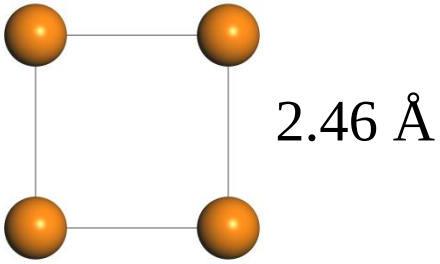
11月9日上机实习安排

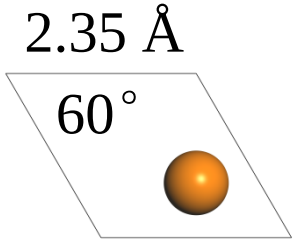
使用MS软件CASTEP模块完成：

Spin-polarized calculation for magnetic Fe membranes:

1. Build slab models for square & triangular Fe membranes
2. **(No Geometry optimizations !!!)** directly perform spin-polarized calculations for different magnetic states
3. Perform spin-polarized calculations for BCC & HCP Fe bulks



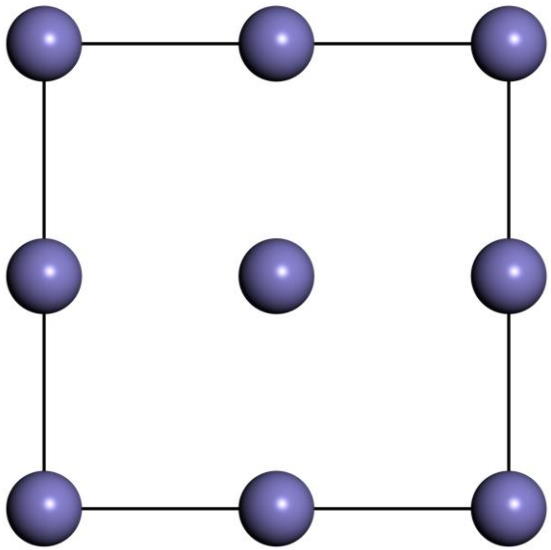
FCC(100)_Square Membrane

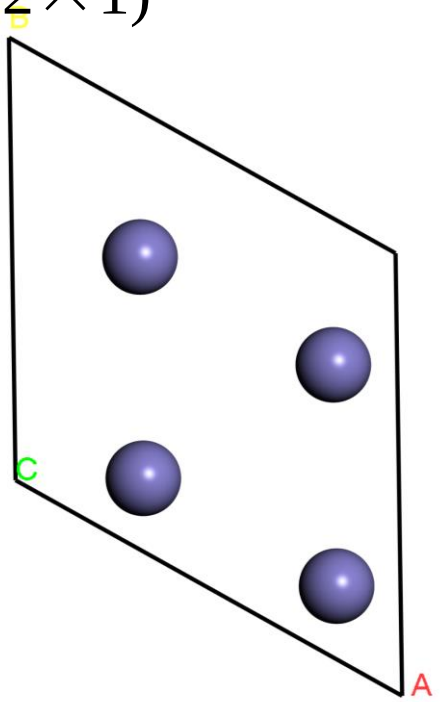


HCP(001)_Rhombic Membrane

1. Build the Slab Models

- Cleave surface along (100) plane of BCC Fe bulk (thickness: 0.5) or along (001) plane of HCP Fe bulk (thickness: 0.5)
- Add 20 Å-vacuum layer
- Build → Symmetry → Supercell (2×2×1)

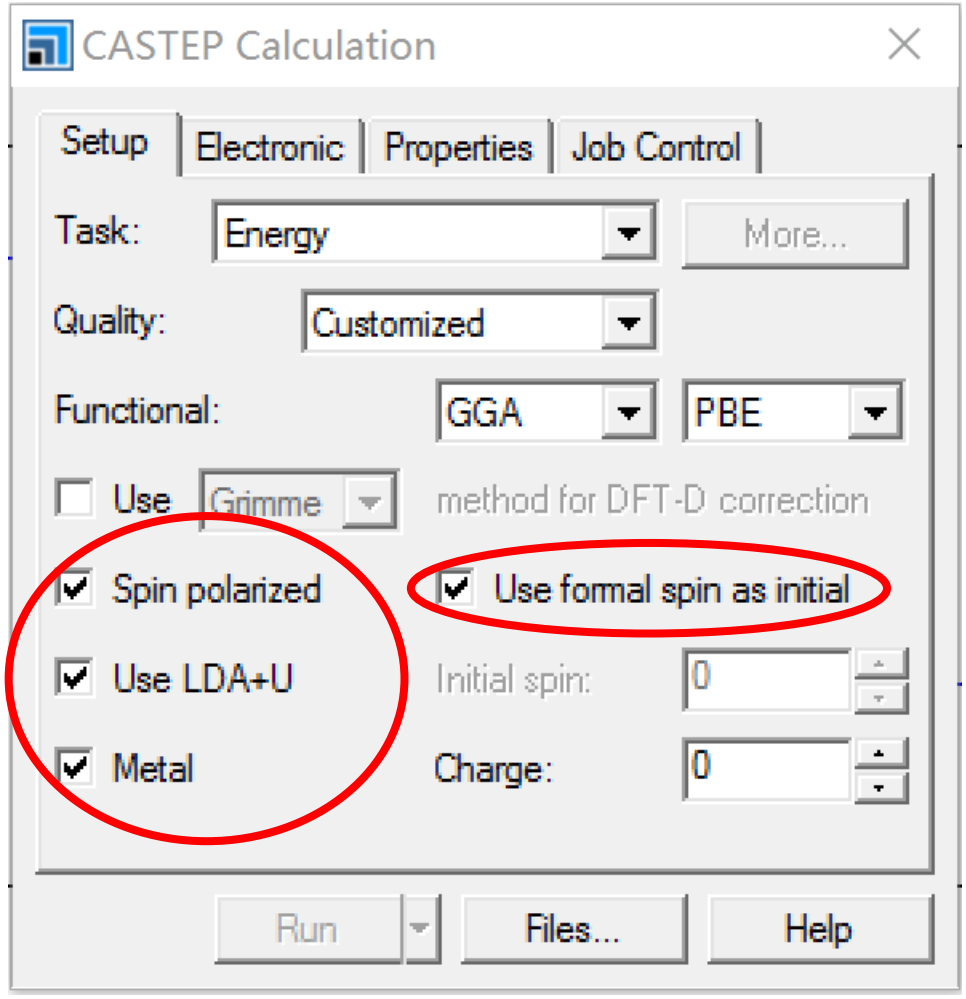




2. Single-Point Calculations for Different Magnetic States

Computational Setting:

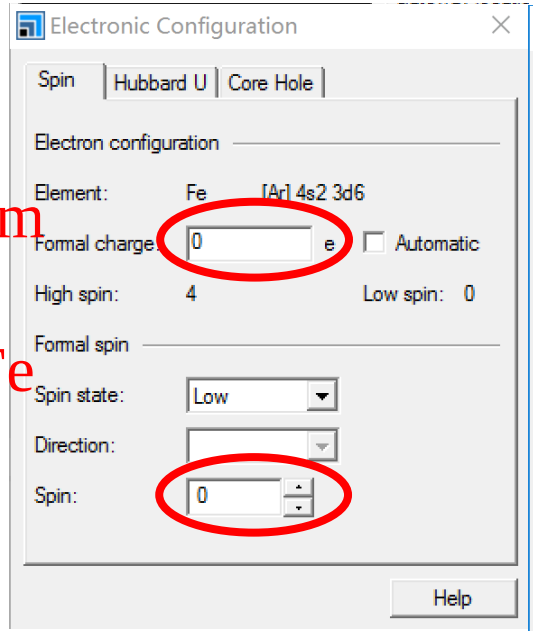
- Method PBE
- Mark “Spin polarized”
- Mark “Use formal spin as initial”
- Mark “Use LDA+U”
- Mark “Metal”
- Cutoff energy: 400 eV
- FFT grid density: standard
- SCF tolerance: 1e-6 eV/atom
- *K* points: 3×3×1 for membranes
  versus 3×3×3 for bulks

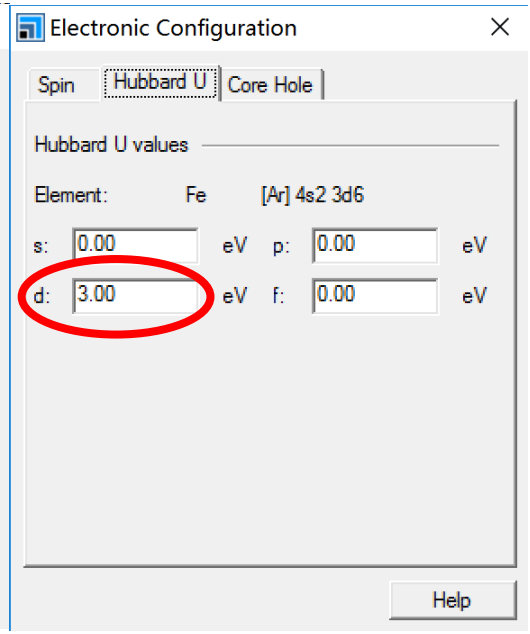


2. Single-Point Calculations for Different Magnetic States

Electronic Configuration Setting:
(Modify → Electronic Configuration)

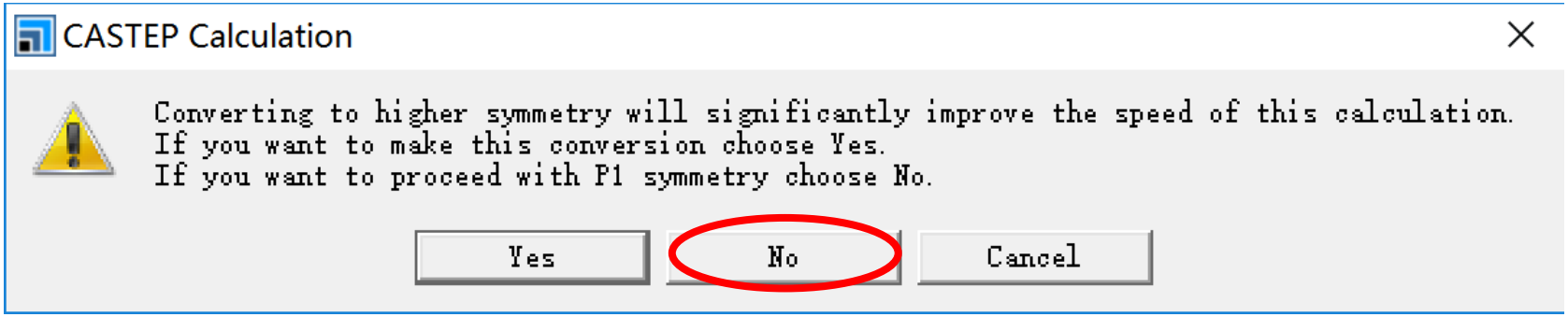
- Formal charge: 0
- Formal spin: changed for different magnetic states from 0 to 4
- Hubbard *U* for *d* orbital of Fe atoms: 3.00 eV





2. Single-Point Calculations for Different Magnetic States

Choose “No” to start the single-point calculations.



2. Single-Point Calculations for Different Magnetic States

- With the variation of formal spin (from 1 to 4), the energies of Fe membranes with different magnetic states are estimated, learning from *.castep file.
- The one with the lowest energy would be the most possible magnetic state that we search for.
- Compare to the Fe bulks and make conclusion.

No.	Formal spin	Initial spin polarization	Initial magnetic moment (μB)	Spin Density vs |Spin Density|	Magnetism	Total Energy (eV)
2	+1	0.125	1.0	2.5 < 5.9	Ferri-	-3441.581316652
3	+2	0.25	2.0	11.7 < 13.4	Ferri-	-3435.849412061
4	**+3**	**0.375**	**3.0**	**12.5 ≈ 12.6**	**Ferro-**	**-3445.891802259**
5	+4	0.5	4.0	13.8 < 16.2	Ferri-	-3439.082098653

Done by VASP

VASP Calculations

- **INCAR (input parameter setting)**
- KPOINTS (*k*-point setting)
- POSCAR (coordination for structure, cif (from MS)→*.vasp generated by **VESTA** software)
- POTCAR (PW-PP information)

INCAR for Geometry Optimization

```
ALGO = Fast
PREC = Normal
ENCUT = 500
EDIFF = 1E-5
EDIFFG = -0.05
ISMEAR = 0       #smearing method for the Gaussian smearing
SIGMA = 0.02     #determines the width of the smearing in eV
LREAL = Auto     #determines the projection operators evaluated in real or reciprocal space
NELM = 100       #the maximum number of electronic SC (selfconsistency) steps
#optimization setting
IBRION = 2       #optimization method for the conjugate gradient algorithm
ISIF = 3         #update lattice parameters, atomic position, force
NSW = 600        #optimization cycle
#print control
LORBIT = 11
LWAVE = .FALSE.
LCHARG = .FALSE.
#add vdW corrections
IVDW = 11        #D3
```

Output: CONTCAR (final structure)
OUTCAR
summary file

KPOINTS File

```
Automatic-mesh
0
Monkhorst-Pack
12  12   1
  0.   0.  0.
```

POSCAR File

CIF file
1.0
2.4600000381 0.0000000000 0.0000000000
-1.2300000191 2.1304225263 0.0000000000
0.0000000000 0.0000000000 20.0000000000
C
2
Direct
0.000000000 0.000000000 0.000000000
0.666670024 0.333330005 0.000000000

POTCAR File

PAW C_GW 28Sep2005
4.00000000000000
parameters from PSCTR are:
VRHFIN =C: s2p2
LEXCH = PE
EATOM = 147.1560 eV, 10.8157 Ry

TITEL = PAW C_GW 28Sep2005
LULTRA = F use ultrasoft PP ?
IUNSCR = 0 unscreen: 0-lin 1-nonlin 2-no
RPACOR = 0.000 partial core radius
POMASS = 12.011; ZVAL = 4.000 mass and valenz
RCORE = 1.500 outmost cutoff radius
RWIGS = 1.630; RWIGS = 0.863 wigner-seitz radius (au A)
ENMAX = 413.992; ENMIN = 310.494 eV
ICORE = 2 local potential
LCOR = T correct aug charges
LPAW = T paw PP
.....

INCAR for **High-Accuracy** Single-Point Calculation (Charge Density)

ALGO = Normal

ENCUT = 500

PREC = Accurate

LREAL = Auto

ISTART = 0 #determines whether to read the file WAVECAR or not

ICHARG = 2 #determines how to construct the 'initial' charge density

ISMEAR = 0

SIGMA = 0.02

LORBIT = 11

LWAVE = .TRUE.

LCHARG = .TRUE.

IVDW = 11

NELM = 300

EDIFF = 10E-6

Enlarge *K* points

Output: CHGCAR

INCAR for Band Structure

ALGO = Normal
ENCUT = 500
PREC = Accurate
LREAL = Auto
LORBIT = 11
LWAVE = .FALSE.
LCHARG = .FALSE.
IVDW = 11
ISTART = 1
ICHARG = 11 #for a given charge density read from CHGCAR
ISMEAR = 0
SIGMA = 0.02
NELM = 300
EDIFF = 10E-6

Output: EIGENVAL

KPOINTS for Band Structure

```
k-points along high symmetry lines
30   ! 30 intersections
Line-mode
rec
0.000  0.000  0.000   ! GM
0.500  0.000  0.000   ! M

0.500  0.000  0.000   ! M
0.500  0.000  0.500   ! L

0.500  0.000  0.500   ! L
0.667  0.333  0.500   ! H

0.667  0.333  0.500   ! H
0.667  0.333  0.000   ! K

0.667  0.333  0.000   ! K
0.000  0.000  0.000   !GM
```

INCAR for DOS

ALGO = Normal
ENCUT = 500
PREC = Accurate
LREAL = Auto
LORBIT = 11
LWAVE = .FALSE.
LCHARG = .FALSE.
IVDW = 11
ISTART = 1
ICHARG = 11
ISMEAR = 0
SIGMA = 0.02
NELM = 300
EDIFF = 10E-6
#control DOS
EMIN = -5.24 #minimum energy for evaluation of DOS
EMAX = 4.76 #maximum energy for evaluation of DOS
NEDOS = 301 #number of grid points in DOS

Output: DOSCAR

Determined by Fermi Level

INCAR for PDOS

ALGO = Normal
ENCUT = 500
PREC = Accurate
LREAL = Auto
IVDW = 11
ISTART = 1
ICHARG = 11
ISMEAR = 0
SIGMA = 0.02
NELM = 300
EDIFF = 10E-6
LORBIT = 11
LWAVE = .FALSE.
LCHARG = .FALSE.
# VB and CB partial charge
LPARD = .TRUE. #Evaluate partial (band and/or k-point) decomposed charge density
IBAND = 261 262
NBMOD = 2 #Number of values in the array IBAND
LSEPB = .TRUE. #Specifies the charge density calculated for every band separately

Output: PARCHG.261.ALLK
PARCHG.262.ALLK

INCAR for Magnetism

#open the spin-orbital
LSORBIT = .TRUE.
LNONCOLLINEAR = .TRUE. #perform fully non-collinear magnetic structure calculations
SAXISR = 0 1 0 #direction of the magnetic field
RWIGS = 1.630 1.100 1.400 2.200 #Wigner Seitz radius read from POTCAR
MAGMOM = 216*0.0 0.866 -0.5 0.0 0.866 0.5 0.0 0.0 1.0 0.0
LMAXMIX = 4 #for d elements
GGA_COMPAT = .FALSE. #apply spherical cutoff on gradient field

Output: OUTCAR