

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

- “Local Density Theory of Polarizability”, G. D. Mahan and K. R. Subbaswamy (1990).
- “Handbook of The Band Structure of Elemental Solids”, D. A. Papaconstantopoulos (1986).
- “Strong Coulomb Correlations in Electronic Structure Calculations”, V. I. Anisimov (2000)
- <http://cms.mpi.univie.ac.at/vasp/vasp/vasp.html>

Review of CMS

- Theoretical considerations for electronic structures of atoms and solids
- Applications: First-principles study on novel and nano materials
- limitations

Theoretical considerations

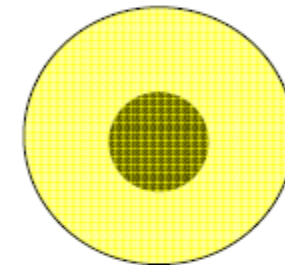
Ab-initio calculation = First-principles study

⇒ **based on quantum mechanics**

(no free parameter to adjust)

Simple example:

Schrodinger eqn. for 1 hydrogen atom



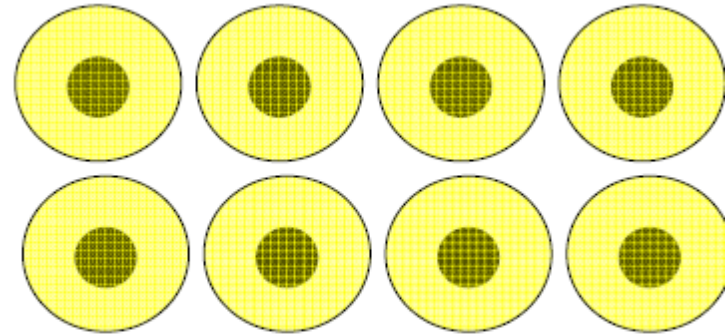
$$-\frac{\hbar^2}{2\mu} \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right] \psi(x, y, z) + V(x, y, z) \psi(x, y, z) = E \psi(x, y, z)$$

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

Real solids

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

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



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

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

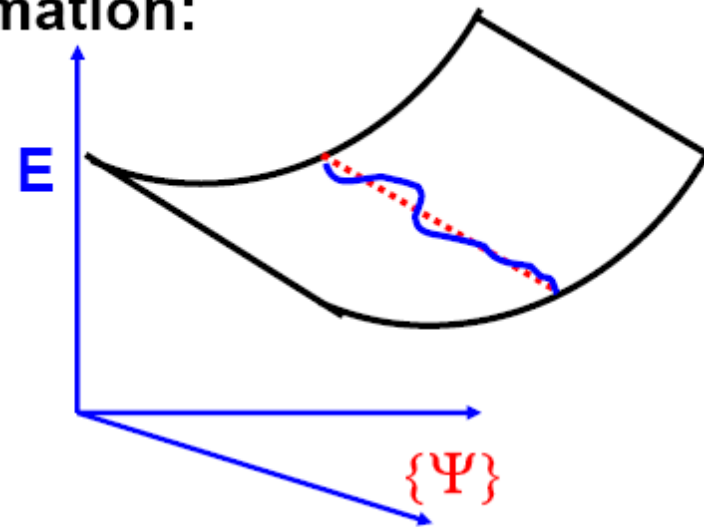
$$\Rightarrow \left[T_N + T_e + V_{ee}(\vec{r}) + V_{NN}(\vec{R}) + V_{Ne}(\vec{r}, \vec{R}) \right] \Psi(\mathbf{x}, \vec{R}) = E \Psi(\mathbf{x}, \vec{R})$$

$$\mathbf{x} \equiv (\vec{r}, s)$$

Adiabatic approximation

Born-Oppenheimer approximation:

Decoupling I and e ($M_I \gg m_e$)



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

$$\begin{cases} \left[T_e + V_{ee}(\vec{r}) + V_{Ne}(\vec{r}, \vec{R}) \right] \psi_n(x, \vec{R}) = \varepsilon_n(\vec{R}) \psi_n(x, \vec{R}) \\ \left[T_N + V_{NN}(\vec{R}) + \varepsilon(\vec{R}) \right] \phi(\vec{R}) = E \phi(\vec{R}) \end{cases}$$

Independent-particle approximation: Hartree-Fock method

- Many-electron wavefunctions = Slater-determinants

$$\begin{aligned}\Psi_{\alpha_1 \dots \alpha_N}^a(q_1, \dots, q_N) &= \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{\alpha_1}(q_1) & \cdots & \phi_{\alpha_1}(q_N) \\ \vdots & & \vdots \\ \phi_{\alpha_N}(q_1) & \cdots & \phi_{\alpha_N}(q_N) \end{vmatrix} \\ &= \frac{1}{\sqrt{N!}} \sum_P (-1)^P P \phi_{\alpha_1}(q_1) \cdots \phi_{\alpha_N}(q_N)\end{aligned}$$

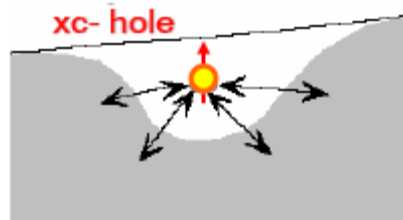
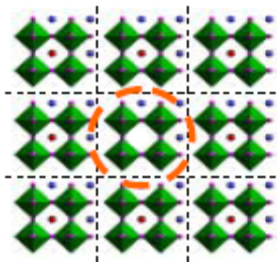
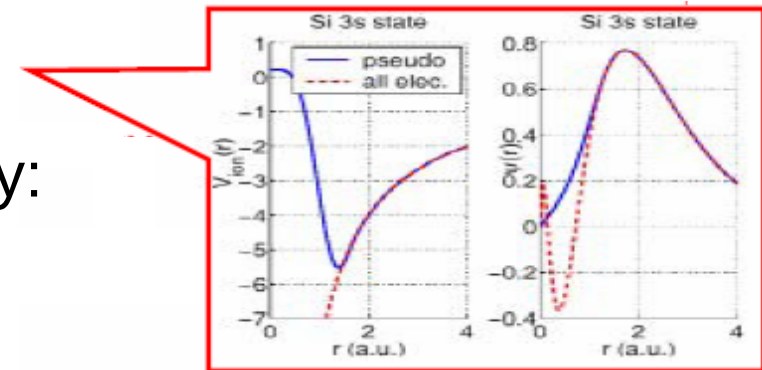
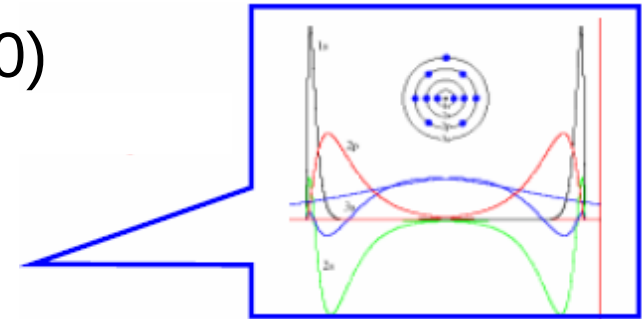
- Variational condition

$$\delta \frac{\langle \Psi^a | H | \Psi^a \rangle}{\langle \Psi^a | \Psi^a \rangle} = 0$$

Variation with respect to the one-electron orbitals ϕ_α

Key ideas (approximations)

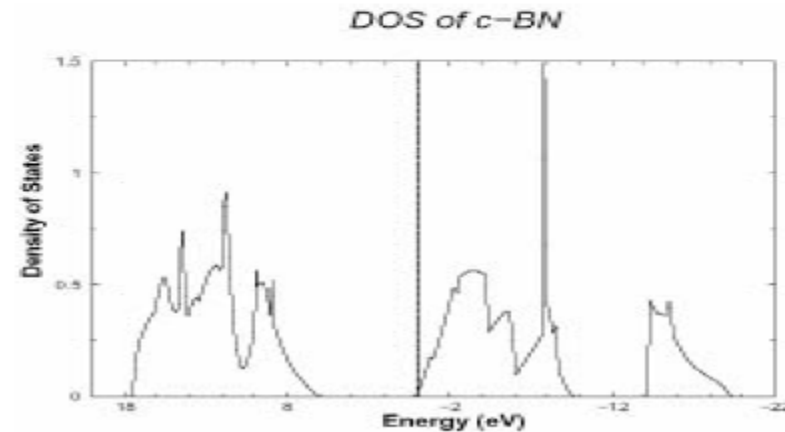
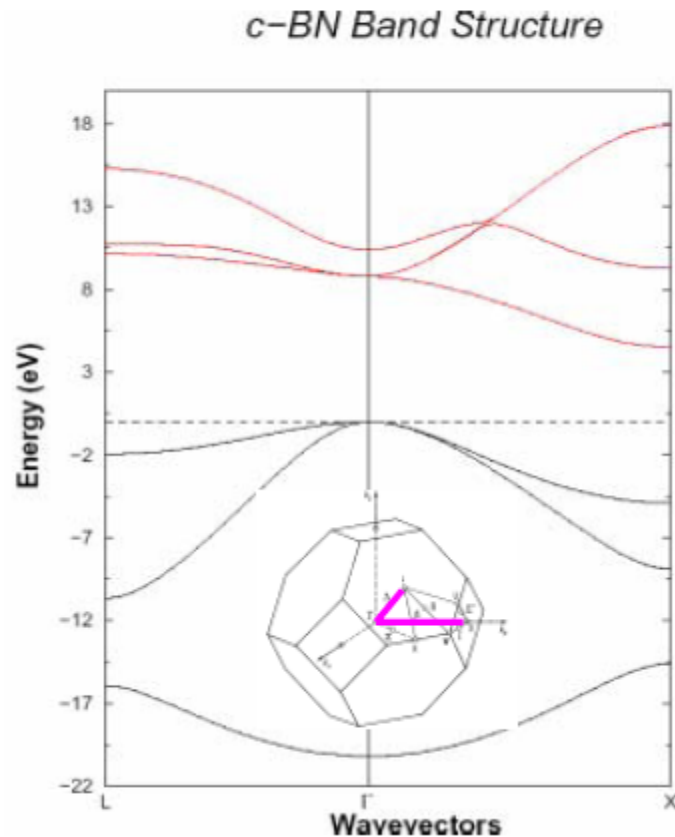
- Periodic boundary condition:
of atom: $O(10^{23}) \rightarrow O(10 \sim 1000)$
- Density functional theory:
 $\Psi_j(r) \rightarrow n(r)$
- Plane wave vs atomic orbital
- All-electron vs pseudopotential:
of e in an atom:
 $O(10 \sim 100) \rightarrow O(1 \sim 10)$
- Exchange-correlation (xc) energy:
mimic many-body effects



Applications to versatile materials

Band structure and density of state

Electronic structures of semiconductors



F-43m	a_0 (Å)	B_0 (GPa)	B_0'
LDA	3.57	376.71	3.68
(GGA)	(3.62)	(365.43)	(3.49)
Expt.	3.62	369-400	4.0

Spectroscopy of Cd₂Re₂O₇: Jeng et. al. JPCM 2009

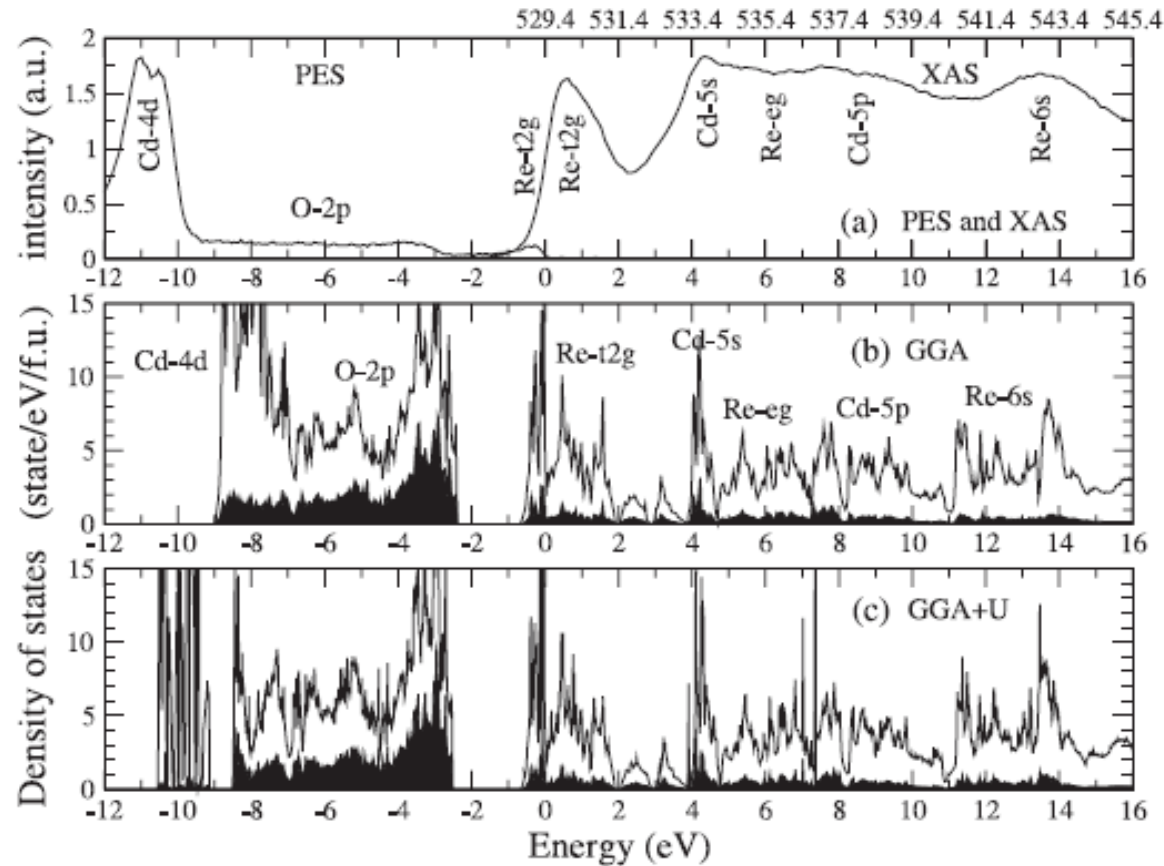
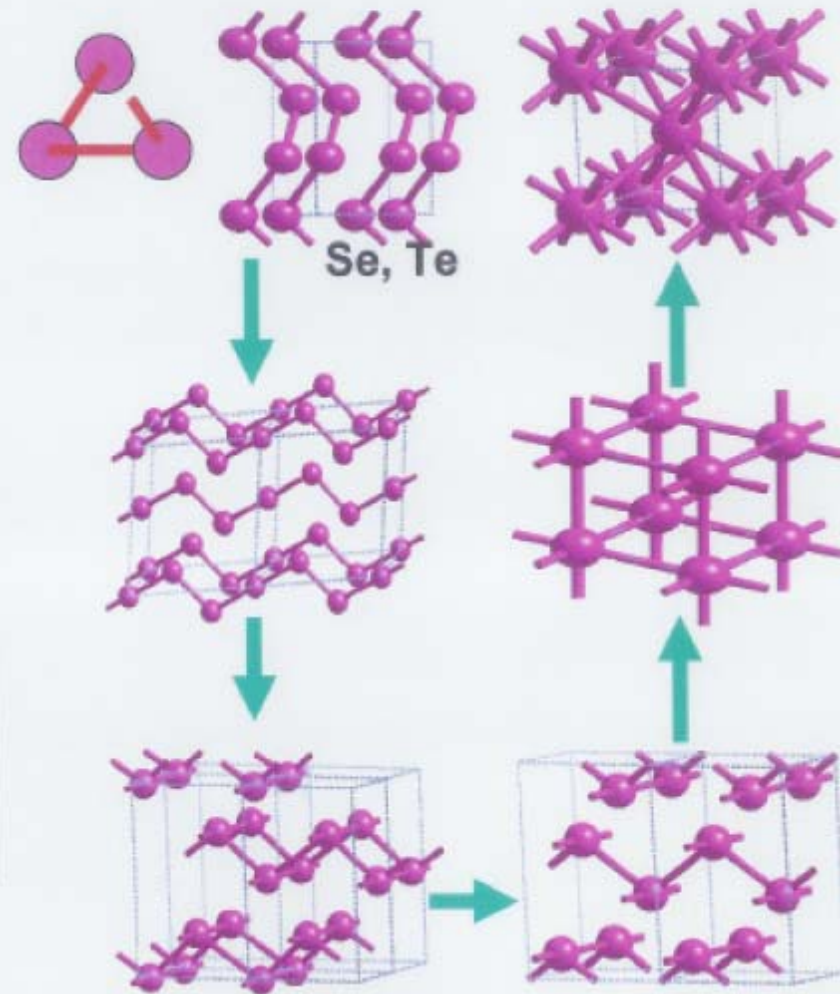
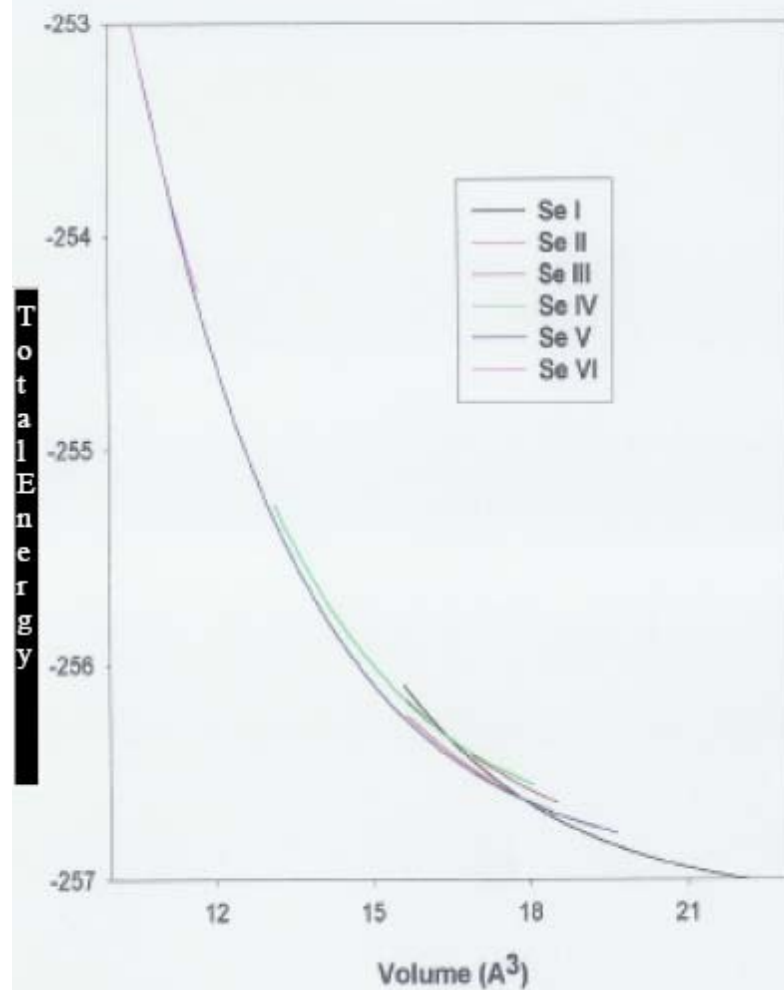


Figure 2. (a) PES [26] and O 1s XAS (this work) spectra of Cd₂Re₂O₇. The Fermi level of XAS is at 529.4 eV (reflection point method). (b) Total density of states from GGA (b) and GGA + *U* (c). The dark area in (b) and (c) are the contributions from O p states.

Phase transitions in Se & Te under compression



Charge and spin density distribution

Jeng et al PRB (2003)

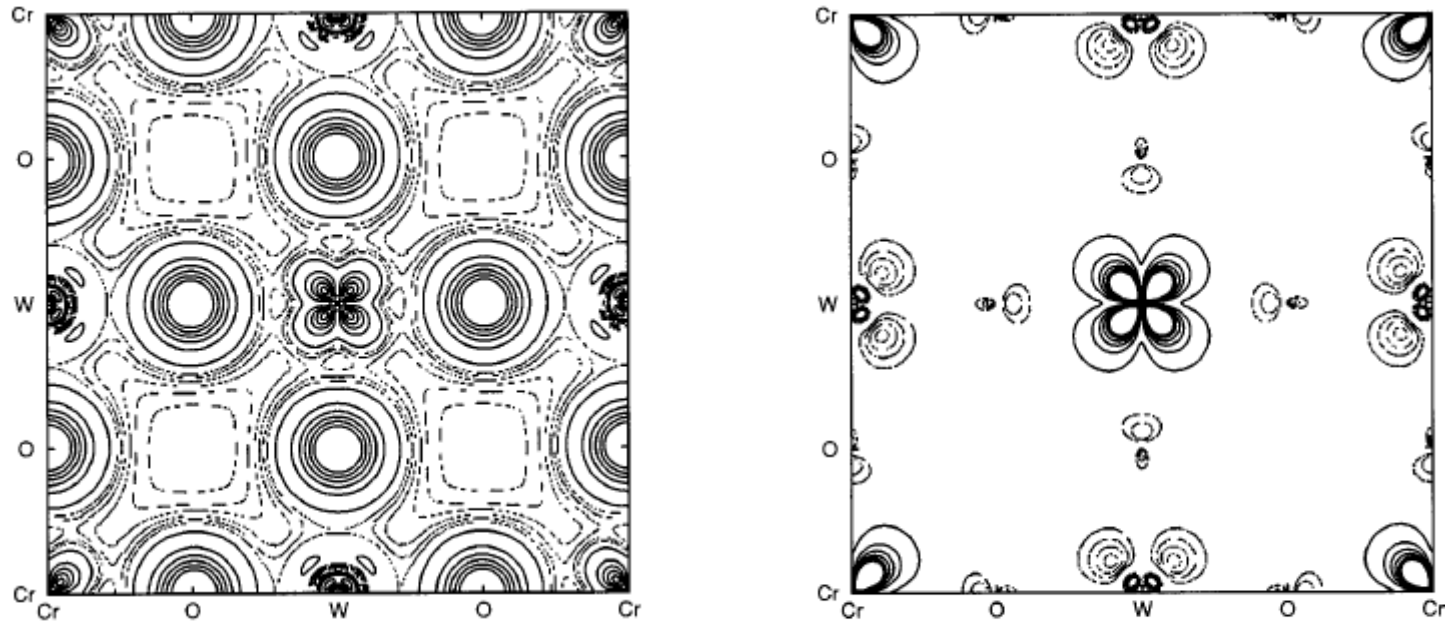


FIG. 4. Valence charge (upper panel) and spin (lower panel) densities of Sr_2CrWO_6 from the GGA. In the upper panel, the contours are along equal charge density lines from 0.015 to $0.065/a_0^3$ (broken lines) with step $0.01/a_0^3$, and from 0.1 to $0.85/a_0^3$ (solid lines) with step $0.15/a_0^3$. 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)

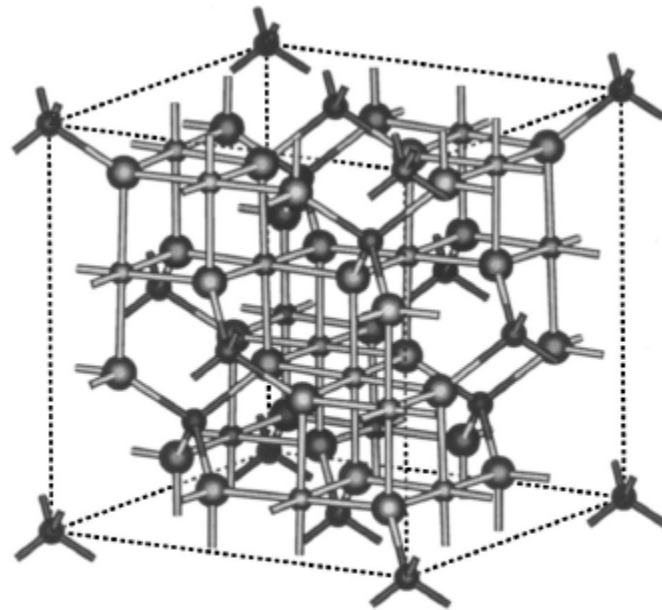


FIG. 1. Crystal structure of Fe_3O_4 . Big balls denote oxygen atoms, small dark balls denote *A*-site (tetrahedral) iron atoms, and small light balls denote *B*-site (octahedral) iron atoms.

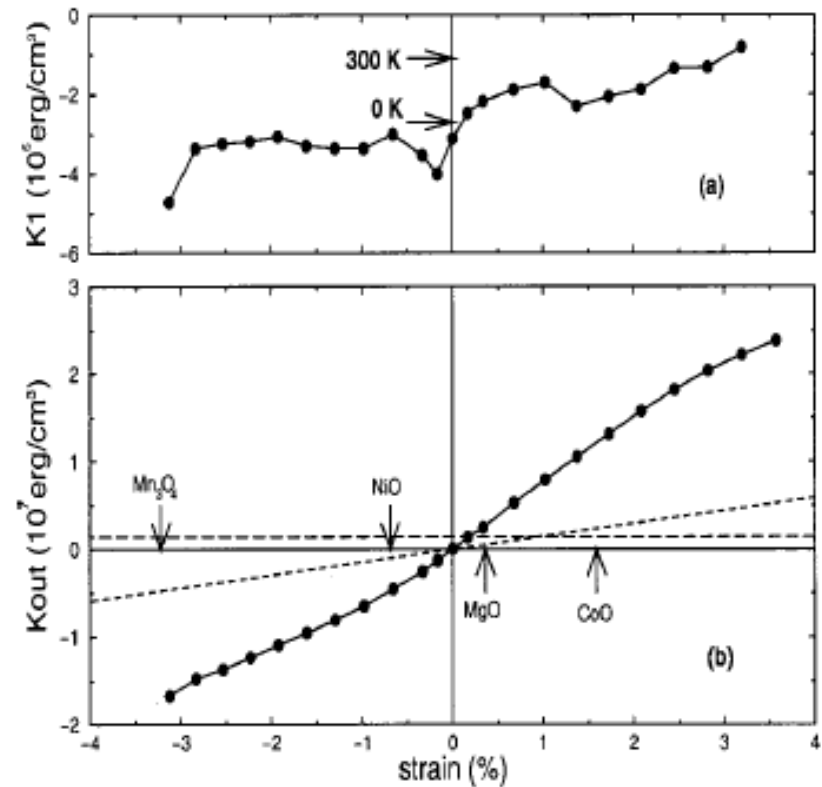
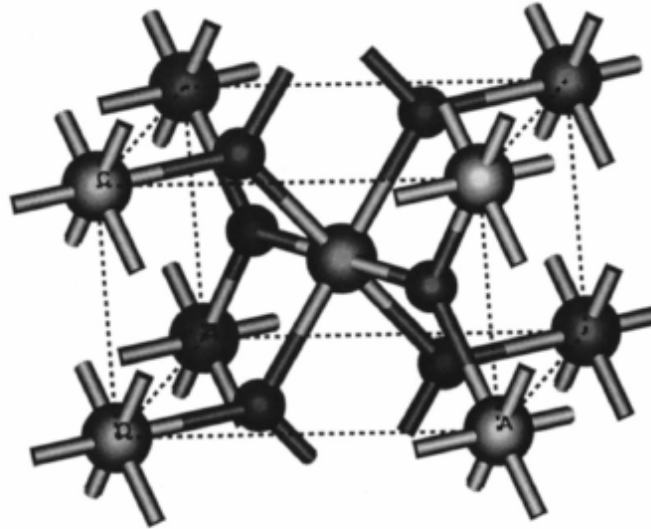


FIG. 8. The fourth-order anisotropy constant K_1 (a) and the out-of-plane anisotropy constant K_{out} (b) as a function of the lateral strain in the (001) plane of Fe_3O_4 . The lines are a guide to the eye only. The arrows in (a) indicate the experimental K_1 value at 300 K and 0 K (see text). The arrows in (b) indicate the possible strain values if an Fe_3O_4 film is grown on Mn_3O_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 for Cr 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.

U (eV)	Cr spin (μ_B)	Orbital (μ_B)	L/S (%)	O spin (μ_B)	Orbital (μ_B)	L/S (%)
0	1.89	-0.037	-2.0	-0.042	-0.0011	2.6
2	1.94	-0.046	-2.4	-0.058	-0.0019	3.2
3	1.99	-0.051	-2.6	-0.079	-0.0025	3.2
4	2.03	-0.056	-2.8	-0.094	-0.0030	3.2
6	2.08	-0.067	-3.2	-0.111	-0.0040	3.6
9	2.12	-0.083	-3.9	-0.124	-0.0047	3.8

Magnetic orbital distribution

Jeng et al PRL (2004)

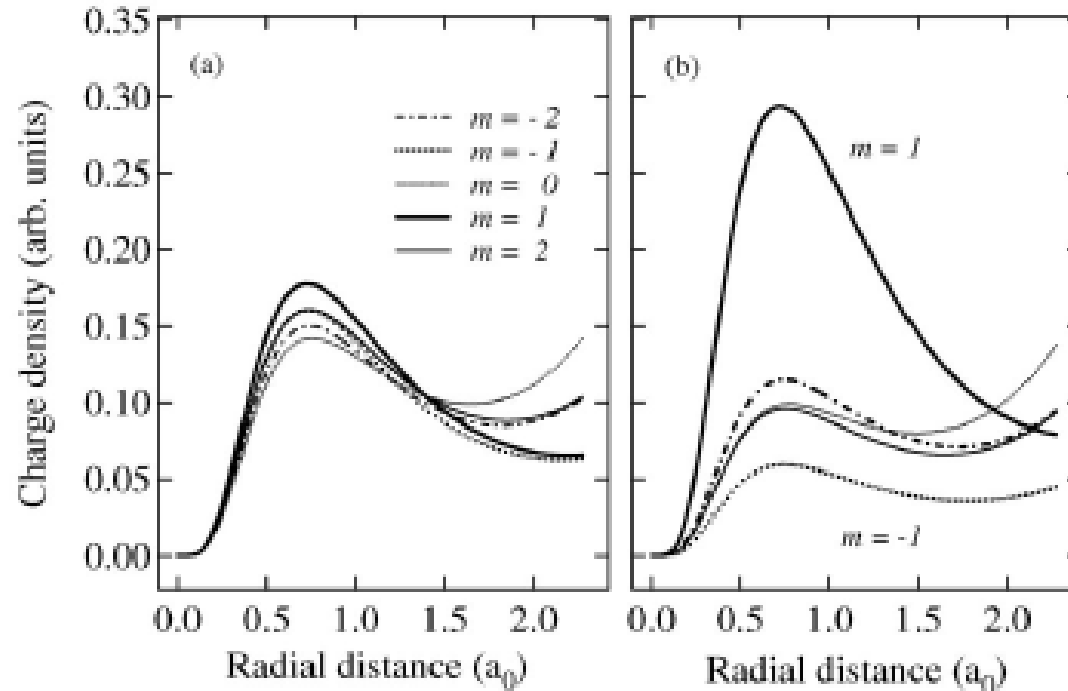


FIG. 2. Charge densities of cubic Fe_3O_4 versus radial distance in units of atomic radius a_0 . The charge densities projected to different orbitals with magnetic quantum number m were obtained from (a) LDA and (b) LDA + U calculations.

Projected density of state

Jeng et al PRB (2005)

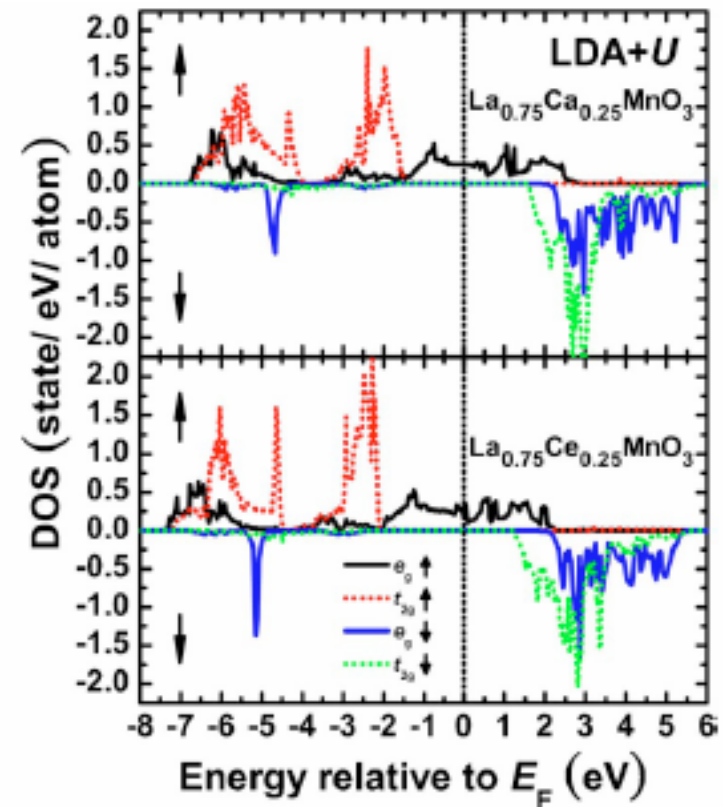
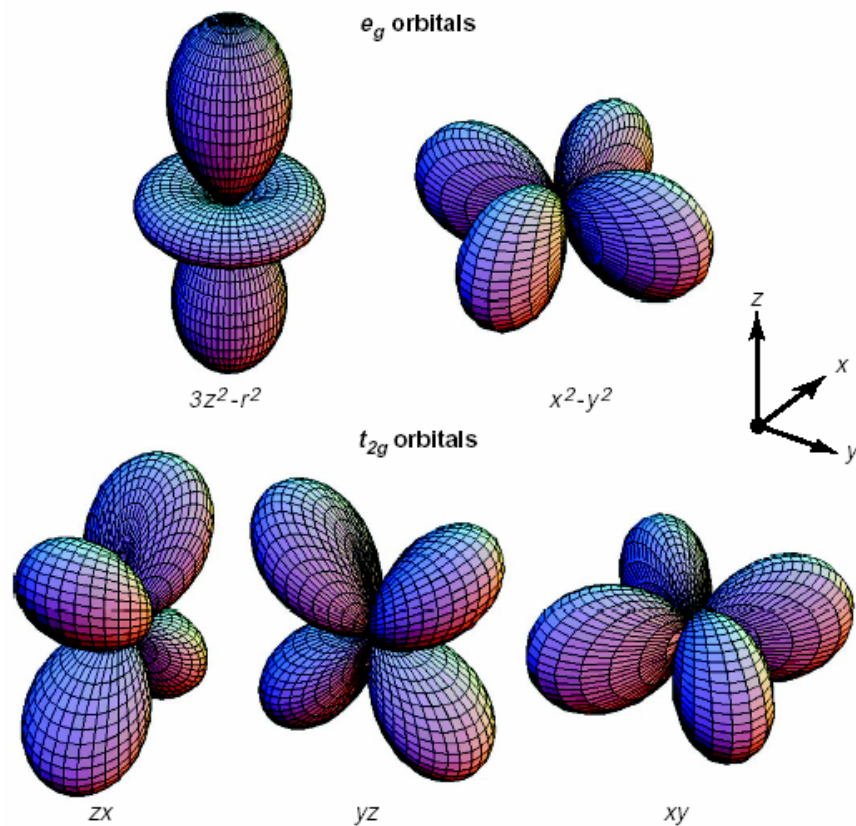


FIG. 2. (Color online) DOS of Mn 3d in LCaMO and LCeMO calculated by LDA+ U method. The parameters used in these calculations are described in the text.

Orbital ordering

Jeng et al PRL (2006)

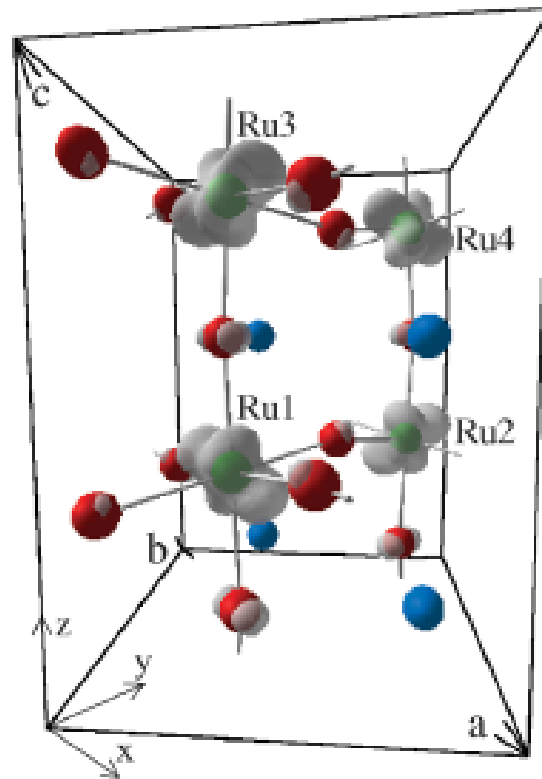


FIG. 4 (color). OO of SrRuO₃. Blue, green, and red balls are, respectively, Sr, Ru, and O ions. The origin has been shifted to $(-1/3, -1/3, -1/3)$.

Charge orbital ordering

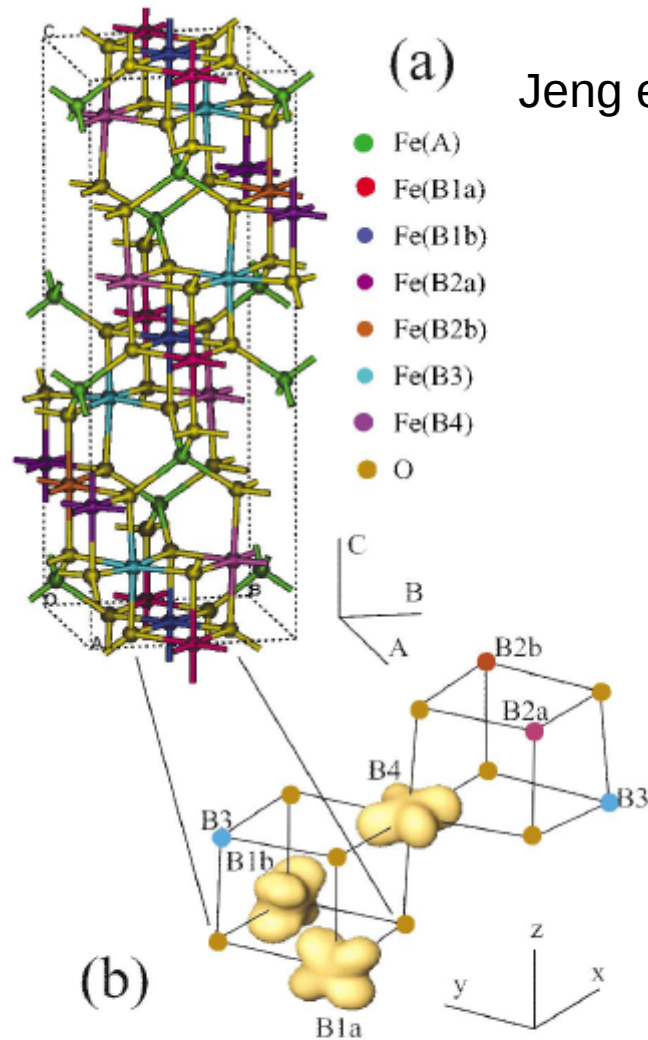


FIG. 1 (color). (a) Crystal structure of the monoclinic Fe_3O_4 . (b) Orbital ordering in B -site sublattice. x - y - z and a - b - c are, respectively, the local and global coordinates.

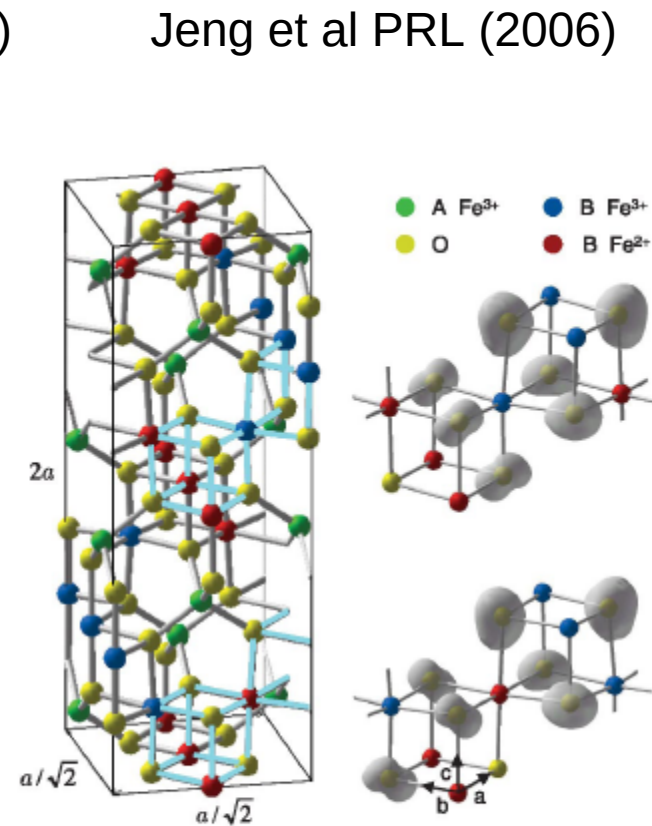
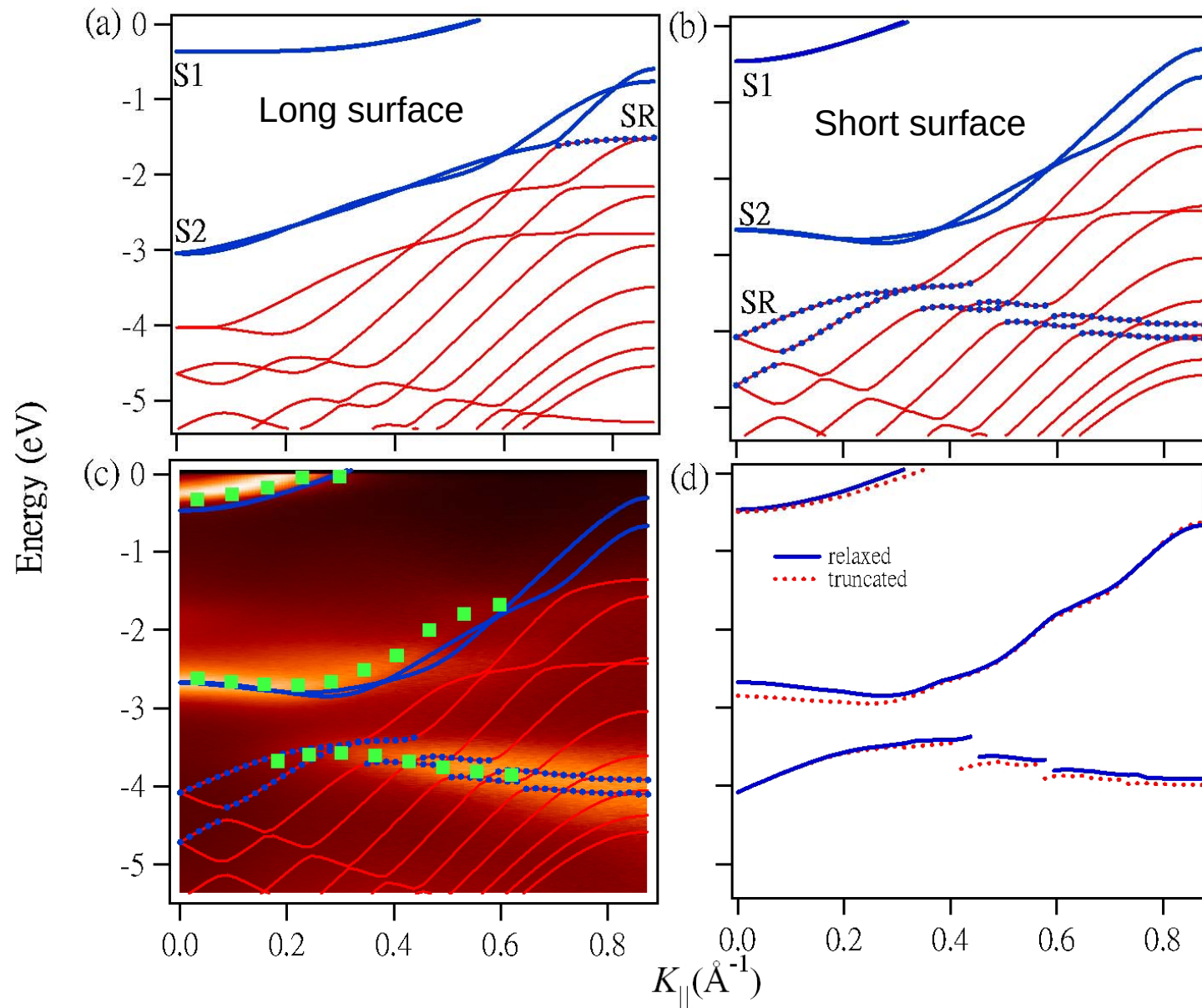


FIG. 2 (color). Left: monoclinic crystal structure of Fe_3O_4 in the low-temperature phase corresponding to a subcell of $\frac{a}{\sqrt{2}} \times \frac{a}{\sqrt{2}} \times 2a$ with $P2/c$ symmetry. Right: 3D isosurfaces of unoccupied density of states of the O $2p$ integrated between the Fermi level and 1 eV above within the corresponding Fe_3O_4 cubes highlighted in the crystal structure. For simplicity, we denote the octahedral Fe site with nominal 2+ and 3+ valences as Fe^{2+} and Fe^{3+} , respectively.

Surface state of Be(1010): Jeng et. al. PRB 2008



Magnetic graphene ribbon: Jeng et. al. PRB 2009

FERROMAGNETISM IN ARMCHAIR GRAPHENE...

PHYSICAL REVIEW B 79, 035405 (2009)

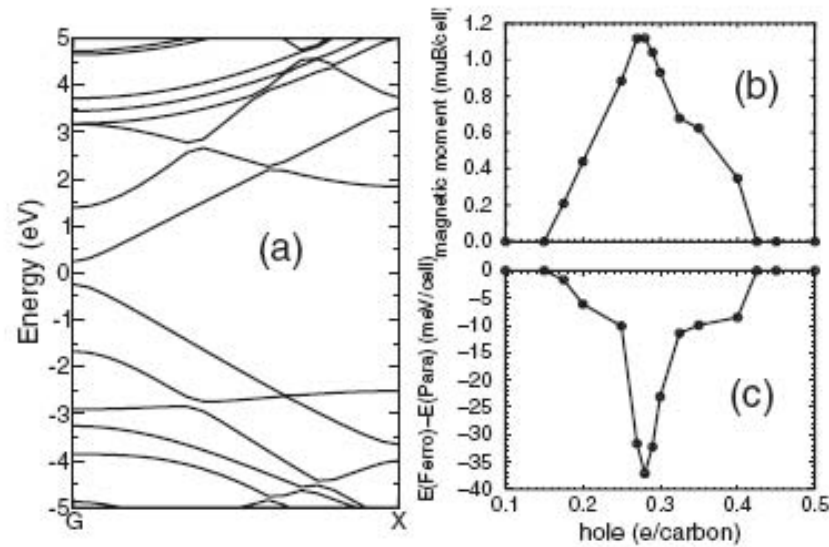


FIG. 4. (a) Band structure of the undoped, infinitely long armchair GNR with $L_y=5$. (b) Doping dependence of the spin polarization per unit cell. (c) Energy difference per unit cell $\Delta(x_h)$ between ferromagnetic and paramagnetic states as a function of the hole doping.

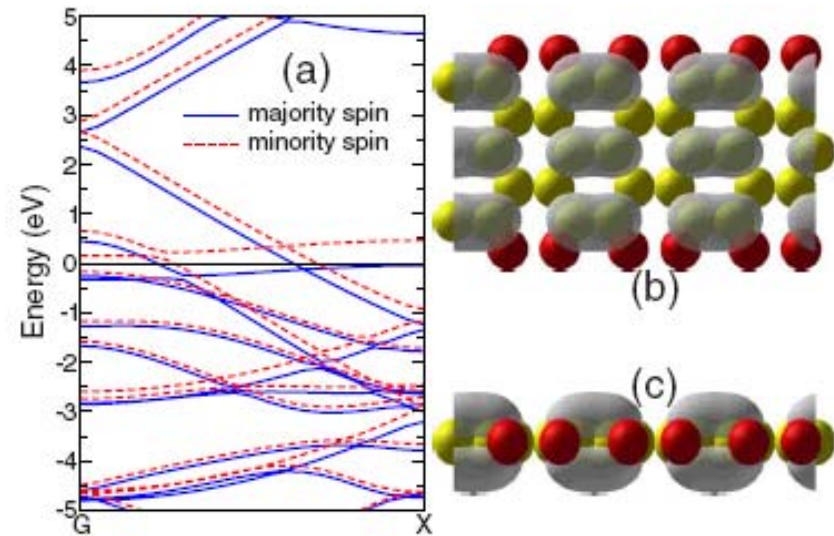


FIG. 5. (Color online) (a) Spin-decomposed band structure of the infinitely long GNR with $L_y=5$ at the optimal hole doping $x_h^* \approx 0.28$. (b) Top and (c) side views of the spin-density distribution (shown in gray color). The yellow (light) and red (dark) spheres denote C and H atoms, respectively.

2d-like Fermi surface in $\text{Cd}_2\text{Re}_2\text{O}_7$: Jeng et. al. JPCM 2009

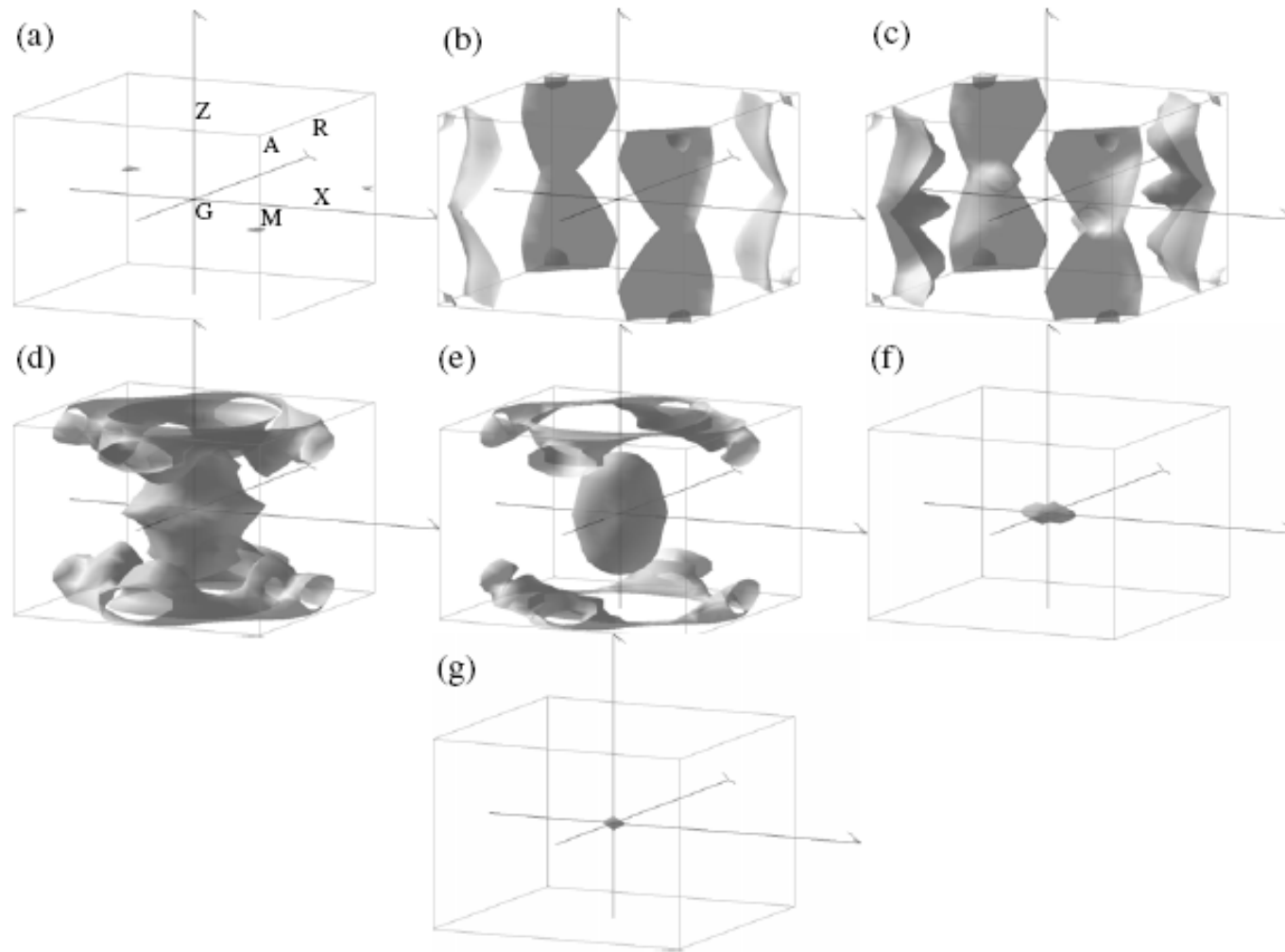
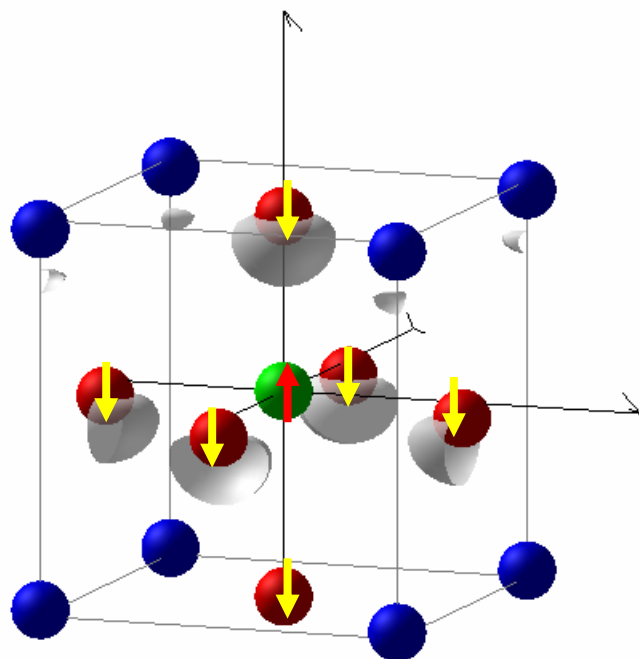


Figure 9. Fermi surfaces of bands 366–372 of the low- T phase from GGA + U . (a) Band 366, (b) band 367, (c) band 368, (d) band 369, (e) band 370, (f) band 371 and (g) band 372.

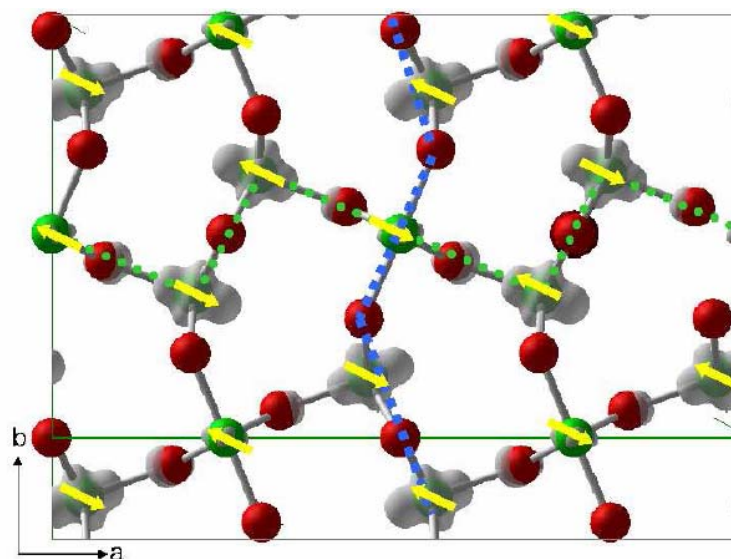
Ferroelectricity: spatial inversion
symmetry breaking $\rightarrow$
ferroelectricity



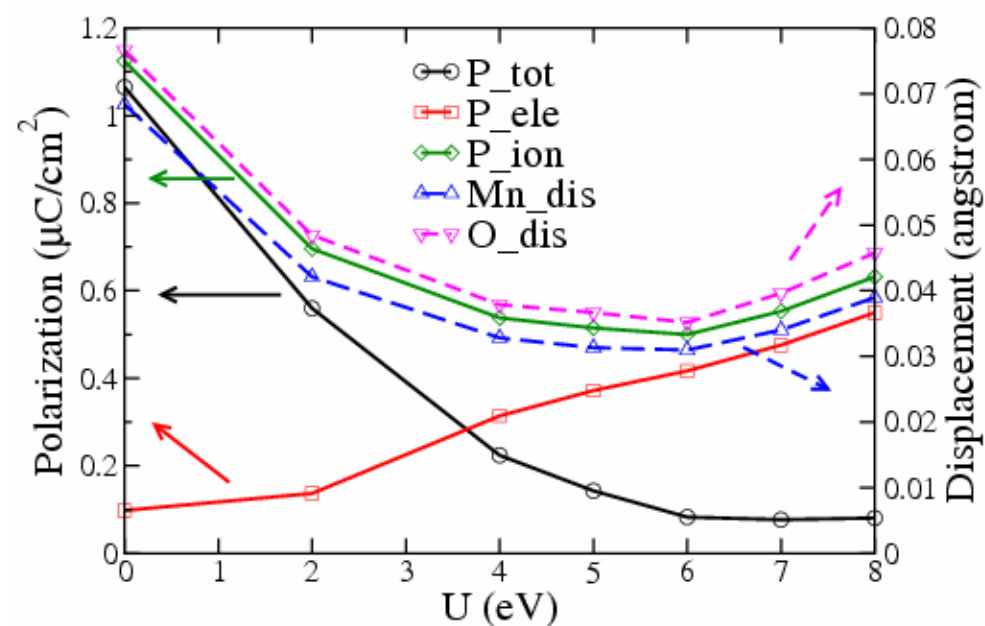
KNbO3 Perovskite ferroelectric

Multiferroism: magnetism
induced spatial inversion
symmetry breaking $\rightarrow$
ferroelectricity

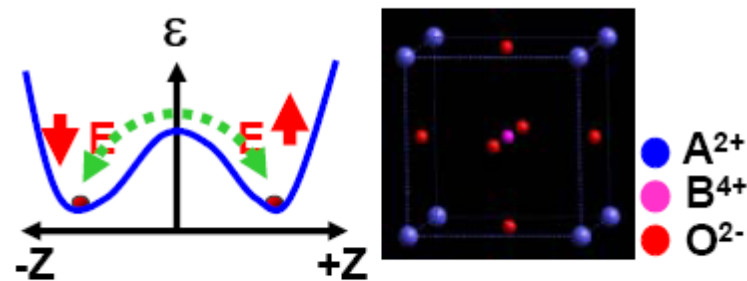
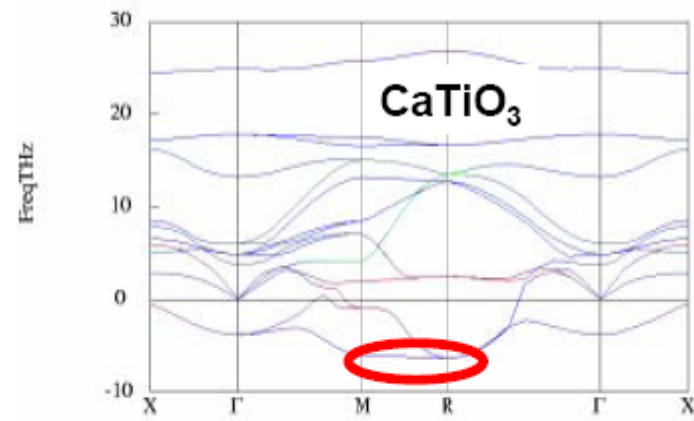
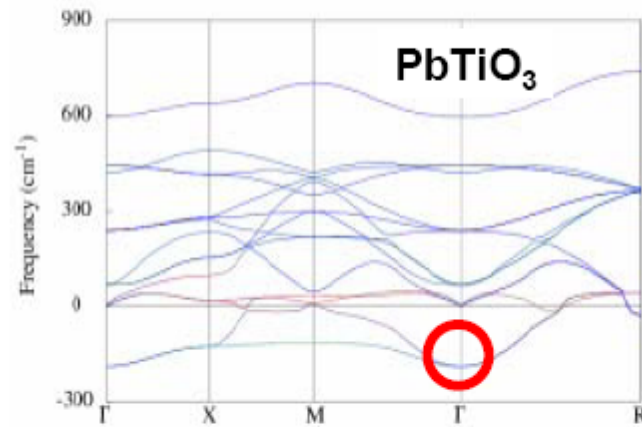
TbMn2O5



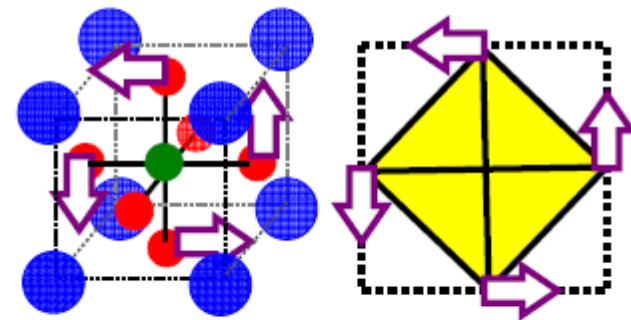
Electrical polarization: Berry phase



Phonon/Structural instability & ferroelectricity in perovskites: Density Functional Perturbation Theory (linear response)



Cubic $\Rightarrow$ Tetragonal



Cubic $\Rightarrow$ Orthorhombic

Ground state properties (LDA)



● Ground-state properties (DFT)

Atomic structure (bond length,
lattice constants)

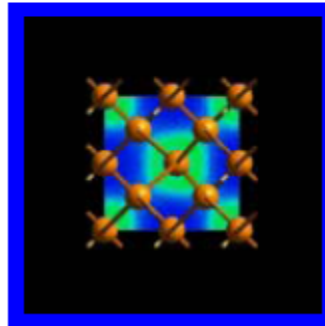
Phase stability

Phonon

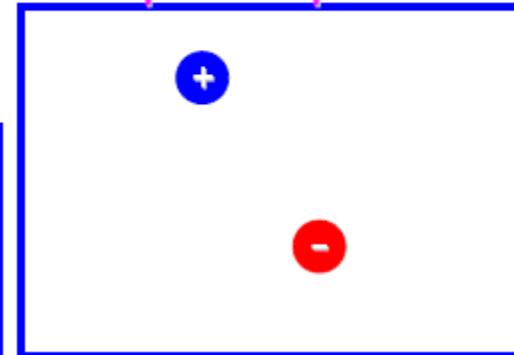
Cohesive energy

Band structure (v)

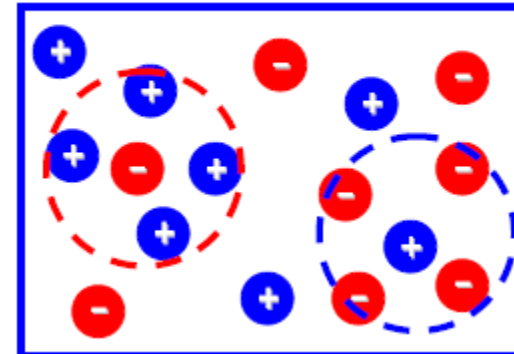
Magnetization ...



independent particles



quasiparticles



● Excitation (beyond DFT)

Optical spectrum

Band structure

(band-gap problem)

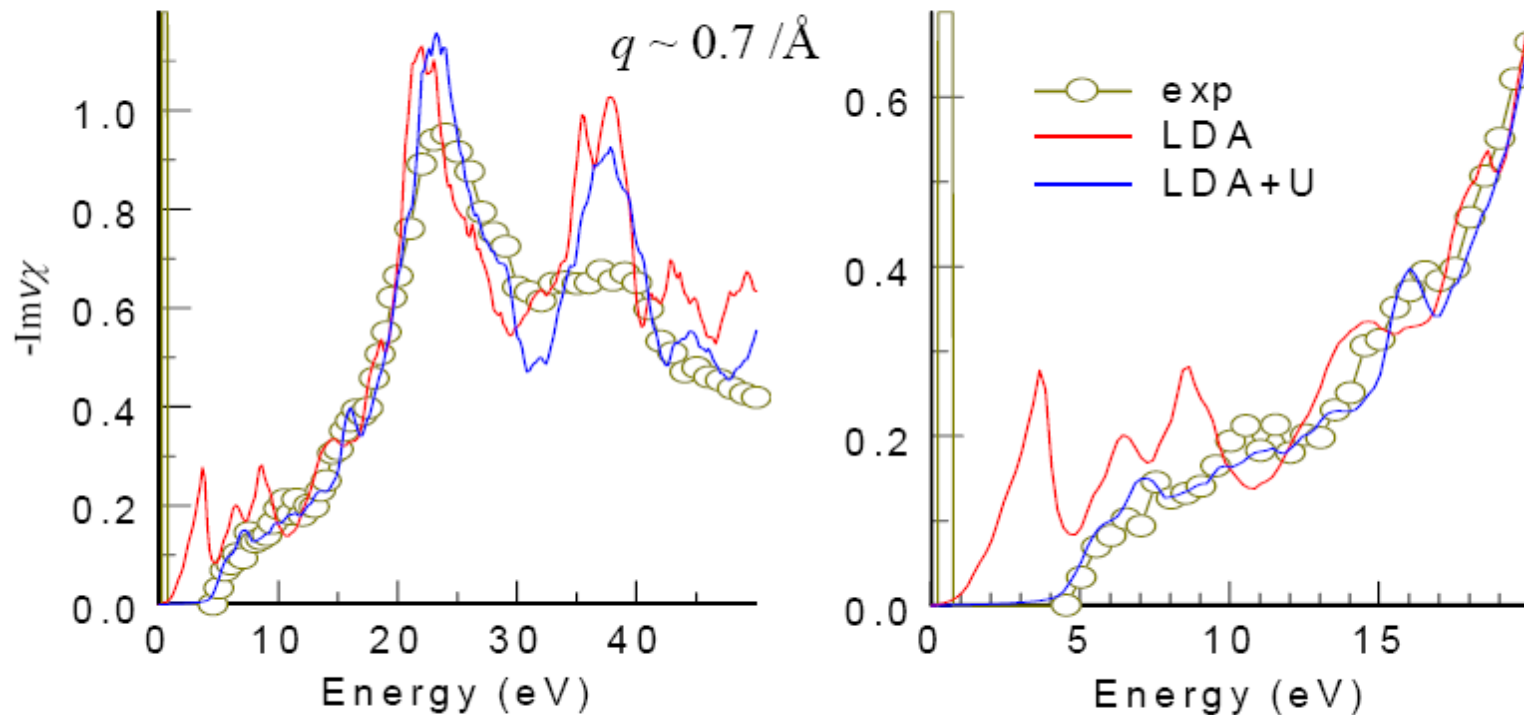
Excitation ...

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)
-

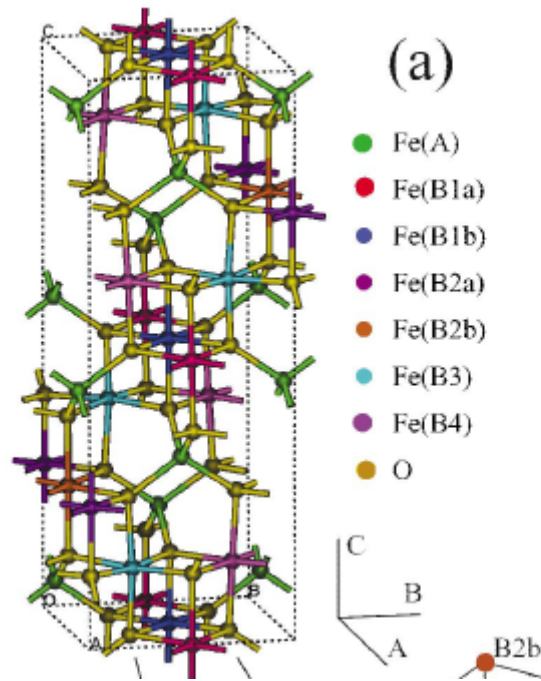
LDA+U for transition metal oxide NiO

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



➔ **LDA+U → great improvement at small q**

LDA+U for low-T magnetite Fe_3O_4



Jeng et al, PRL (2004), PRB (2006)

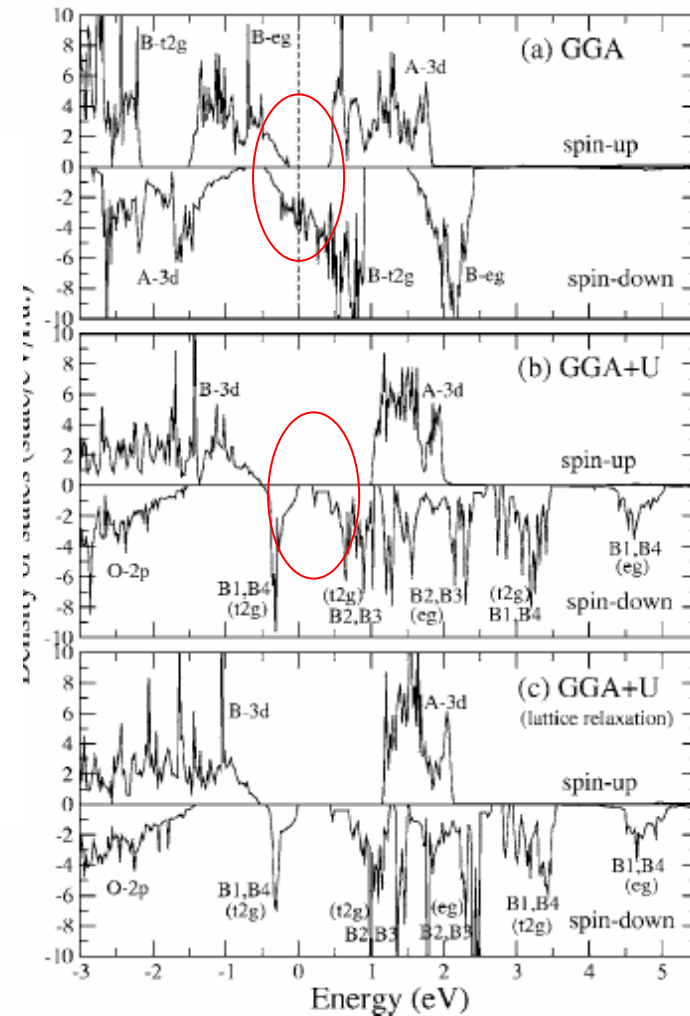
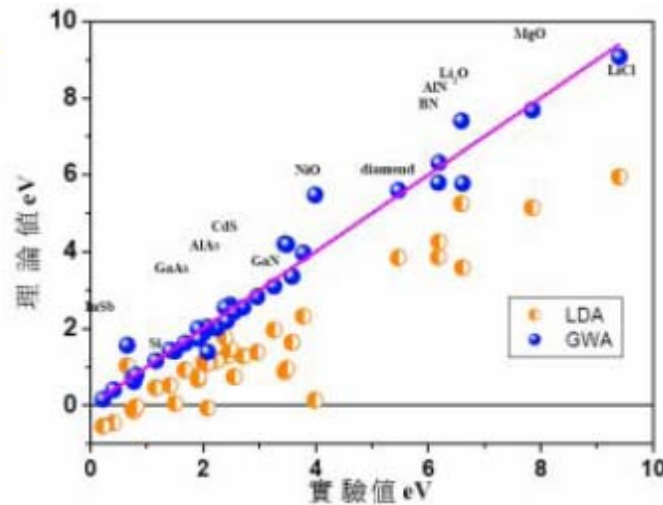


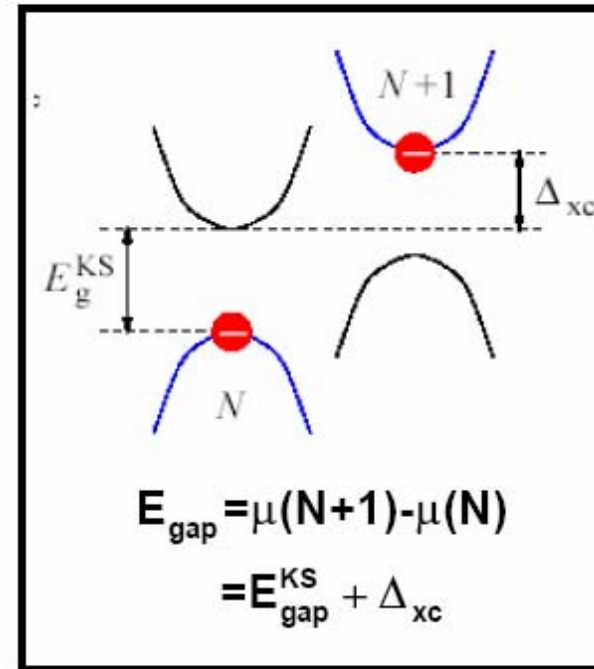
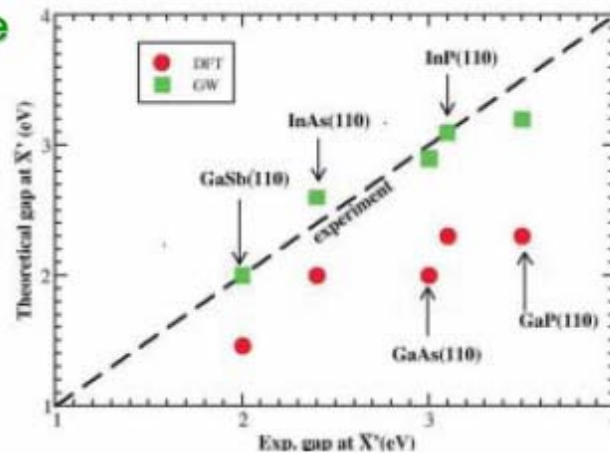
FIG. 2. Spin-resolved density of states of Fe_3O_4 in low- T monoclinic $P2/c$ structure from GGA (a), GGA+ U (b), and GGA+ U under lattice relaxation (c). The Fermi level is at zero energy.

Band gap problem in semiconductors: GWA

Bulk



Surface



CMS II-1 Hands-on: Unix, vi, VASP, total energy, and convergence

Horng-Tay Jeng

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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
```

↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑

u g o owner group size date time name

% 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)

0	000	---
1	001	--x
2	010	-w-
3	011	-wx
4	100	r--
5	101	r-x
6	110	rw-
7	111	rwx

% 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

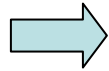
alias: Show the available alias

Vi editor

% vi filename

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

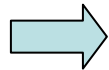
i,a,o,I,A,O



insert mode

To key-in characters

ESC



command mode

To handle the file

h(←), j(↓), k(↑), l(→)

nG

go to the nth line

G

go to the last line

^g

show line number of the cursor

^f

next page

^b

last page

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, ...)

Working 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&

OUTPUT FILES

OUTCAR
OSZICAR
CONTCAR
CHGCAR
WAVECAR
EIGENVAL
PROCAR
XDATCAR
LOCPOT
DOSCAR
CHG

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

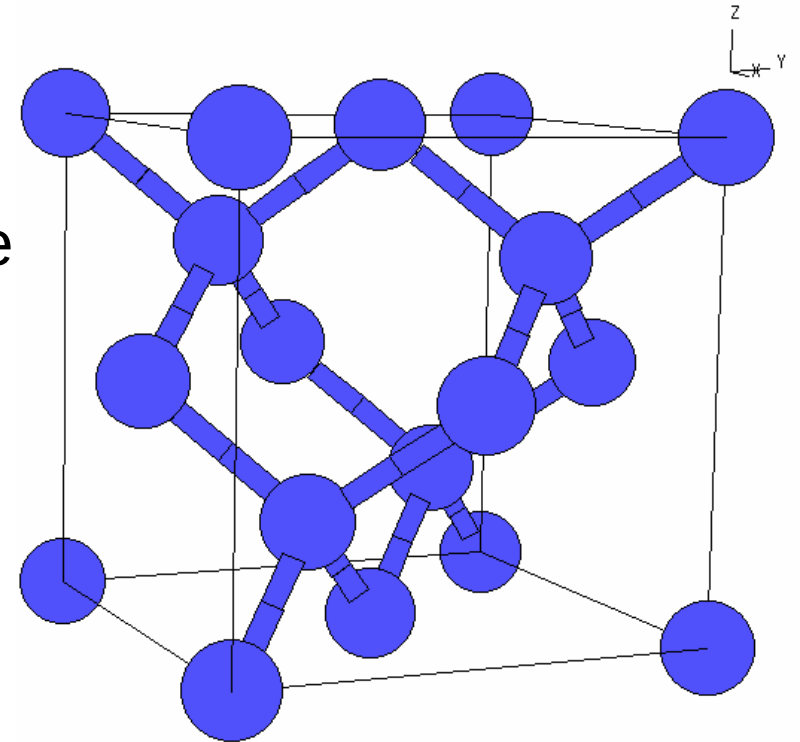
Automatic mesh

Mondhorst-Pack type mesh

K-point density in BZ

Shift of the mesh

Diamond structure



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 A

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)

Example : fcc structure

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

$$\vec{a}_1 = \frac{a}{2} (\vec{j} + \vec{k})$$

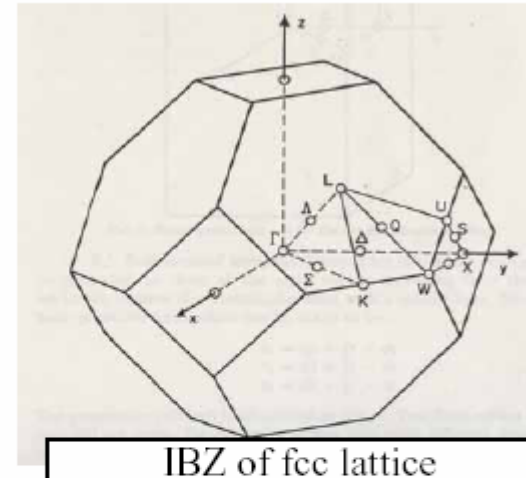
$$\vec{a}_2 = \frac{a}{2} (\vec{i} + \vec{k})$$

$$\vec{a}_3 = \frac{a}{2} (\vec{i} + \vec{j})$$

$$\vec{b}_1 = \frac{4\pi}{a} \frac{1}{2} (-\vec{i} + \vec{j} + \vec{k})$$

$$\vec{b}_2 = \frac{4\pi}{a} \frac{1}{2} (\vec{i} - \vec{j} + \vec{k})$$

$$\vec{b}_3 = \frac{4\pi}{a} \frac{1}{2} (\vec{i} + \vec{j} - \vec{k})$$



Point	Cartesian coordinates (units of $2\pi/a$)	Reciprocal coordinates (units of b_1, b_2, b_3)
G	(0 0 0)	(0 0 0)
X	(0 0 1)	(1/2 1/2 0)
W	(1/2 0 1)	(1/2 3/4 1/4)
K	(3/4 3/4 0)	(3/8 3/8 3/4)
L	(1/2 1/2 1/2)	(1/2 1/2 1/2)

POTCAR

Copy POTCAR from potpaw Si directory

Ex: POTCAR of W

```
PAW W 19Jan2001
6.000000000000000000
parameters from PSCTR are:
VRHFIN =W: 5p6s5d
LEXCH = CA
EATOM = 206.5370 eV, 15.1800 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
distr: 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:
      Coordinates      Weight
    .050000 .050000 .000000  4.000000
.....

ion position      nearest neighbor table
  1 .000 .000 .180-  2 2.44  2 2.44  2 2.44  2 2.44  3 2.82
  2 .500 .500 .090-  1 2.44  3 2.44  1 2.44  3 2.44  1 2.44  3 2.44
.....
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 absolut eigen values
```

grep E-fermi OUT*

k-point 1 : .0500 .0500 .0000
 band No. band energies occupation
 1 -7.1007 1.00000
 2 -5.6294 1.00000

.....
 24 -.0812 1.00000
 25 .0452 1.00000
 26 .4166 .98757
 27 .4330 .98331
 28 .5655 .88306
 29 1.1510 .00159
 30 3.0240 .00000
 31 4.8957 .00000
 32 5.1413 .00000

k-point 2 : .1500 .0500 .0000

.....
 POSITION TOTAL-FORCE (eV/Angst)

 .00000 .00000 2.80979 .000000 .000000 .044768
 1.41120 1.41120 1.44005 .000000 .000000 .023860

external pressure = 783.50 kB Pullay stress = 0.00 kB

.....
 external pressure = 0.54 kB Pullay stress = 0.00 kB

.....
 direct lattice vectors reciprocal lattice vectors
 -1.532408821 1.532408821 1.532408821 0.000000000 0.326283687 0.326283687
 1.532408821 -1.532408821 1.532408821 0.326283687 0.000000000 0.326283687
 1.532408821 1.532408821 -1.532408821 0.326283687 0.326283687 0.000000000

.....

total charge

# of ion	s	p	d	tot
1	.391	.281	6.106	6.778
2	.411	.433	6.211	7.054
3	.411	.434	6.163	7.008
4	.411	.433	6.211	7.054
5	.391	.281	6.106	6.778
tot	2.01	1.86	30.80	34.67

magnetization (x)

# of ion	s	p	d	tot
1	.011	.003	2.867	2.880
2	-.012	-.036	2.271	2.223
3	-.001	-.036	2.462	2.425
4	-.012	-.036	2.271	2.223
5	.011	.003	2.867	2.880
tot	.00	-.10	12.74	12.63

.....

-----Iteration 1(1) -----

POTLOK: VPU time 2.28; CPU time 2.28

SETDIJ: 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.

grep LOOP OU*

OSZCAR

	N	E	dE	d eps	neg	rms	rms(c)
DAV: 1		.335885869262E+02	.33589E+02	-.42225E+03	17288	.695E+02	
DAV: 2		-.429448425975E+01	-.37883E+02	-.34709E+02	14040	.191E+02	
DAV: 3		-.472026980215E+01	-.42579E+00	-.42552E+00	16554	.232E+01	
DAV: 4		-.472147266739E+01	-.12029E-02	-.12028E-02	15730	.115E+00	
DAV: 5		-.472148218577E+01	-.95184E-05	-.95179E-05	15418	.942E-02	.316E+00
DAV: 6		-.442946208768E+01	.29202E+00	-.98533E-01	14907	.126E+01	.817E-01
DAV: 7		-.440595084829E+01	.23511E-01	-.53654E-02	16133	.244E+00	.305E-01
DAV: 8		-.440083611401E+01	.51147E-02	-.18624E-03	14174	.672E-01	.115E-02
DAV: 9		-.440083792741E+01	-.18134E-05	-.94978E-06	7237	.266E-02	
1 F= -.44008379E+01 E0= -.43980580E+01 d E =-.440084E+01							

E0: Total energy

Cohesive energy: Bulk total energy –
atomic total energy (spin-polarized)

PROCAR

PROCAR new format

of k-points: 1 # of bands: 9 # of ions: 2

k-point 1 : .00000000 .00000000 .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	.781

XDATCAR

2 2 50

.5000000E+03 .1000000E-08 .1000000E-08 .1000000E-08 .5000000E-15
0.100000000000000005E-03

CAR

bcc Fe

.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 .94272265

.00000000 .00000000 .05571192
.00000000 .00000000 .94428808

.00000000 .00000000 .05710243
.00000000 .00000000 .94289757

~

CHGCAR

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

```
bcc Fe
10.0000000000000000
 1.000000 .000000 .000000
 .000000 1.000000 .000000
 .000000 .000000 1.000000
 1 1
Direct
.000000 .000000 .057102
.000000 .000000 .942898

 84 84 84
.41098271954E+04 .38580593547E+04 .32056173636E+04 .23907855172E+04 .16323134731E+04
.10440737881E+04 .64952106325E+03 .40394464342E+03 .25149651632E+03 .15428370958E+03
.92653834837E+02 .55483939720E+02 .34042823873E+02 .21474147940E+02 .13548327933E+02
.....
augmentation occupancies 1 33
.5244394E+00 -.3805205E+00 .8687841E-32 .9745050E-01 -.8804372E-32
.....
.1622568E-01 -.1784093E-33 -.2752412E-18
augmentation occupancies 2 33
.5478642E+00 .1011510E+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
.1329580E+01 .0000000E+00 -.7399463E-33 .8218637E-01 .8516730E-33
-.1488428E-16 .3152197E+00 .1110142E-31 .3496585E-33 .6753791E-01
.1884802E-33 .4810138E-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
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