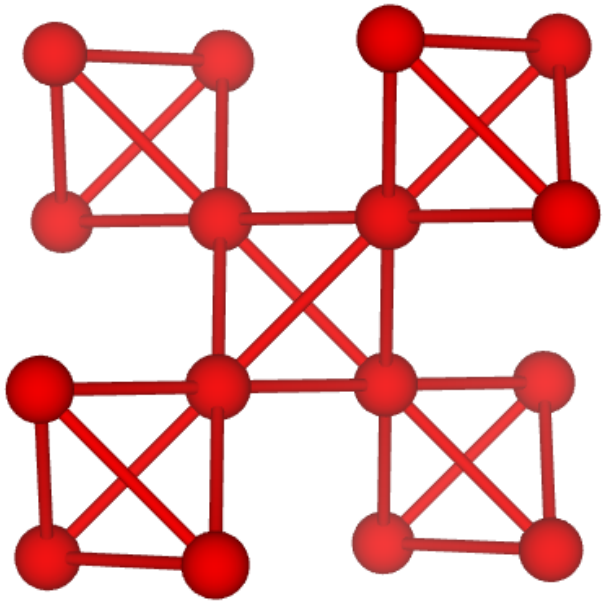

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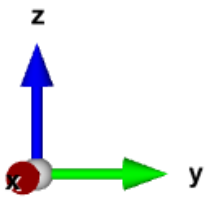

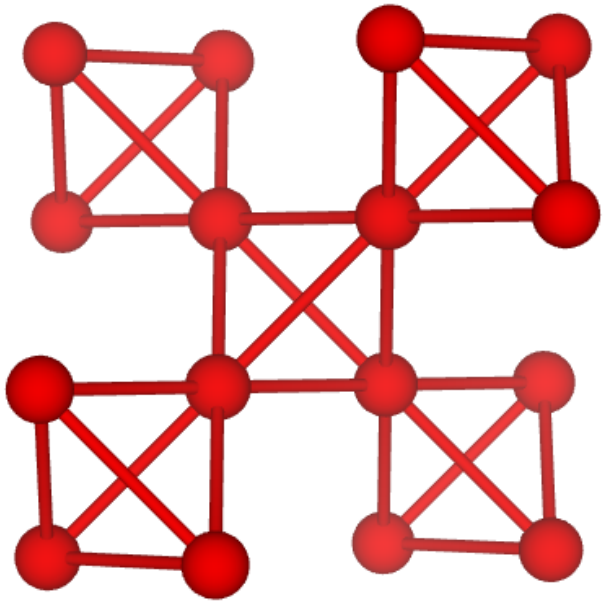

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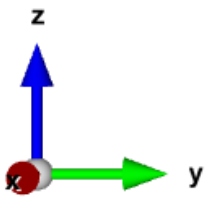

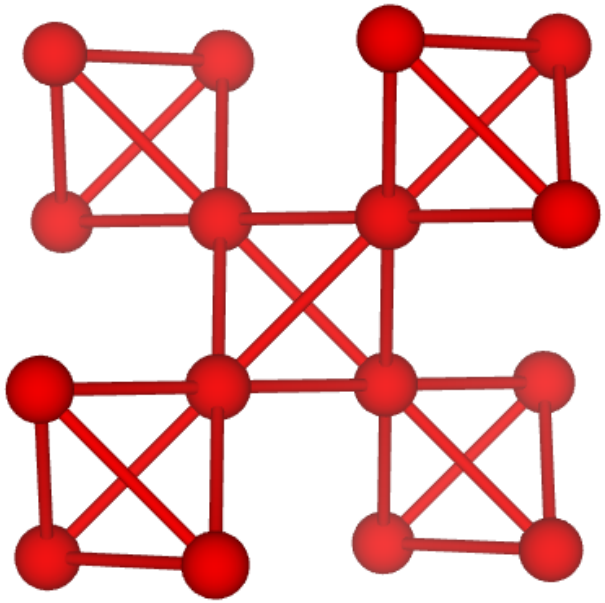

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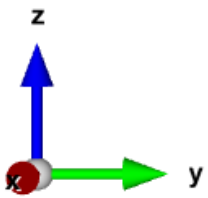

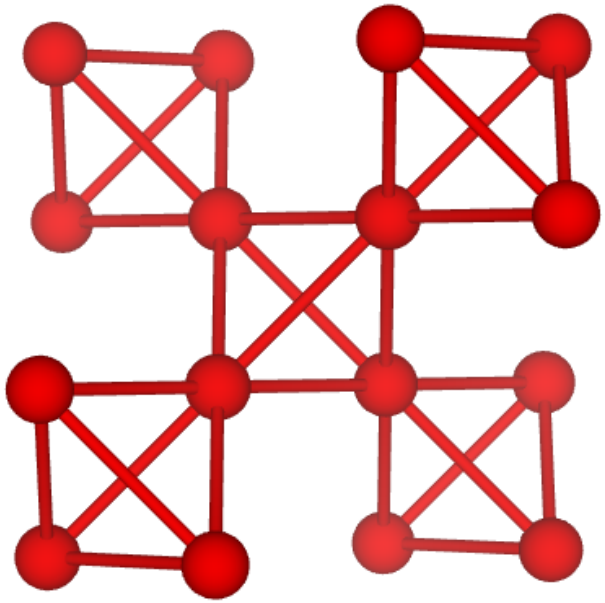

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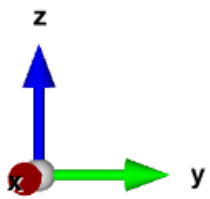

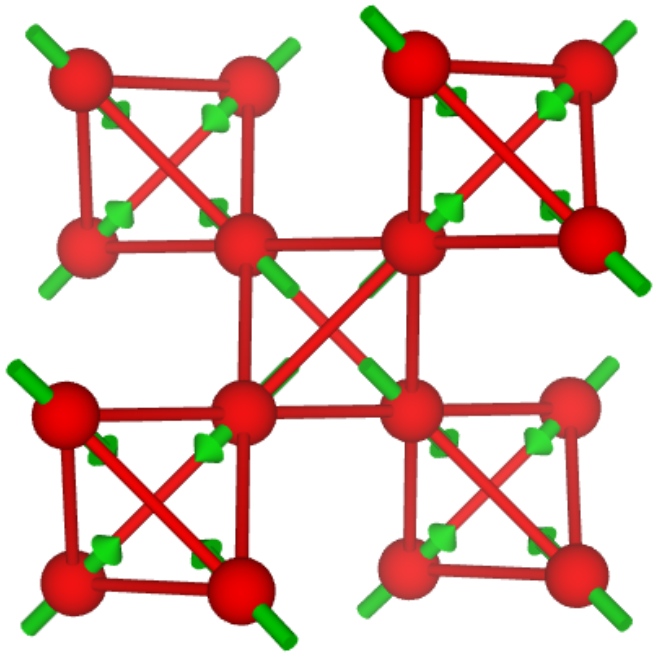

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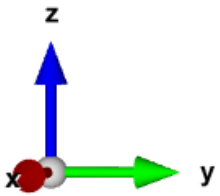

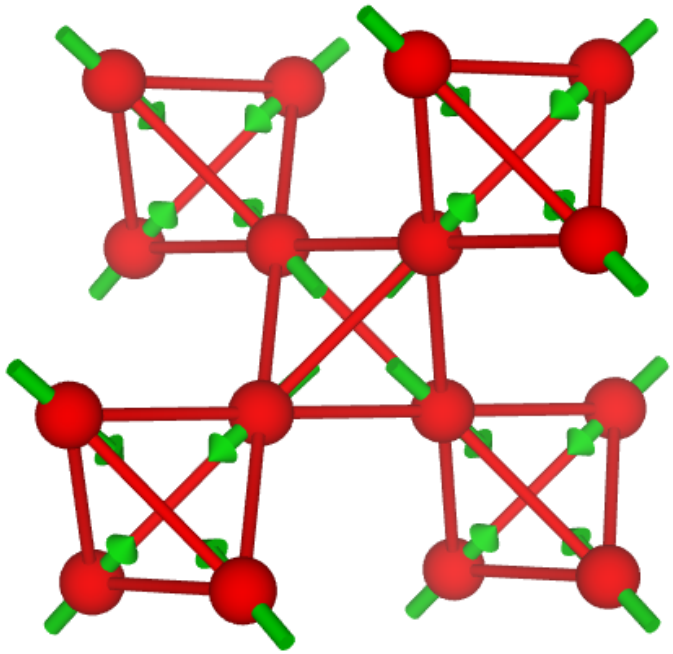

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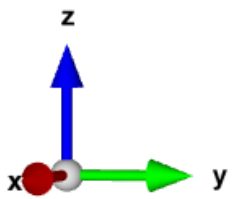

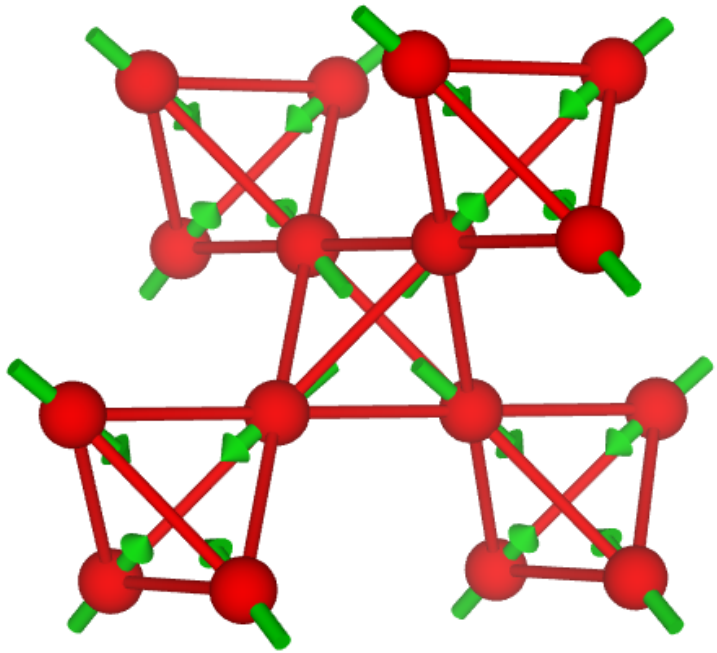

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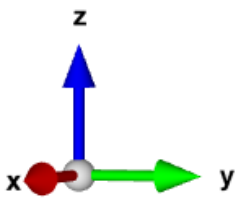

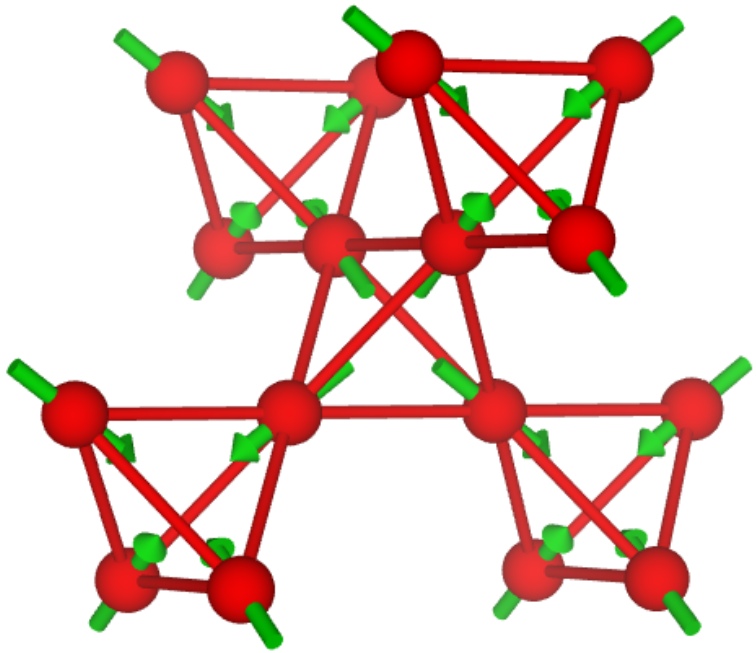

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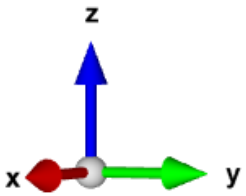

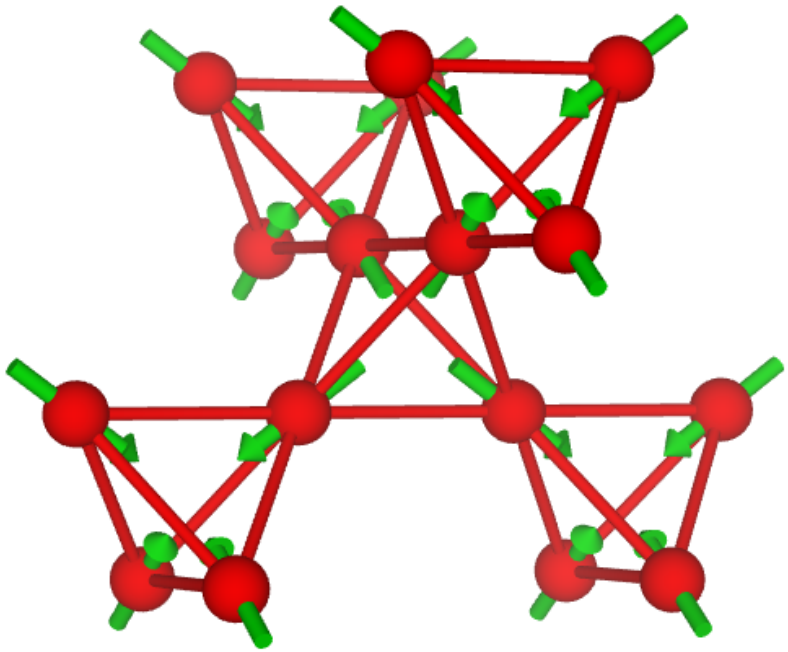

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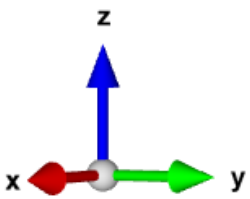

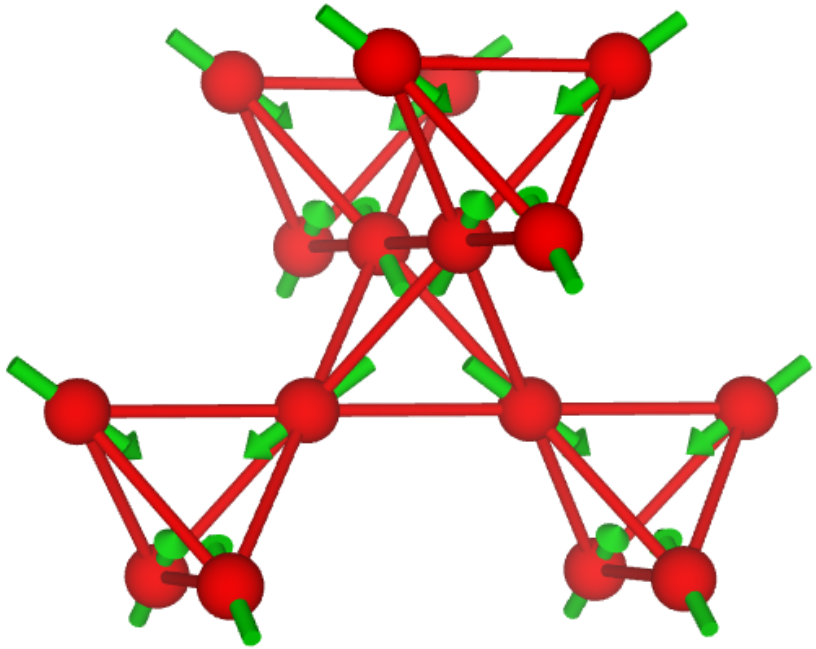

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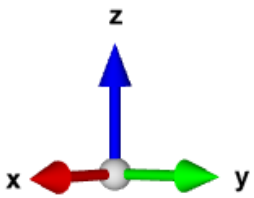

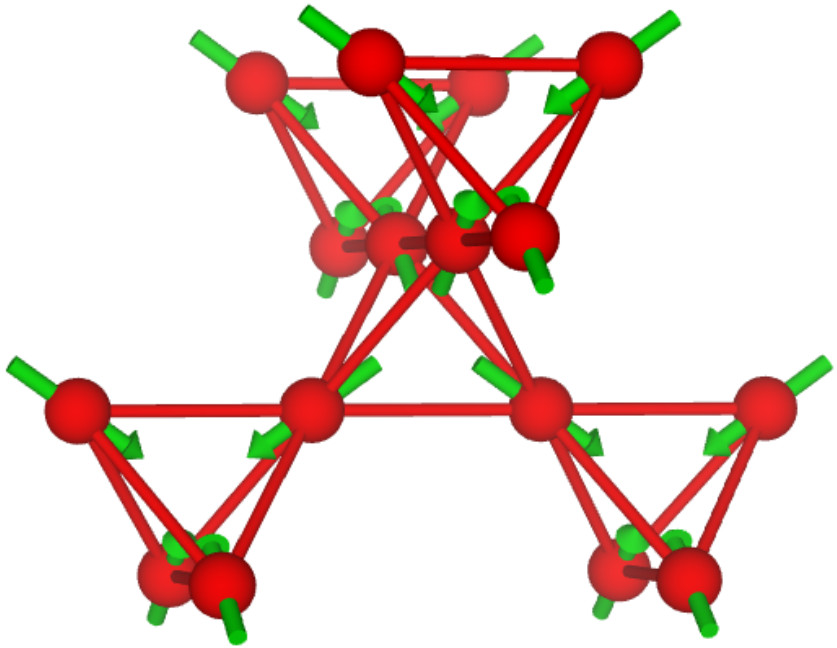

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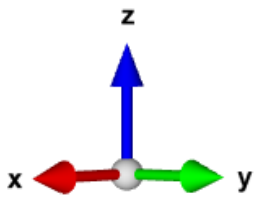

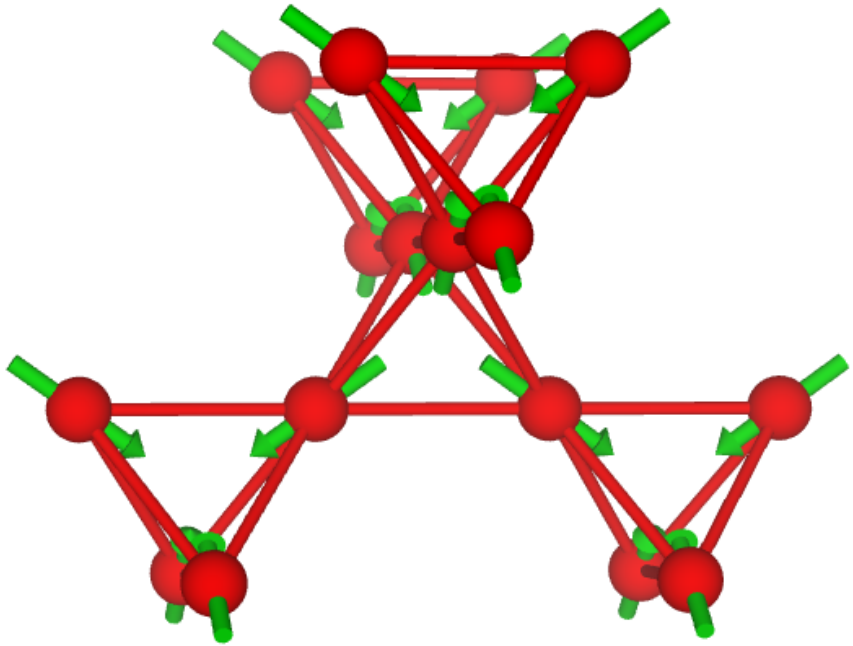

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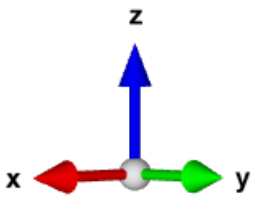

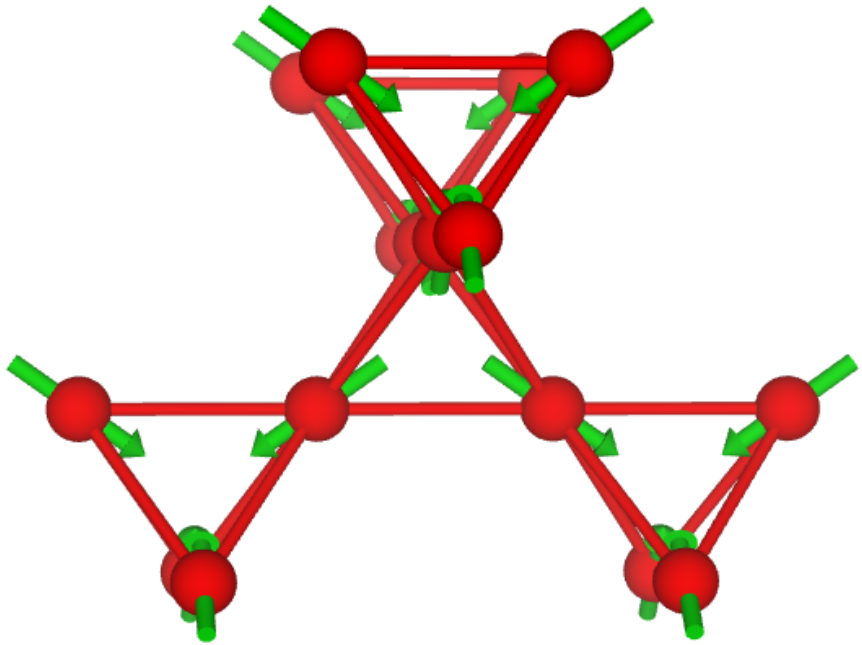

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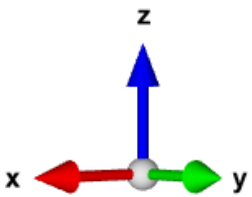

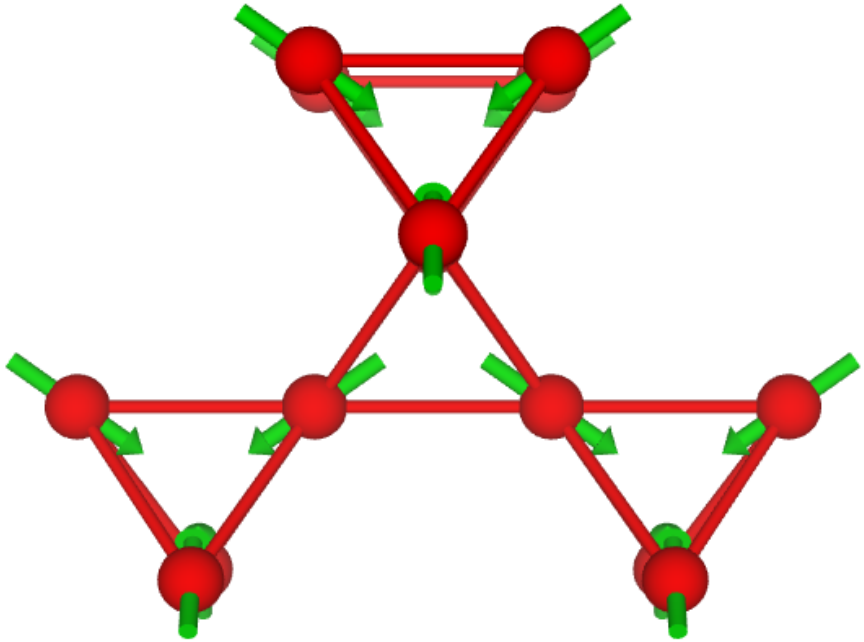

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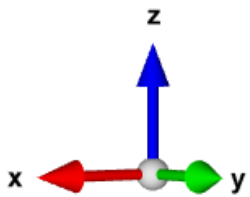

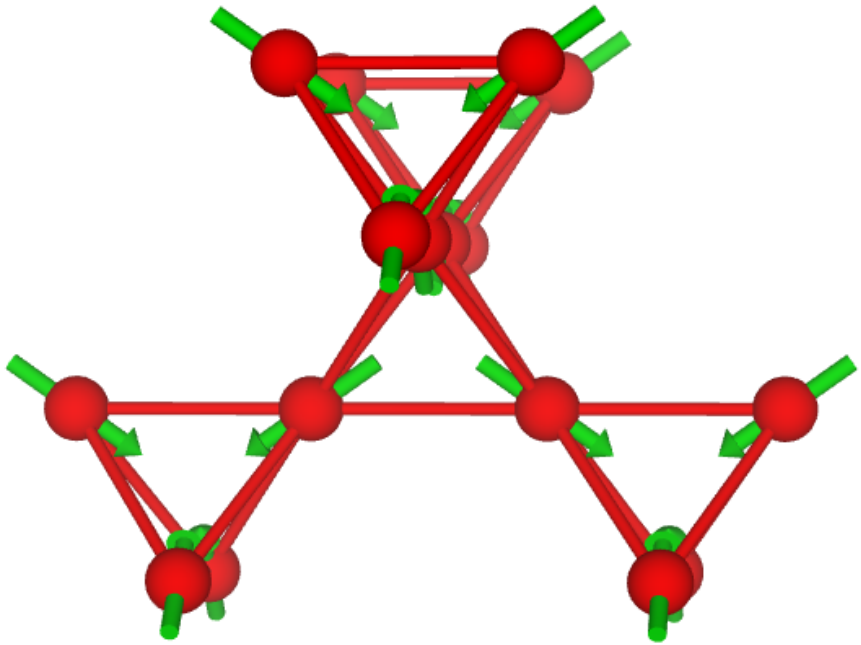

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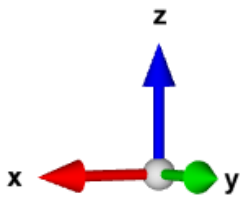

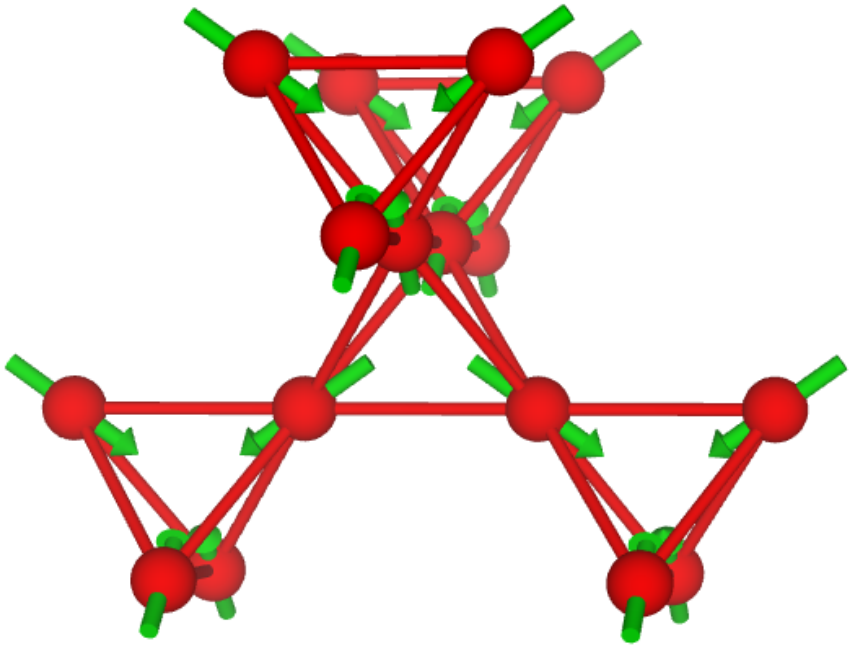

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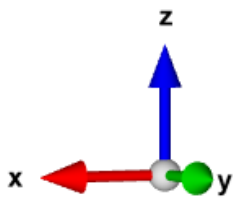

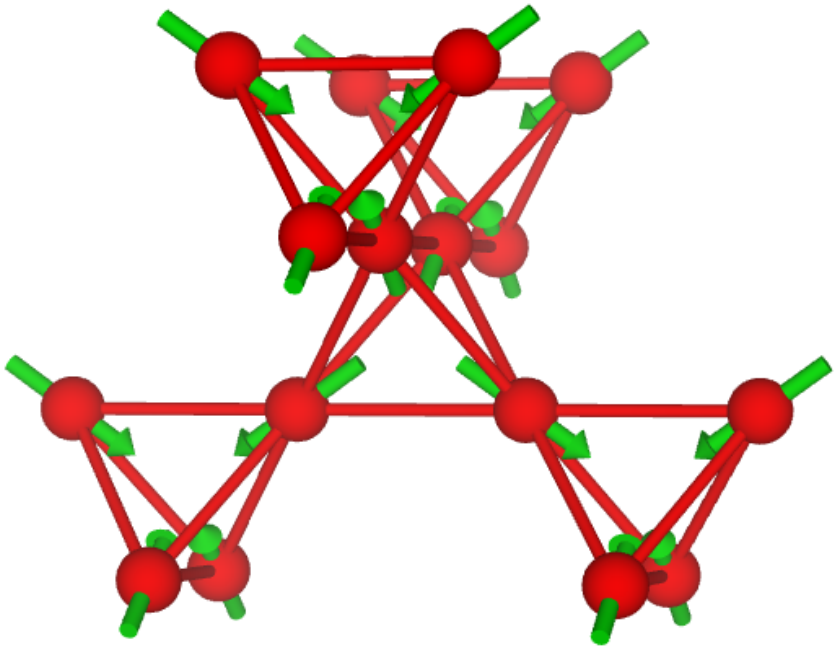

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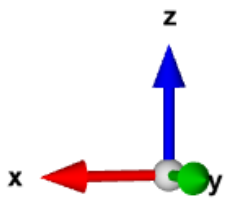

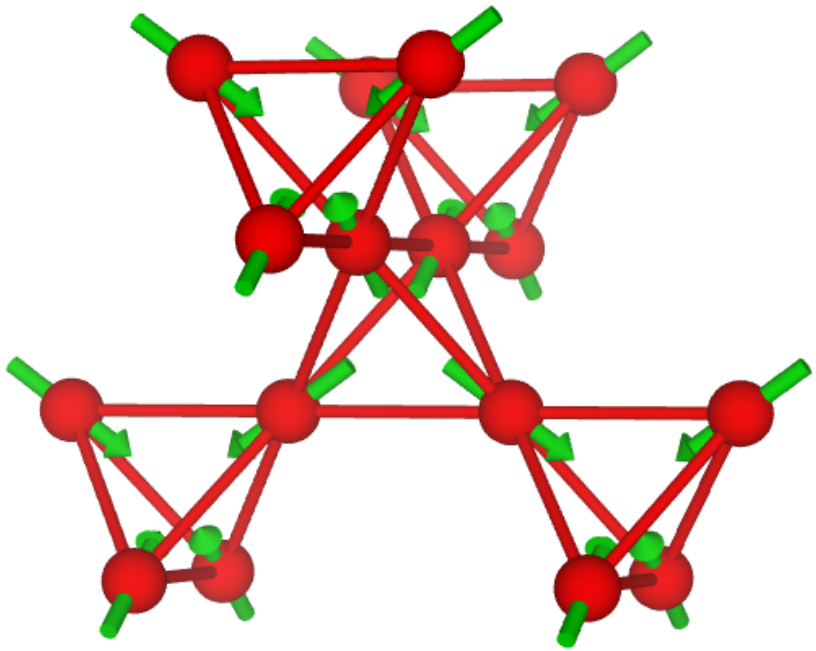

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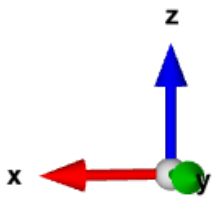

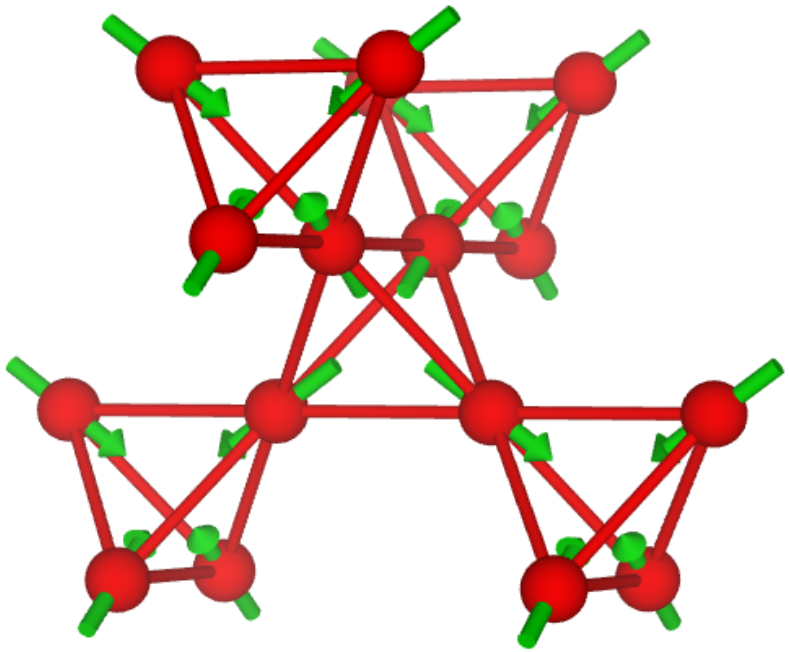

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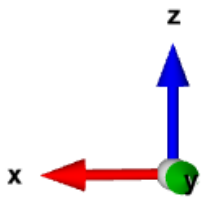

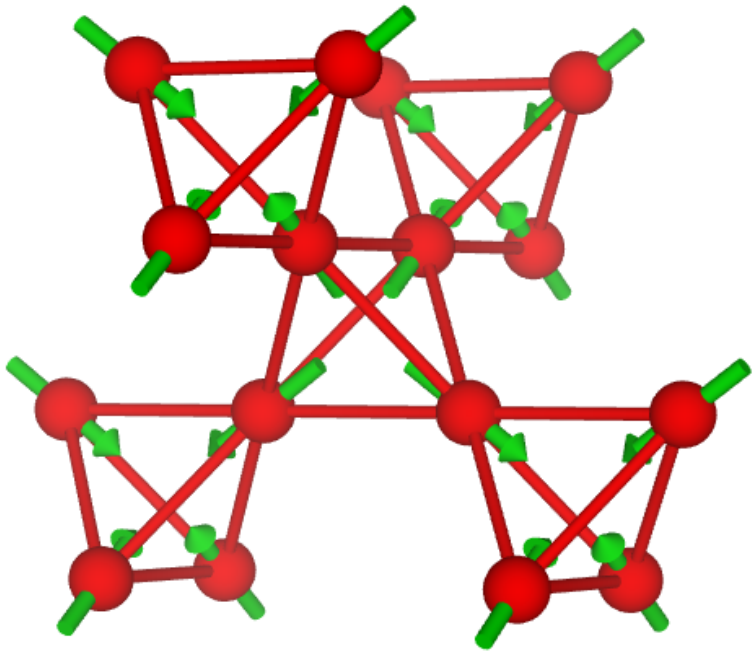

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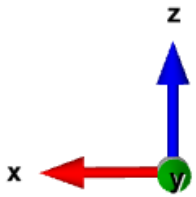

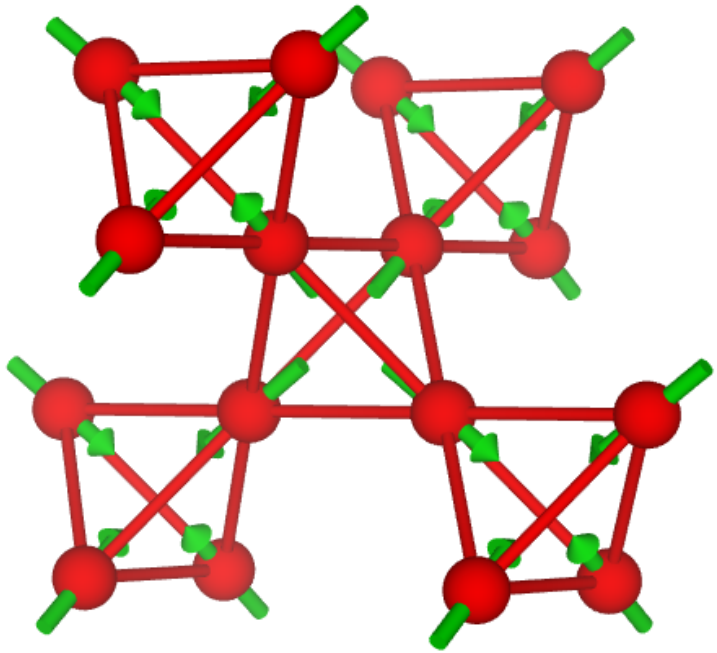

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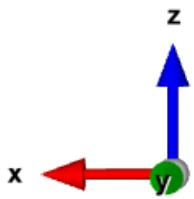

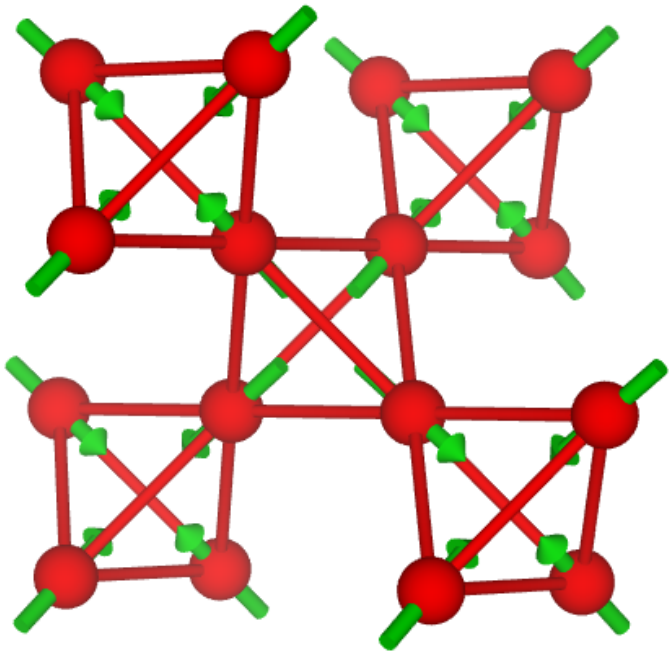

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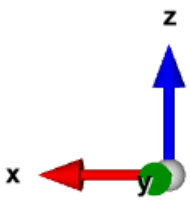

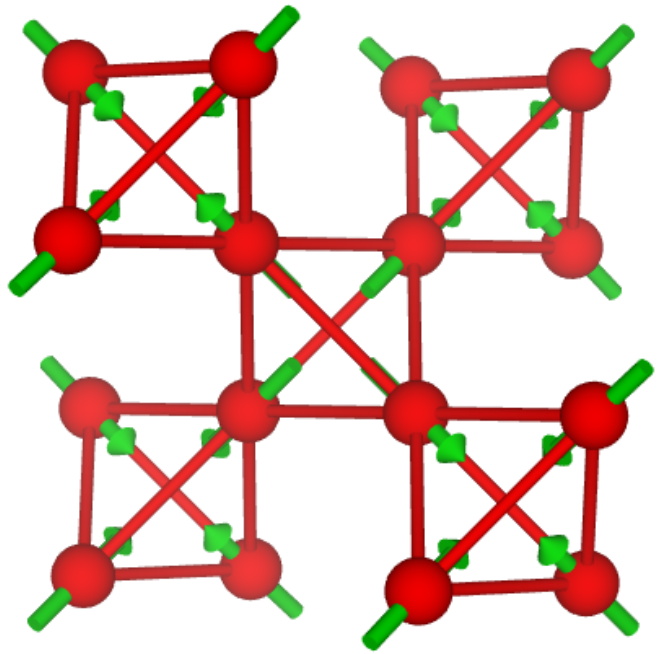

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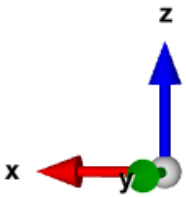
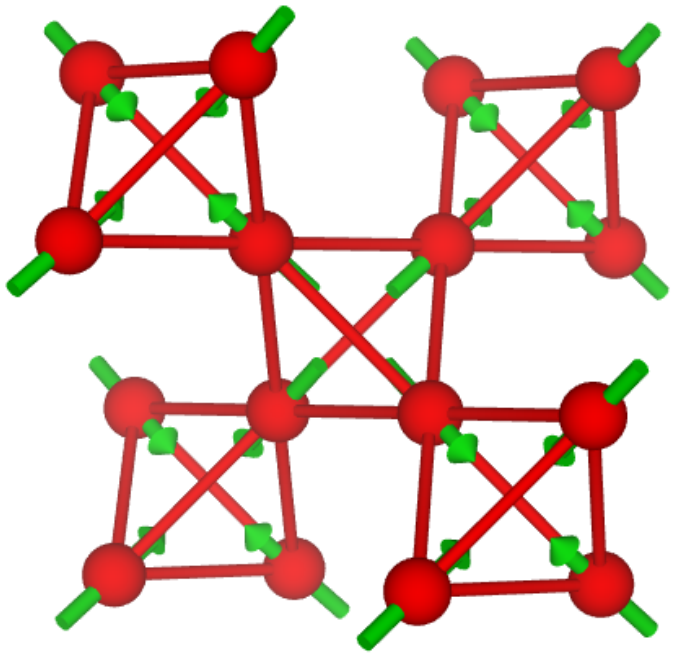
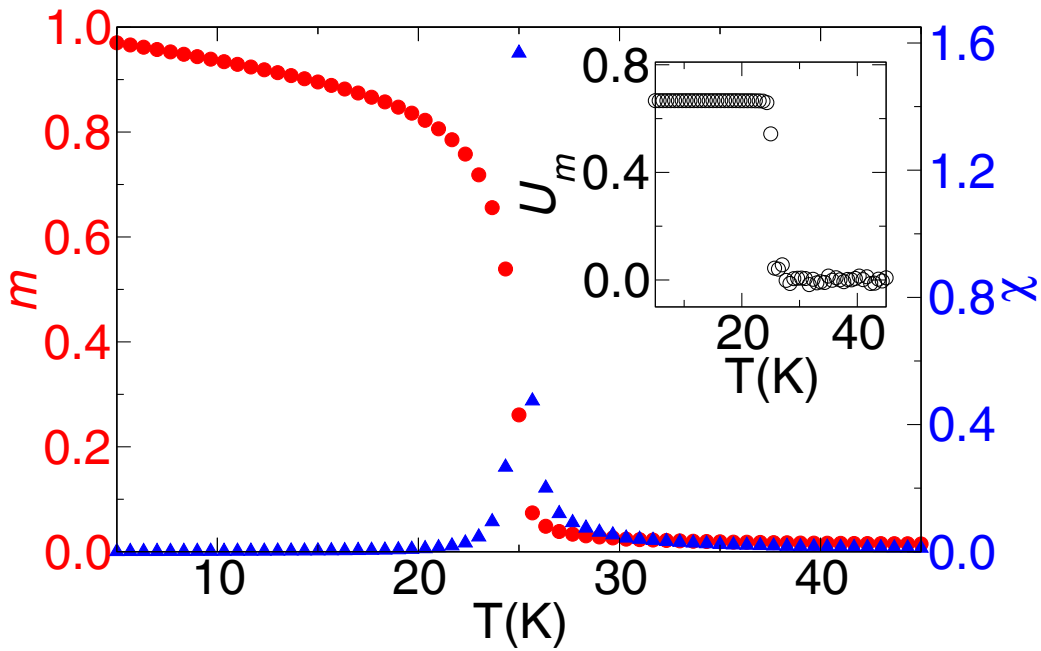




Pyrochlore FeF_3: A geometrical frustrated system

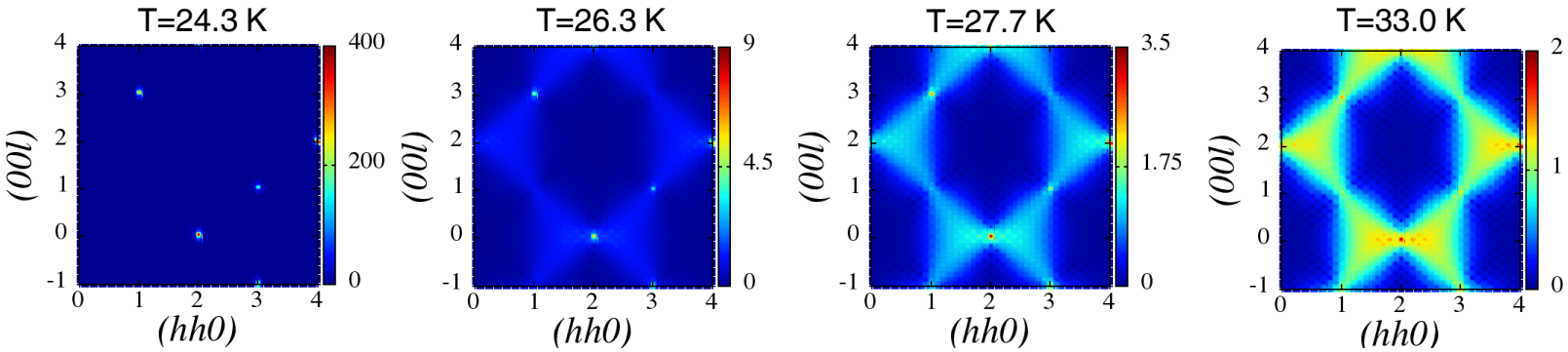
MC result: order parameter



"The AIAO order parameter is $m = \sum_i \mathbf{S}_i.\mathbf{d}_i/N$, where $\mathbf{d}_i$ indicates a local unit vector at the ith site, which points to the center of the related tetrahedron of site i."

Pyrochlore FeF_3: A geometrical frustrated system

MC result: neutron structure factor



The peaks in the graph (T=24.3 K) are related to the all-in/all-out order.

N. Rezaei, M. Alaei, H. Akbarzadeh, Computational Materials Science, 202, 110947 (2022)

Implementing a more general Hamiltonian

$$H = \sum_{i,j>i} \mathbf{S}_i^T \mathbb{J}_{ij} \mathbf{S}_j + \sum_i \mathbf{S}_i^T \mathbb{A}_i \mathbf{S}_i$$

- $\mathbb{J}_{ij}$: J matrix
- $\mathbb{A}_i$: single-ion anisotropy matrix

$$\mathbb{J}_{ij} = J_{ij}\mathbb{I} + \mathbb{D}_{ij} + \mathbb{K}_{ij}$$

- $J_{ij} = (\mathbb{J}_{ij,xx} + \mathbb{J}_{ij,yy} + \mathbb{J}_{ij,zz})/3$
- $\mathbb{D}_{ij} = (\mathbb{J}_{ij} - \mathbb{J}_{ij}^T)/2$
- $\mathbb{K}_{ij} = (\mathbb{J}_{ij} + \mathbb{J}_{ij}^T)/2 - J_{ij}\mathbb{I}$

maintenance and financial support

Thanks to

- Dr. Akbarzadeh,
- Dr. Shahbazi,
- Dr. Hashemifar

Thank you for your attention