Computational Material Science
Part II-1: introduction

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Outline

• Introduction of Computational Material Science (CMS)
• Density Functional Theory (DFT) and local-density approximation (LDA)
• Crystal structure, reciprocal lattice, and Brillouin Zone
• Band theory, band structure, k-points sampling, and density of state
• Plane wave, pseudopotential, LDA, and LSDA
• Transition-metal oxides, strong correlations, and LDA+U method
• Structure optimization
• Surface and molecule
Hands-on during the lectures

- unix or linux: operating systems
- VASP (Vienna Ab-initio Simulation Package): perform first-principles calculations
- Xmgrace (or gnuplot): plot the calculated density of states and band structures
- Vaspview: visualize the lattice structure, charge distribution, and spin density
References

- http://cms.mpi.univie.ac.at/vasp/vasp/vasp.html
Review of CMS

- Atomic and electronic structure of solids
- Theoretical considerations
- Applications: ground state property calculations
- First-principles study on novel and nano materials
- Limitations
Theoretical considerations

Ab-initio calculation = First-principles study
\[ \Rightarrow \text{based on quantum mechanics} \]

Simple example:
Schrodinger eqn. for 1 hydrogen atom

\[
-\frac{\hbar^2}{2\mu} \left[ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right] \psi(x, y, z) + V(x, y, z) \psi(x, y, z) = E \psi(x, y, z)
\]

\[
\frac{V(r) = -\frac{Ze^2}{r}}{\psi(r) = R(r)Y(\theta, \phi)} \rightarrow \left[ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + \frac{2\mu}{\hbar^2} \left( E + \frac{Ze^2}{r} - \frac{\hbar^2 l(l+1)}{2\mu r^2} \right) \right] R(r) = 0
\]
Real solids

Ions: \( \left( \{ \vec{R}_I \}, \{ \vec{P}_I \}, \{ Z_I \}, \{ M_I \} \right) \)

Electrons: \( \left( \{ \vec{r}_i \}, \{ \vec{p}_i \}, m \right) \)

\[
H = \sum_{I=1}^{N} \frac{\vec{p}_I^2}{2M_I} + \sum_{i=1}^{N} \frac{\vec{p}_i^2}{2m} + \sum_{i>j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} + \sum_{i>j} \frac{Z_I Z_J e^2}{|\vec{R}_I - \vec{R}_J|} - \sum_{i,j} \frac{Z_i e^2}{|\vec{R}_I - \vec{r}_i|}
\]

\[
= T_N + T_e + V_{ee}(\vec{r}) + V_{NN}(\vec{R}) + V_{Ne}(\vec{r}, \vec{R})
\]

\[
\Rightarrow \left[ T_N + T_e + V_{ee}(\vec{r}) + V_{NN}(\vec{R}) + V_{Ne}(\vec{r}, \vec{R}) \right] \Psi(x, \vec{R}) = E \Psi(x, \vec{R})
\]

\[
x \equiv (\vec{r}, s)
\]
Adiabatic approximation

Born-Oppenheimer approximation:
Decupling I and e ($M_1 \gg m_e$)

$$\Psi(x, \vec{R}) = \psi(x, \vec{R}) \phi(\vec{R})$$

$$\begin{align*}
\left[ T_e + V_{ee}(\vec{r}) + V_{Ne}(\vec{r}, \vec{R}) \right] \psi_n(x, \vec{R}) &= \epsilon_n(\vec{R}) \psi_n(x, \vec{R}) \\
\left[ T_N + V_{NN}(\vec{R}) + \epsilon(\vec{R}) \right] \phi(\vec{R}) &= E \phi(\vec{R})
\end{align*}$$
Independent-particle approximation: Hartree-Fock method

- Many-electron wavefunctions = Slater-determinants

\[
\Psi^{\alpha}_{\alpha_1 \ldots \alpha_N} (q_1, \ldots, q_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix}
\phi_{\alpha_1}(q_1) & \cdots & \phi_{\alpha_1}(q_N) \\
\vdots & & \vdots \\
\phi_{\alpha_N}(q_1) & \cdots & \phi_{\alpha_N}(q_N)
\end{vmatrix}
\]

\[= \frac{1}{\sqrt{N!}} \sum_{P} (-1)^P P \phi_{\alpha_1}(q_1) \cdots \phi_{\alpha_N}(q_N)\]

- Variational condition

\[
\delta \left( \frac{\langle \Psi^a | H | \Psi^a \rangle}{\langle \Psi^a | \Psi^a \rangle} \right) = 0
\]

Variation with respect to the one-electron orbitals \(\phi_\alpha\)
Key ideas (approximations)

- Periodic boundary condition:
  \# of atom: \(O(10^{23}) \rightarrow O(10^{1000})\)

- Density functional theory:
  \[ j(r) \rightarrow n(r) \]

- Plane wave vs atomic orbital

- All-electron vs pseudopotential:
  \# of e in an atom:
  \(O(10\sim 100) \rightarrow O(1\sim 10)\)

- Exchange-correlation (xc) energy:
  mimic many-body effects
Applications to versatile materials

Band structure and density of state

Electronic structures of semiconductors

<table>
<thead>
<tr>
<th>Method</th>
<th>$a_0$ (Å)</th>
<th>$B_0$ (GPa)</th>
<th>$B_0'$</th>
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<tr>
<td>LDA (GGA)</td>
<td>3.57 (3.62)</td>
<td>376.71 (365.43)</td>
<td>3.68 (3.49)</td>
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<tr>
<td>Expt.</td>
<td>3.62</td>
<td>369-400</td>
<td>4.0</td>
</tr>
</tbody>
</table>
Phase transitions in Se & Te under compression
Phonon/Structural instability & ferroelectricity in perovskites:
Density Functional Perturbation Theory (linear response)
Charge and spin density distribution

Jeng et al PRB (2003)

FIG. 4. Valence charge (upper panel) and spin (lower panel) densities of Sr$_2$CrWO$_6$ from the GGA. In the upper panel, the contours are along equal charge density lines from 0.015 to 0.065$a_0^3$ (broken lines) with step 0.01$a_0^3$, and from 0.1 to 0.83$a_0^3$ (solid lines) with step 0.15$a_0^3$. In the lower panel, they are from −0.005 to −0.03$a_0^3$ (broken lines) with step −0.005$a_0^3$, and from 0.01 to 0.16$a_0^3$ (solid lines) with step 0.03$a_0^3$. 
Magnetocrystalline anisotropy

Jeng et al PRB (2002)

FIG. 1. Crystal structure of Fe$_3$O$_4$. Big balls denote oxygen atoms, small dark balls denote A-site (tetrahedral) iron atoms, and small light balls denote B-site (octahedral) iron atoms.

FIG. 8. The fourth-order anisotropy constant $K_1$ (a) and the out-of-plane anisotropy constant $K_{out}$ (b) as a function of the lateral strain in the (001) plane of Fe$_3$O$_4$. The lines are a guide to the eye only. The arrows in (a) indicate the experimental $K_1$ value at 300 K and 0 K (see text). The arrows in (b) indicate the possible strain values if an Fe$_3$O$_4$ film is grown on Mn$_2$O$_4$, NiO, MgO, and CoO substrates, respectively.
Spin and orbital magnetic moment

Jeng et al JAP (2002)

FIG. 1. Rutile structure of CrO$_2$. Big light balls denote Cr atoms and small dark balls denote O atoms.

TABLE II. Calculated spin and orbital magnetic moments and O in CrO$_2$ from the LSDA ($U=J=0$ eV) and from the LSDA+$U$. The on-site Coulomb energy $U$ is in units of eV and the exchange parameter $J=0.87$ eV.

<table>
<thead>
<tr>
<th>$U$ (eV)</th>
<th>Cr spin ($\mu_B$)</th>
<th>Orbital ($\mu_B$)</th>
<th>$L/S$ (%)</th>
<th>O spin ($\mu_B$)</th>
<th>Orbital ($\mu_B$)</th>
<th>$L/S$ (%)</th>
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<tr>
<td>0</td>
<td>1.89</td>
<td>-0.037</td>
<td>-2.0</td>
<td>-0.042</td>
<td>-0.0011</td>
<td>2.6</td>
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<td>-0.046</td>
<td>-2.4</td>
<td>-0.058</td>
<td>-0.0019</td>
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<td>3</td>
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<td>-0.051</td>
<td>-2.6</td>
<td>-0.079</td>
<td>-0.0025</td>
<td>3.2</td>
</tr>
<tr>
<td>4</td>
<td>2.03</td>
<td>-0.056</td>
<td>-2.8</td>
<td>-0.094</td>
<td>-0.0030</td>
<td>3.2</td>
</tr>
<tr>
<td>6</td>
<td>2.08</td>
<td>-0.057</td>
<td>-3.2</td>
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<td>-0.083</td>
<td>-3.9</td>
<td>-0.124</td>
<td>-0.0047</td>
<td>3.8</td>
</tr>
</tbody>
</table>
Projected density of state

FIG. 2. (Color online) DOS of Mn 3d in LCaMO and LCeMO calculated by LDA+U method. The parameters used in these calculations are described in the text.
FIG. 2. Charge densities of cubic Fe$_3$O$_4$ versus radial distance in units of atomic radius $a_0$. The charge densities projected to different orbitals with magnetic quantum number $m$ were obtained from (a) LDA and (b) LDA + U calculations.
Charge orbital ordering

FIG. 1 (color). (a) Crystal structure of the monoclinic Fe₃O₄, (b) Orbital ordering in B-site sublattice, x-y-z and a-b-c are, respectively, the local and global coordinates.

FIG. 2 (color). Left: monoclinic crystal structure of Fe₃O₄ in the low-temperature phase corresponding to a subcell of \( \frac{a}{\sqrt{2}} \times \frac{a}{\sqrt{2}} \times 2a \) with \( P2_1/c \) symmetry. Right: 3D isosurfaces of unoccupied density of states of the O 2p integrated between the Fermi level and 1 eV above within the corresponding Fe₃O₄ cubes highlighted in the crystal structure. For simplicity, we denote the octahedral Fe site with nominal 2+ and 3+ valences as Fe²⁺ and Fe³⁺, respectively.

 Orbital ordering

Jeng et al PRL (2006)

FIG. 4 (color). OO of SrRuO$_3$. Blue, green, and red balls are, respectively, Sr, Ru, and O ions. The origin has been shifted to ($-1/3, -1/3, -1/3$).
Novel magnetic materials

- **Magnetic carbon** in pure carbon system (polymerized C$_{60}$), Makarova *et al.* found a ferromagnetic signal at room temperature. ([Nature 413 (2001)](https://www.nature.com/articles/nature00798))

- **C/BN zigzag nanotubes** periodic arrangements of C/BN hetero-junctions can lead to the formation of a one-dimensional itinerant ferromagnetic state. ([PRB 67 (2003)](https://journals.aps.org/prb/abstract/10.1103/PhysRevB.67.014411))

- **Ferromagnetic fullerenes** a moderate large $m$ (\(~10$ μB\)) at the open edge of defective C$_{60}$ ([PRB 68 (2003)](https://journals.aps.org/prb/abstract/10.1103/PhysRevB.68.205405))
Ground state properties (LDA)

- Ground-state properties (DFT)
  Atomic structure (bond length, lattice constants)
  Phase stability
  Phonon
  Cohesive energy
  Band structure (v)
  Magnetization ...

- Excitation (beyond DFT)
  Optical spectrum
  Band structure (band-gap problem)
  Excitation ...

[Diagram showing independent particles and quasiparticles]
Beyond LDA

- LDA+U
- Self-Interaction Correction (SIC)
- GW Approximation (GWA)
- Optimized Effective Potential method (OEP)
- Time-Dependent Density Functional Theory (TDDFT)
- Quantum Monte-Carlo method (QMC)
- Dynamical Mean Field Theory (DMFT)
- . . . .
LDA+U for transition metal oxide NiO

- Excitation: LDA, LDA+U vs. experiment (inelastic X-ray scattering)

- LDA+U ➔ great improvement at small q
LDA+U for low-T magnetite Fe$_3$O$_4$


FIG. 2. Spin-resolved density of states of Fe$_3$O$_4$ in low-T monoclinic $P2_1/c$ structure from GGA (a), GGA+U (b), and GGA+U under lattice relaxation (c). The Fermi level is at zero energy.
Band gap problem in semiconductors: GWA

\[ E_{\text{gap}} = \mu(N+1) - \mu(N) = E_{\text{gap}}^{\text{KS}} + \Delta_{\text{xc}} \]
CMS II-1 Hands-on: Unix, vi, VASP, total energy, and convergence

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Unix

Login: guest ← account name
Password: ******* (abcdef) ← password

Change password: %passwd

Frequently used command

% pwd  show the full path of the current directory

% cd ../Fe  change directory

% ls *.f  list all files with extension name of .f

% ls -l  (long list)
% ls -l
-rwxrwxrwx 1 users user 4564 Jun11 20:45 love
dr--r----- 2 users user 547 Jun11 22:50 sub/
-rw-rw-r-- 1 users user 4135 Jun21 11:20 t1

% chmod u+x filename
% chmod 741 filename

% ls -a (list hidden files, eg .csrch .login)
% ls -F (add * at the end of executable files, add / at the end of directories)
% mkdir dname

% rmdir dname, rm -rf dname

% rm filename (delete filename)

% mv filename1 filename2 (change name)

% cp [-i p r ] filename target (copy)
   i:to make sure
   p:keep the original time
   r:copy directory

% cat filename (>test)
   Show the content of filename and put into another file (test)

% more filename, less filename
   Show the content of filename page by page
% head –n filename
    Show the first n lines of filename

% tail –n filename (>>test)
    Show the last n lines of filename and put at the end of test

% grep –i string filename
    Find all lines of filename containing string ignoring upper or lower cases

% grep ‘total energy’ filename

% find directory –name filename –print
    Find filename in directory and list the full path
ls hw? → hw2, hw3, hw4
ls hw?? → hw11, hw12
ls hw* → hw2, hw3, hw4, hw11, hw12
ls hw[2-11] → hw2, hw3, hw4, hw11
ls hw{2,12} → hw2, hw12
ls test[a-c] → testa, testb, testc

**alias**

alias la ls-a;
alias ch1 ‘cd /usr/john ; ls-l’
alias rm ‘rm –i’;
alias hm ‘history | more ’

**unalias**

Unalias ch1

**alias:** Show the available alias
Vi editor

% vi filename

There are 2 modes in vi editor: (1) insert mode, (2) command mode

- **insert mode**: To key-in characters
  - i, a, o, I, A, O

- **command mode**: To handle the file
  - ESC
  - h(←), j(↓), k(↑), l(→)

- Go to the nth line: nG
- Go to the last line: G
- Show line number of the cursor: ^g
- Next page: ^f
- Last page: ^b
x               delete a character
dd              delete a line
ndd             delete n lines
u               undo the last command
p,P             paste
/string         search for string
:q!             Quit
:wq             save and quit
:w filename     save as filename
:set nu         show line number
:1,$ s/string1/string2/g replace string1 by string2
:n1,n2 w filename write line n1 to n2 into filename
:r filename     read from filename
VASP
Vienna Ab-initio Simulation Package

- **VASP Home Page**
  http://cms.mpi.univie.ac.at/vasp/

- **Hands-on tutorial course on VASP**
  http://cms.mpi.univie.ac.at/vasp-workshop/

- **VASP Manual**
  http://cms.mpi.univie.ac.at/vasp/vasp.html
Total energy calculation: Si(Dia)

- Many properties depend on the total energy of the system
- Equilibrium Lattice constant
- Bulk module, Elastic constant
- Phase transition, surface reconstruction
- Bonding, Structure, …
- The most important point is to make sure your calculation is convergent (vs # of kpoints, cutoff energy, …)
Work list

- Setup bulk calculation for Si(Dia) using experimental lattice structure as input
- Increase the number of k-points (density of k-mesh) from (4 4 4), (8 8 8), ..., till the calculated total energy is convergent
- Increase the cutoff energy from default value to 1.2, 1.4, ... times of default value to see the convergence of the total energy
Setup bulk calculation for Si(Dia)

• Make a working directory for Si
  \%mkdir si
• Goto the working directory si
  \%cd si
• Prepare the four input files
  INCAR: control parameters
  KPOINTS: BZ integration
  POSCAR: lattice structure
  POTCAR: pseudopotential
• Run the VASP code
  \%vasp4620s&
INCAR

SYSTEM = Si Diamond
DOS related values
ISMEAR = -5
RWIGS = 1.1

Title

comment
Tetrahedron method
Atomic radius

KPOINTS

Si Diamond
0
Mondhorst-Pack
16 16 16
0 0 0

title
Automatic mesh
Mondhorst-Pack type mesh
K-point density in BZ
Shift of the mesh
POSCAR

Si Diamond
5.43
0.0 0.5 0.5
0.5 0.0 0.5
0.5 0.5 0.0
2
Direct
0.0 0.0 0.0 ! Si
0.25 0.25 0.25 ! Si

Title
Lattice constant in Å
a1 a2 a3
b1 b2 b3
c1 c2 c3
# of atoms in unit cell
Use a, b, c as the basis vectors
Atomic positions (in a,b,c)
Atomic positions (in a,b,c)

Diamond structure
Example: fcc structure

\[ \bar{k} = x_1 \bar{b}_1 + x_2 \bar{b}_2 + x_3 \bar{b}_3 \quad \bar{k} = \frac{2\pi}{a} (x_1, x_2, x_3) \]

\[ \bar{a}_1 = \frac{a}{2} (\bar{i} + \bar{k}) \]
\[ \bar{a}_2 = \frac{a}{2} (\bar{j} + \bar{k}) \]
\[ \bar{a}_3 = \frac{a}{2} (\bar{i} + \bar{j}) \]

\[ \bar{b}_1 = \frac{4\pi}{a} \frac{1}{2} (-\bar{i} + \bar{j} + \bar{k}) \]
\[ \bar{b}_2 = \frac{4\pi}{a} \frac{1}{2} (\bar{i} - \bar{j} + \bar{k}) \]
\[ \bar{b}_3 = \frac{4\pi}{a} \frac{1}{2} (\bar{i} + \bar{j} - \bar{k}) \]

<table>
<thead>
<tr>
<th>Point</th>
<th>Cartesian coordinates (units of 2\pi/a)</th>
<th>Reciprocal coordinates (units of b1,b2,b3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( G )</td>
<td>(0 0 0)</td>
<td>(0 0 0)</td>
</tr>
<tr>
<td>( X )</td>
<td>(0 0 1)</td>
<td>(1/2 1/2 0)</td>
</tr>
<tr>
<td>( W )</td>
<td>(1/2 0 1)</td>
<td>(1/2 3/4 1/4)</td>
</tr>
<tr>
<td>( K )</td>
<td>(3/4 3/4 0)</td>
<td>(3/8 3/8 3/4)</td>
</tr>
<tr>
<td>( L )</td>
<td>(1/2 1/2 1/2)</td>
<td>(1/2 1/2 1/2)</td>
</tr>
</tbody>
</table>

IBZ of fcc lattice
POTCAR
Copy POTCAR from potpaw Si directory

Ex: POTCAR of W

```
PAW W 19Jan2001
6.00000000000000000000000000000000
parameters from PSCTR are:
VRHFIN =W: 5p6s5d
LEXCH = CA
EATOM = 206.5370 eV, 15.1806 Ry

TITEL = PAW W 19Jan2001
LULTRA = F use ultrasoft PP?
IUNSCR = 1 unscreen 0-lin 1-nonlin 2-no
RPACOR = 2.330 partial core radius
POMASS = 183.850; ZVAL = 6.000 mass and valenz
RCORE = 2.750 outmost cutoff radius
RWIGS = 2.750; RWIGS = 1.455 wigner-seitz radius (au A)
ENMAX = 223.126; ENMIN = 167.344 eV
RCLOC = 2.147 cutoff for local pot

Description
 1 E  TYP  RCUT  TYP  RCUT
 2 .000  23 2.500
```

OUTCAR

vasp.4.6.9 24Apr03 complex
executed on SP2/3/4 date 2005.03.16 15:42:04
running on 1 nodes
cistr: one band on 1 nodes, 1 groups

I would recommend the setting:
dimension x,y,z NGX - 11 NGY - 11 NGZ - 63

NGX is ok and might be reduce to 16
NGY is ok and might be reduce to 16
NGZ is ok and might be reduce to 82

Found 15 irreducible k-points:
Following reciprocal coordinates:

<table>
<thead>
<tr>
<th>Coordinates</th>
<th>Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>.050000</td>
<td>.050000</td>
</tr>
<tr>
<td>.000000</td>
<td>4.000000</td>
</tr>
</tbody>
</table>

ion position nearest neighbor table

| 1  | .000 | .000 | .180 | 2.44 | 2.44 | 2.44 | 2.44 | 3.282 |
| 2  | .500 | .500 | .000 | 1.244| 3.244| 1.244| 3.244| 1.244 | 3.244 |

k-point 1: .0500 .0500 .0000 plane waves: 1255
k-point 2: .1500 .0500 .0000 plane waves: 1249

E-fermi: .7339 XC(G=0): -7.2761 alpha+bet : -6.2180
add alpha+bet to get absolute eigen values

grep E-fermi OUT*
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<th>k-point 1:</th>
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<th>0.0500</th>
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| k-point 2: | 0.1500 | 0.0500 | 0.0000 |

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<table>
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<th>Pullay stress</th>
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<table>
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<tr>
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<th>0.54 kB</th>
<th>Pullay stress</th>
<th>0.00 kB</th>
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<table>
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<tr>
<th>direct lattice vectors</th>
<th>reciprocal lattice vectors</th>
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<tbody>
<tr>
<td>-1.532408821 1.532408821 1.532408821 0.000000000 0.326283687 0.326283687</td>
<td>0.326283687 0.326283687 0.326283687 0.000000000 0.326283687 0.326283687</td>
</tr>
<tr>
<td>1.532408821 -1.532408821 1.532408821 0.326283687 0.000000000 0.326283687</td>
<td>0.326283687 0.326283687 0.326283687 0.000000000 0.326283687 0.326283687</td>
</tr>
</tbody>
</table>
### total charge

<table>
<thead>
<tr>
<th># of ion</th>
<th>s</th>
<th>p</th>
<th>d</th>
<th>tot</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>.291</td>
<td>.281</td>
<td>6.106</td>
<td>6.778</td>
</tr>
<tr>
<td>2</td>
<td>.411</td>
<td>.433</td>
<td>6.211</td>
<td>7.654</td>
</tr>
<tr>
<td>3</td>
<td>.411</td>
<td>.434</td>
<td>6.163</td>
<td>7.088</td>
</tr>
<tr>
<td>4</td>
<td>.411</td>
<td>.435</td>
<td>6.211</td>
<td>7.654</td>
</tr>
<tr>
<td>5</td>
<td>.291</td>
<td>.281</td>
<td>6.106</td>
<td>6.778</td>
</tr>
<tr>
<td>tot</td>
<td>2.01</td>
<td>1.86</td>
<td>30.89</td>
<td>34.67</td>
</tr>
</tbody>
</table>

### magnetization (x)

<table>
<thead>
<tr>
<th># of ion</th>
<th>s</th>
<th>p</th>
<th>d</th>
<th>tot</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>.011</td>
<td>.003</td>
<td>2.867</td>
<td>2.880</td>
</tr>
<tr>
<td>2</td>
<td>.012</td>
<td>.036</td>
<td>2.271</td>
<td>2.223</td>
</tr>
<tr>
<td>3</td>
<td>.001</td>
<td>.036</td>
<td>2.462</td>
<td>2.425</td>
</tr>
<tr>
<td>4</td>
<td>.012</td>
<td>.036</td>
<td>2.271</td>
<td>2.223</td>
</tr>
<tr>
<td>5</td>
<td>.011</td>
<td>.003</td>
<td>2.867</td>
<td>2.880</td>
</tr>
<tr>
<td>tot</td>
<td>.00</td>
<td>-.10</td>
<td>12.74</td>
<td>12.63</td>
</tr>
</tbody>
</table>

---

Iteration 1(1)

- POTLOK: VPU time 2.28; CPU time 2.28
- SETDII: VPU time .27; CPU time .27
- EDDAV: VPU time 8.15; CPU time 8.16
- DOS: VPU time .00; CPU time .00

LOOP: VPU time 10.72; CPU time 10.77

LOOP+: VPU time 271.30; CPU time 271.92

---

Iteration 2(1)

---

General timing and accounting informations for this job:

- Total CPU time used (sec): 519.130
- User time (sec): 518.960
- System time (sec): .170
- Elapsed time (sec): 521.628

- Maximum memory used (kb): 53852.
- Average memory used (kb): 514.
E0: Cohesive energy:
Bulk total energy-atomic total energy
PROCAR

PROCAR new format
# of k-points: 1  # of bands: 9  # of ions: 2

k-point 1:
0.00000000 0.00000000 0.00000000 weight = 1.00000000

band 1 # energy -29.19030270 # occ. 2.00000000

ion  s  p  d  tot
1  .162  .138  .025  .325
2  .581  .089  .006  .676
tot  .743  .227  .031  1.001

band 2 # energy -13.97365697 # occ. 2.00000000

ion  s  p  d  tot
1  .181  .017  .001  .199
2  .158  .418  .006  .582
tot  .339  .435  .007  .814
<table>
<thead>
<tr>
<th>XDATCAR</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 2 50</td>
</tr>
<tr>
<td>.5000000E+03  .1000000E-08  .1000000E-08  .1000000E-08  .5000000E-15</td>
</tr>
<tr>
<td>0.100000000000000000000005E-03</td>
</tr>
<tr>
<td>CAR</td>
</tr>
<tr>
<td>bcc Fe</td>
</tr>
</tbody>
</table>


| .00000000  .00000000  .05500000 |
| .00000000  .00000000  .94500000 |
| .00000000  .00000000  .08205172 |
| .00000000  .00000000  .91794828 |
| .00000000  .00000000  .06383446 |
| .00000000  .00000000  .93616554 |
| .00000000  .00000000  .05825907 |
| .00000000  .00000000  .94174093 |
| .00000000  .00000000  .05727735 |
| .00000000  .00000000  .94272268 |
| .00000000  .00000000  .05571192 |
| .00000000  .00000000  .94428808 |
| .00000000  .00000000  .05710243 |
| .00000000  .00000000  .94289757 |

~
CHGCAR

((( chg ( i, j, k ) , i=1, nx ), j=1, ny ), k=1, nz )

beec Fe
1.0000000000000000
1.0000000000000000
0.0000000000000000
0.0000000000000000
1.0000000000000000
0.0000000000000000
0.0000000000000000
1.0000000000000000

Direct
0.0000000000000000
0.0000000000000000
0.0000000000000000
0.0000000000000000

84 84 84
.41098271954E+04 .38580593547E+04 .32456173636E+04 .23907855172E+04 .16323134731E+04
.10440738818E+04 .69452163253E+03 .48394643428E+03 .25149651632E+03 .15428370956E+03
.92653834837E+02 .55483939720E+02 .34042823873E+02 .21474147940E+02 .13548327933E+02
........
augmentation occupancies 1 33
.5244394E+00 -.3895205E+00 .6867841E-32 .9745050E-01 -.8804372E-32
........
.1622568E-01 -.1784093E-33 -.2752412E-18
augmentation occupancies 2 33
.5478642E+00 .1011816E+00 -.1371290E-33 -.5095633E-01 .6053117E-33
-.2851393E-33 .4943223E-01 -.2869968E-34 .1850662E-01 .3013137E-32
.1147544E+00 -.1892876E-32 -.2537948E-33 .3431420E-01 .2348182E-33
.1329508E+01 .0000000E+00 -.7399463E-33 .8218637E-01 .8516730E-33
.1488428E-16 .3152197E+00 .1110142E-31 .3496585E-33 .6755791E-01
.1888023E-33 .8410138E-17 .2572049E-01 .0000000E+00 .9750446E-34
.1262313E-01 -.6911072E-34 -.3365055E-19
K-point convergence test

- Use (4 4 4) k-mesh density in KPOINTS to calculate the cohesive energy
- Redo (8 8 8) record the cohesive energies
- Redo (12 12 12) … till a convergent cohesive energy is obtained
cutoff energy convergence test

- Use sufficient k-points KPOINTS to do the following calculations
- Find out the default cutoff energy (ENCUT) in OUTCAR
- Set a new line in INCAR to increase cutoff energy by 1.2 times larger and redo the calculation
  \[ \text{ENCUT} = ??? \]
- Set ENCUT 1.4 times larger … till convergent cohesive energy is obtained
Homework
please Email to jeng@phys.sinica.edu.tw

• K-point convergence test for Si(Dia) and C(Dia) using experimental lattice constant
• Cutoff energy convergence test for Si(Dia) and C(Dia) using experimental lattice constant