CMS II-5: plane wave, pseudopotential, LDA, and LSDA

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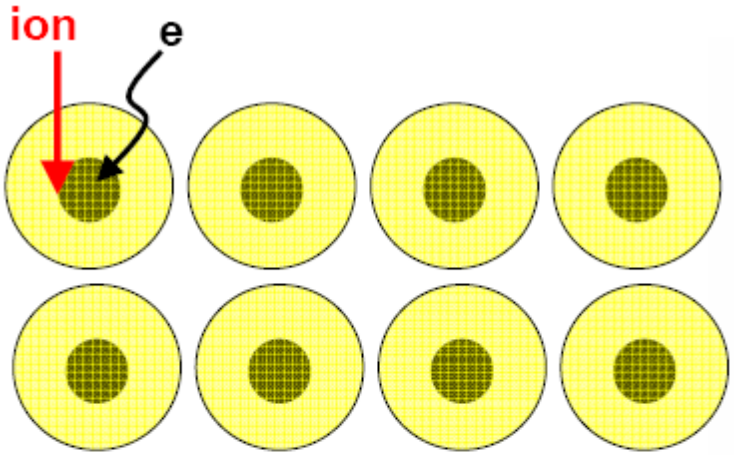
The periodic potential



- In principle, we are faced with a many electron problem
- But we can make a lot of progress using the

single electron picture

- We investigate the properties of the Schrödinger equation for a single electron:
  $H\Psi = (-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}))\Psi = E\Psi$
  with $U(\mathbf{r}+\mathbf{R}) = U(\mathbf{r})$

Bloch theorem

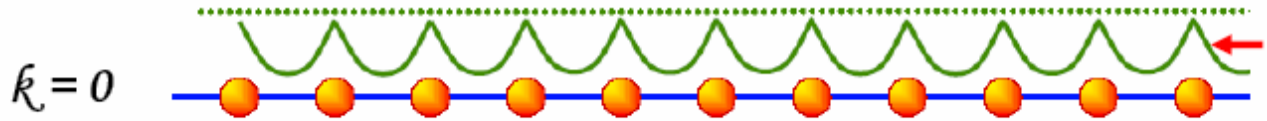
'When I started to think about it, I felt that the main problem was to explain how the electrons could sneak by all the ions in a metal....
By straight Fourier analysis I found to my delight that the wave differed from the plane wave of free electrons only by a periodic modulation'

F. BLOCH

$$\psi_{nk}(r) = e^{ik\cdot r} u_{nk}(r) \qquad \left[u_{nk}(r) = u_{nk}(r+R) \right]$$

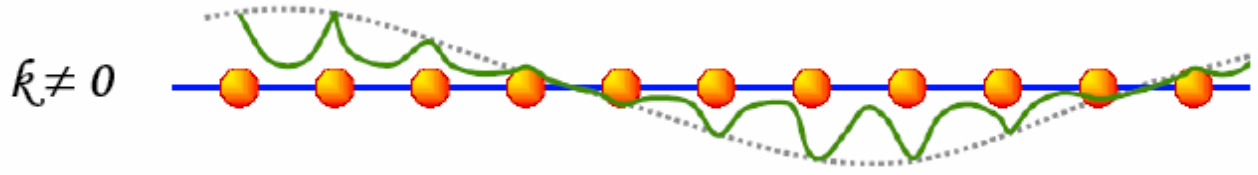
Bloch theorem in 1D

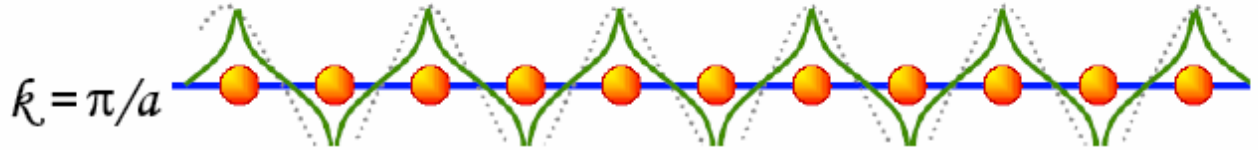
$$\psi(r) = e^{ik\cdot r} u(r - na)$$



Γ

at zone center





at zone boundary

Plane wave basis set and energy cutoff

- introduce the cell periodic part $u_{n,\mathbf{k}}$ of the wavefunctions

$$\psi_{n,\mathbf{k}}(\mathbf{r}) = u_{n,\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\mathbf{r}},$$

$u_{n,\mathbf{k}}(\mathbf{r})$ is cell periodic (insert into Bloch theorem) to treat them equally

- all cell periodic functions are now written as a sum of plane waves

$$u_{n,\mathbf{k}}(\mathbf{r}) = \frac{1}{\Omega^{1/2}}\sum_{\mathbf{G}} C_{\mathbf{G}n\mathbf{k}}e^{i\mathbf{G}\mathbf{r}}, \quad \psi_{n,\mathbf{k}}(\mathbf{r}) = \frac{1}{\Omega^{1/2}}\sum_{\mathbf{G}} C_{\mathbf{G}n\mathbf{k}}e^{i(\mathbf{G}+\mathbf{k})\mathbf{r}}$$

$$\rho(\mathbf{r}) = \sum_{\mathbf{G}} \rho_{\mathbf{G}}e^{i\mathbf{G}\mathbf{r}},$$

$$V(\mathbf{r}) = \sum_{\mathbf{G}} V_{\mathbf{G}}e^{i\mathbf{G}\mathbf{r}},$$

- in practice only those plane waves $|\mathbf{G}+\mathbf{k}|$ are included which satisfy

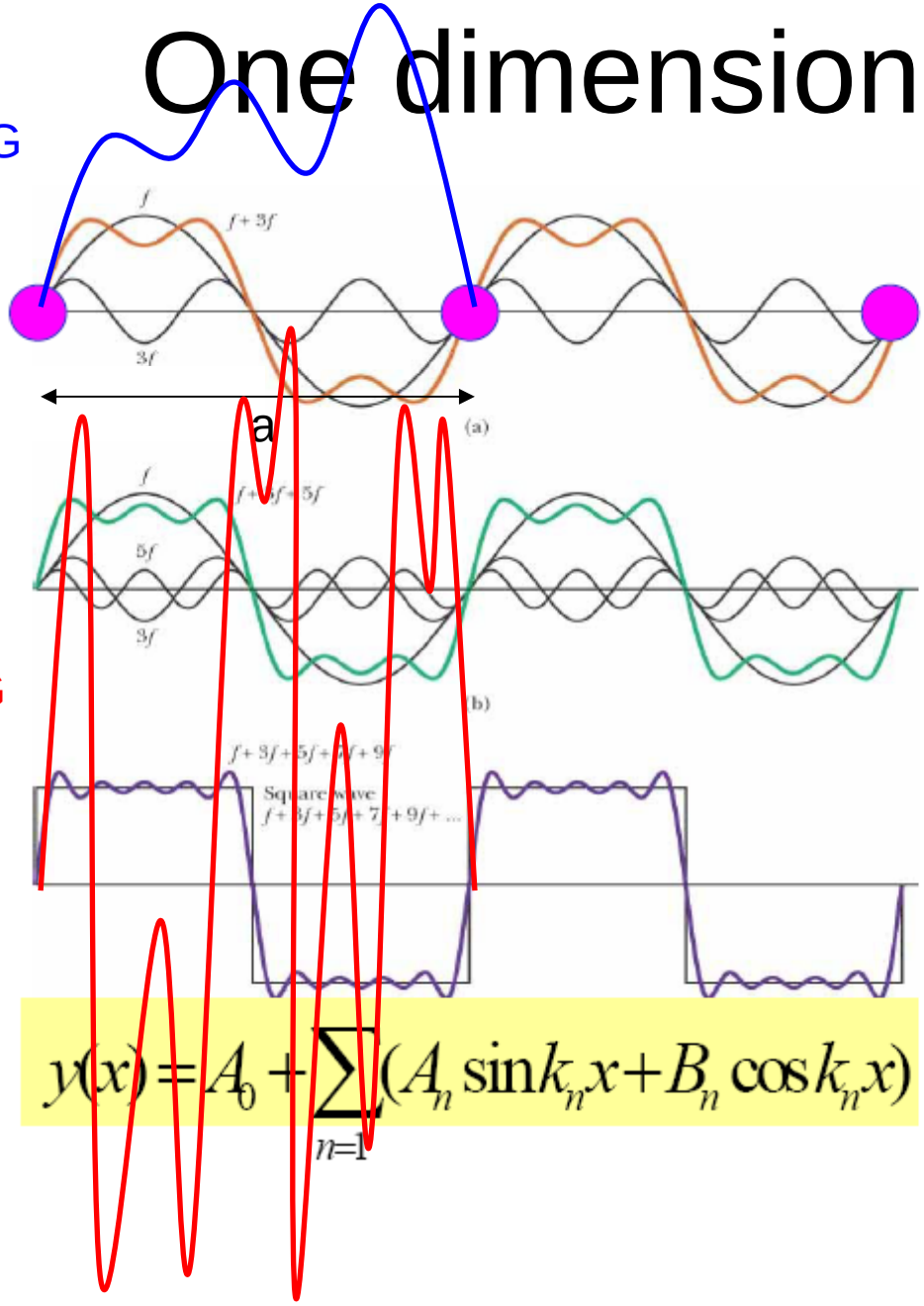
$$\frac{\hbar^2}{2m_e}|\mathbf{G}+\mathbf{k}|^2 < E_{\text{cutoff}}$$

Wave length of **G** is smaller than **k**, and |**G**| could be much larger than |**k**|, depending on how sharp is the periodic part u_{nk} (**r**)

One dimensional lattice

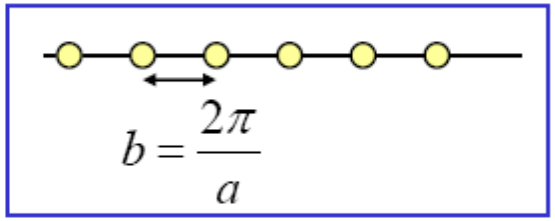
small G

large G



$$y(x) = A_0 + \sum_{n=1} (A_n \sin k_n x + B_n \cos k_n x)$$

Reciprocal Lattice



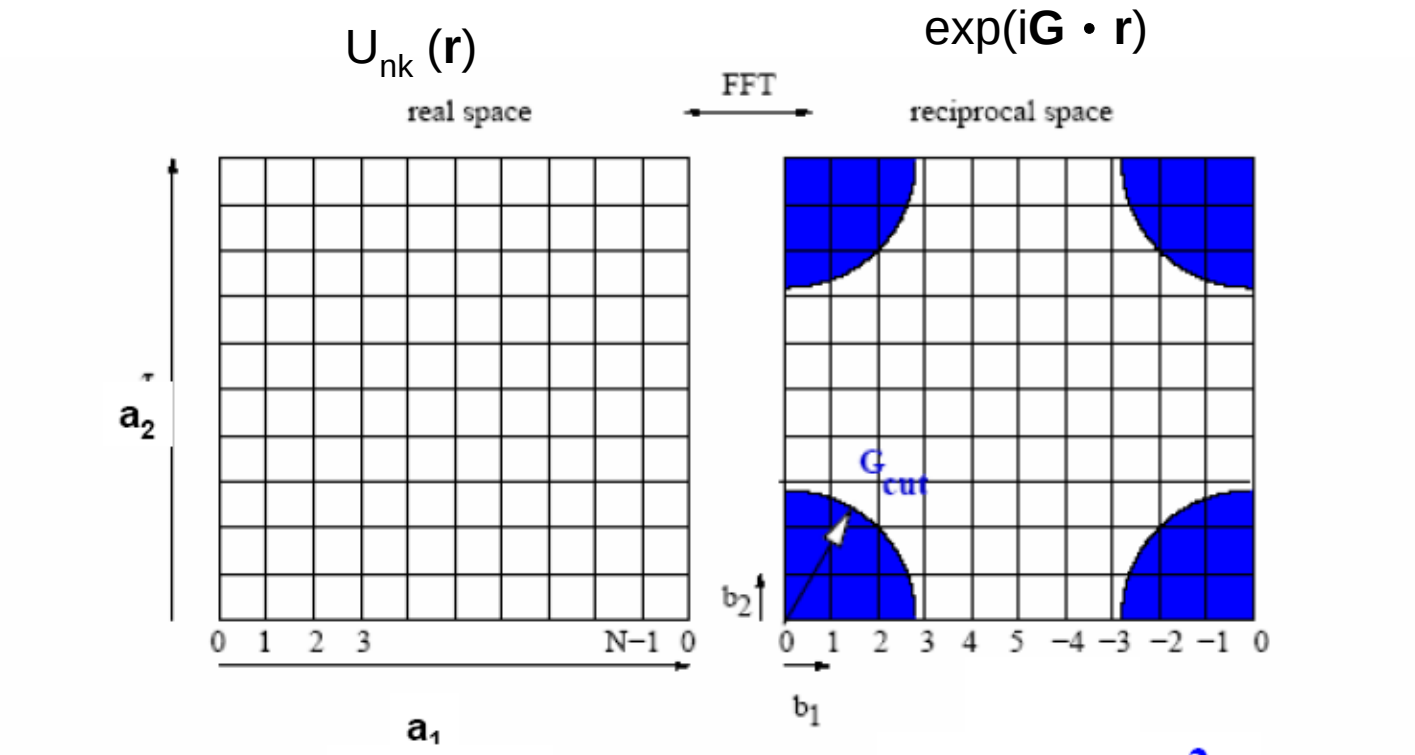
$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$$

$$b = \frac{2\pi}{a}$$

$$k_n = n\frac{2\pi}{a}$$

$$y(x) = \sum_n C_n e^{ik_n x}$$

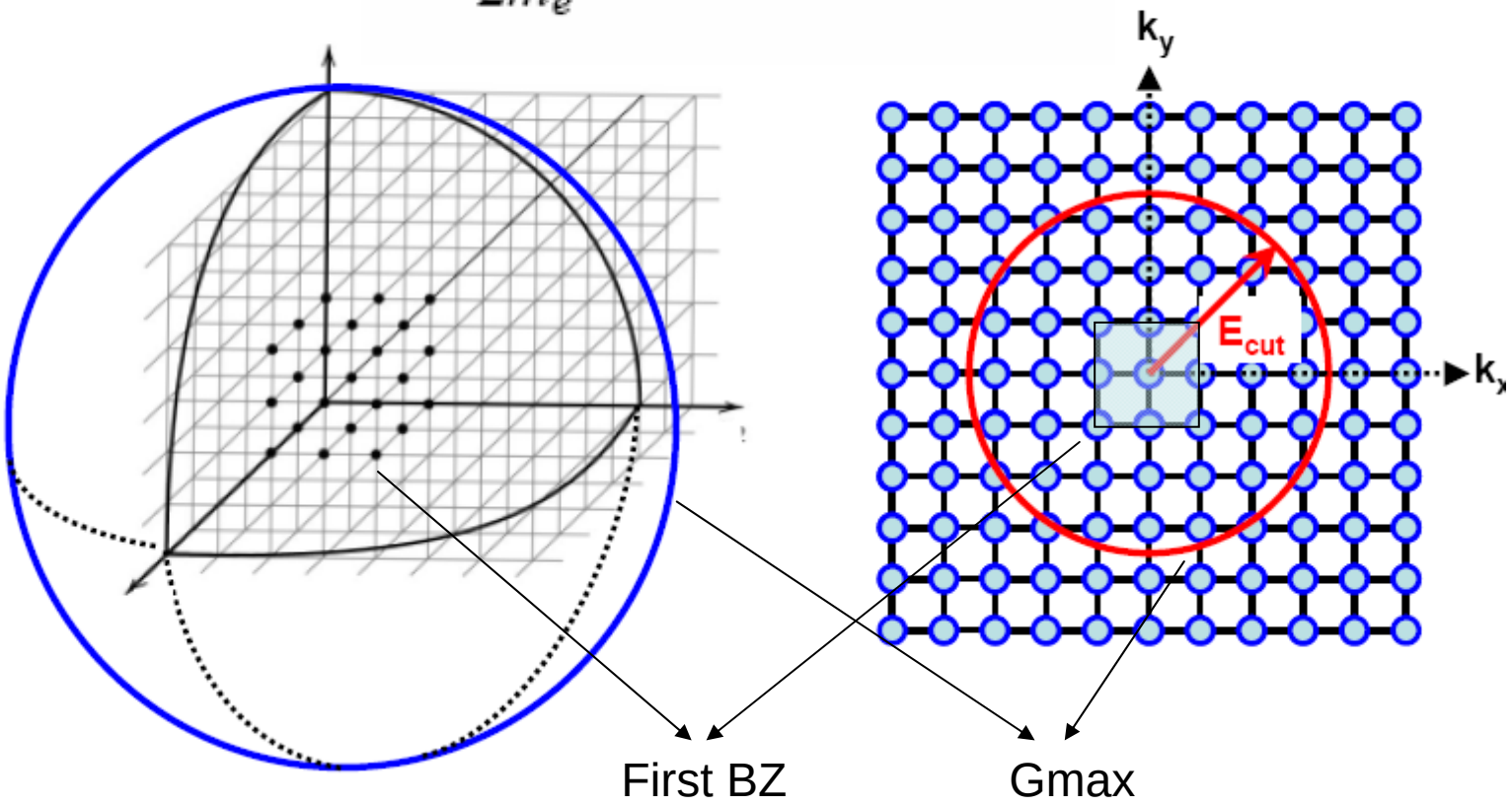
Fast Furier transform



$$x_1 = \frac{n_1}{N} a_1 \qquad g_1 = n_1 b_1 = n_1 \frac{2\pi}{a_1}$$

$$C_{\mathbf{r}n\mathbf{k}} = \sum_{\mathbf{G}} C_{\mathbf{G}n\mathbf{k}} e^{i\mathbf{G}\mathbf{r}} \quad C_{\mathbf{G}n\mathbf{k}} = \frac{1}{N_{\mathrm{FFT}}} \sum_{\mathbf{r}} C_{\mathbf{r}n\mathbf{k}} e^{-i\mathbf{G}\mathbf{r}} \quad \psi_{n,\mathbf{k}}(\mathbf{r}) = \frac{1}{\Omega^{1/2}} C_{\mathbf{r}n\mathbf{k}} e^{i\mathbf{k}\mathbf{r}}.$$

$$\frac{\hbar^2}{2m_e}|\mathbf{G}+\mathbf{k}|^2 < E_{\text{cutoff}}$$



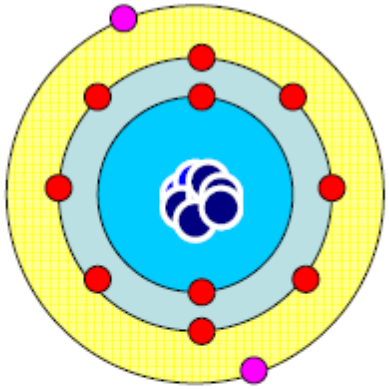
Usually the default value in VASP is good enough,
Increase ENCUT for problematic cases if necessary

Advantages of plane wave basis set

- Natural choice for system with periodic boundary conditions
- It is easy to pass from real- to reciprocal space representation (and vice versa) by FFT **$N^2 \log N$!**
- No Pulay correction to forces on atoms
- Basis set convergence easy to control

Note: order-N scheme needs localized basis set
(eg. Atomic orbitals → siesta or openmx)

Pseudopotential: core vs valence electrons



Mg: [Ne] $3S^2$

Core + valence

- Chemical bonds between atoms are formed by sharing /transferring valence electrons.
- Core electrons do not take part in bonding!
- Wavefunctions of valence electrons change significantly once the bond is formed ,whereas ones of core electrons change slightly.

Wavefunctions in 3D

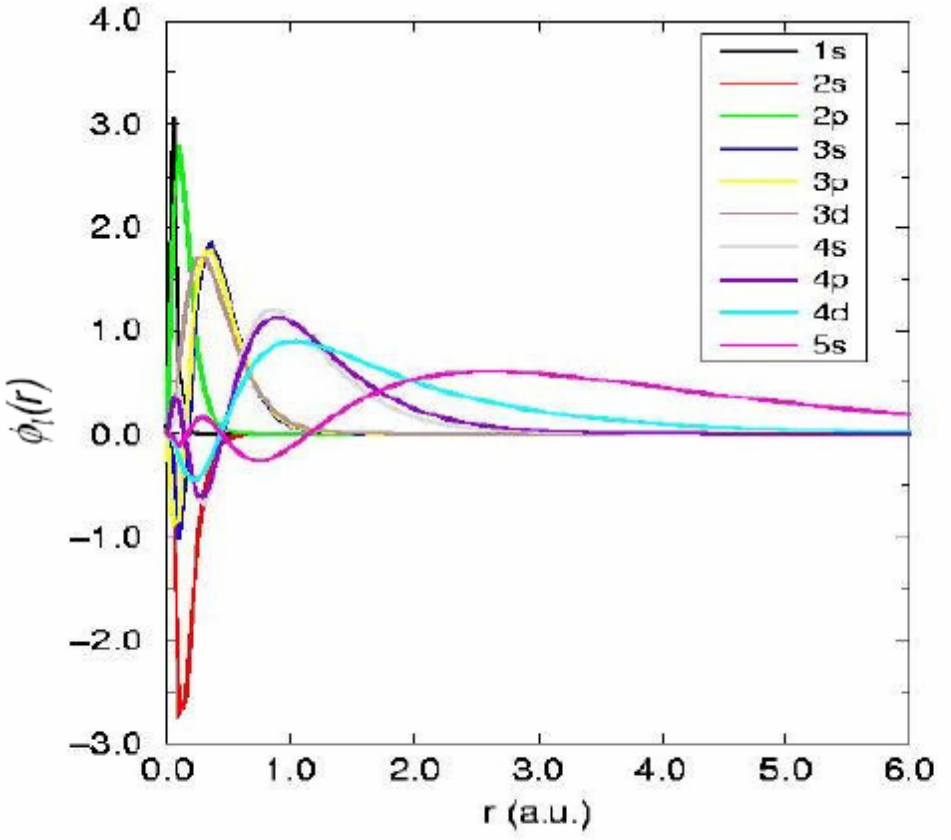
- Hydrogen(ic) atoms: solve exactly (analytically).

$$\psi_{lm}(r) = \psi_l(r) Y_{lm}(\theta,\varphi) = \frac{\phi_l(r)}{r} Y_{lm}(\theta,\varphi)$$

- When there are many interacting electrons: have to solve numerically.
  - Schrödinger equation / Dirac equation
  - Hartree-Fock equations
  - Kohn-Sham equations
  - The core electrons are treated in spherical symmetry, whereas the valence electrons are not spherical symmetric

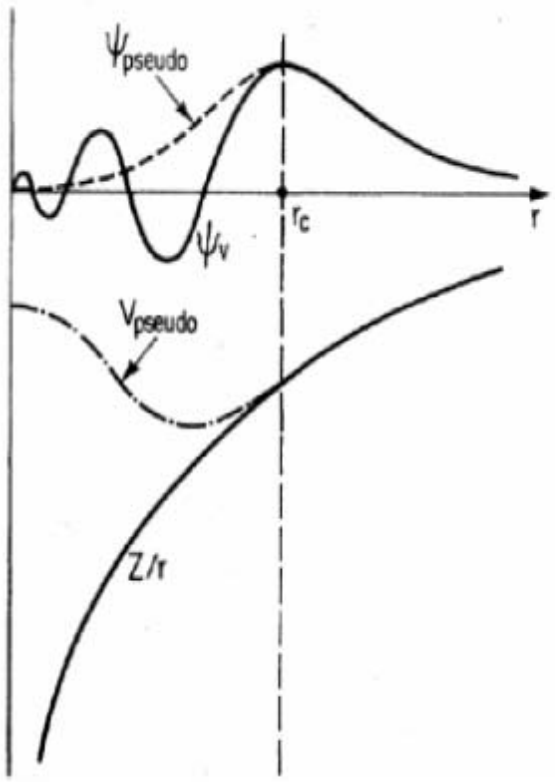
- All-electron calculations: both core and valence e-s included (whether for atom or solid).

Core vs valence electrons



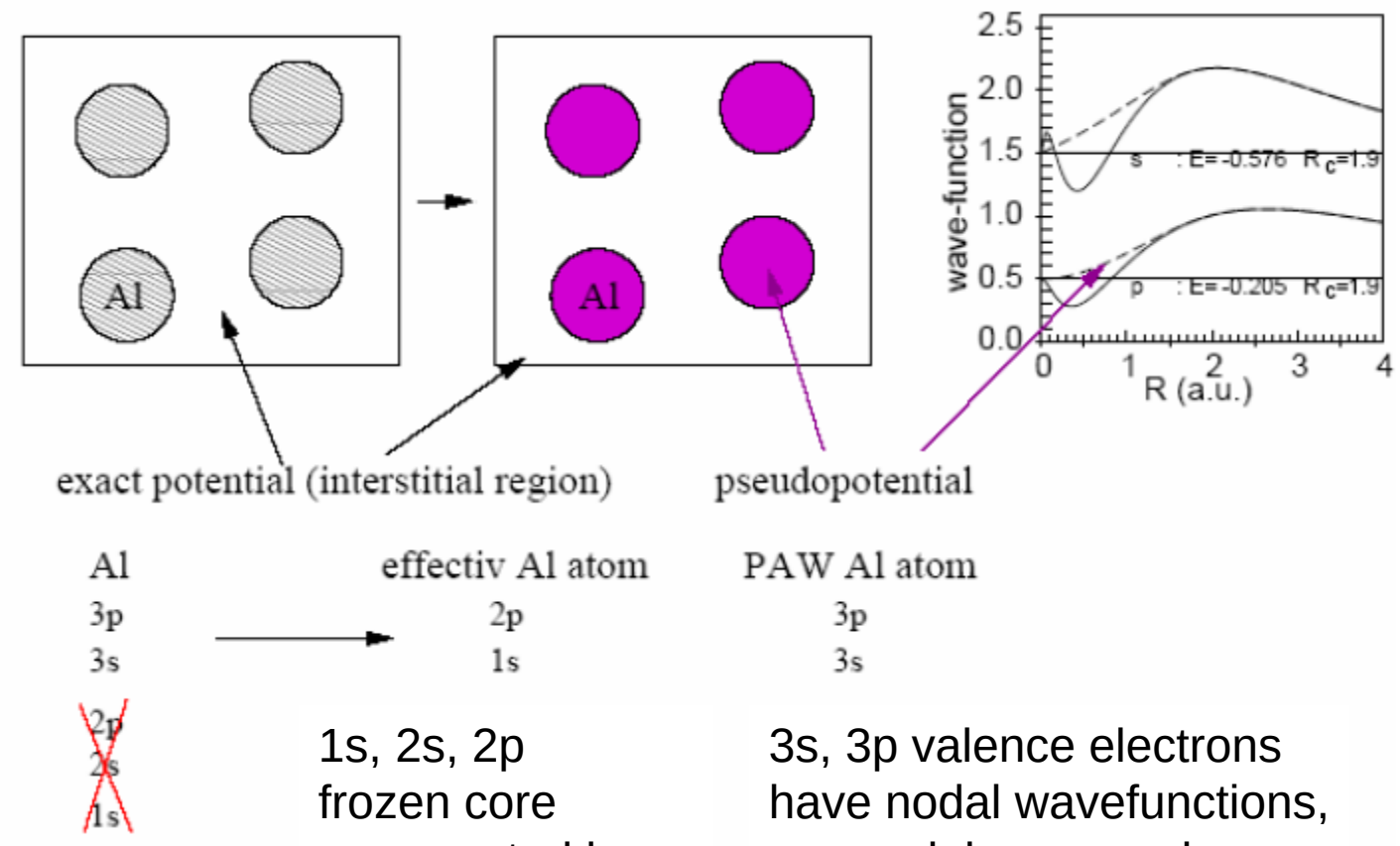
Ag=[Kr] $4d^{10}$ $5s^{1}$

Pseudopotential and pseudowavefunction



- Too many planewaves needed for core states, and related orthogonality
- Physical properties depend on valence electrons - throw away cores
- Pseudopotential constructed so that
  - Scattering properties preserved
  - Potential and Ψ identical outside core
  - Norm conserved (can be relaxed)
- Transferability . . .
- Local/Non-local and realspace potentials . . .

Essential idea



1s, 2s, 2p
frozen core
represented by
a pseudopotential

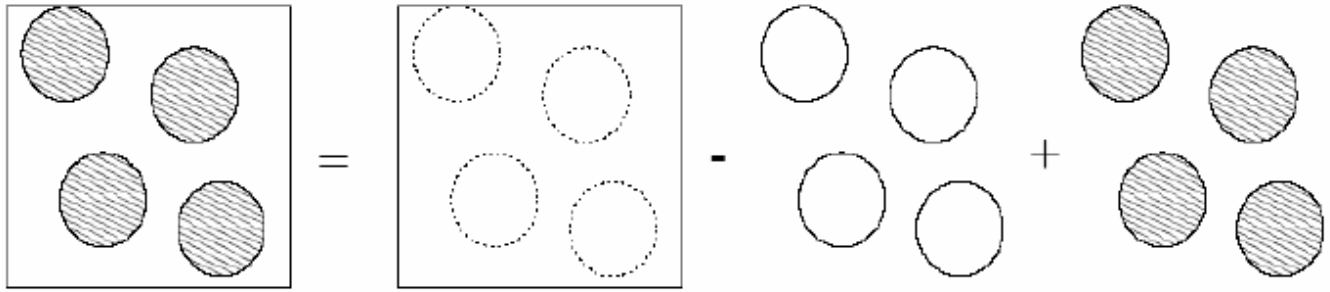
3s, 3p valence electrons
have nodal wavefunctions,
use nodeless pseudo
wavefunctions instead

3 types of pseudopotential

- **Norm-conserving pseudopotentials (NCP)**
- **Ultra-soft pseudopotentials (US-PP)**
  D. Vanderbilt, PRB 41 p. 7892 (1990)
- **PAW potentials**
  P.E. Blochl, PRB, 50 p.17953 (1994)

PAW

- character of wavefunction: $c_{lm\varepsilon} = \langle \tilde{p}_{lm\varepsilon} | \tilde{\Psi}_n \rangle$
- $|\Psi_n\rangle = |\tilde{\Psi}_n\rangle - \sum |\tilde{\phi}_{lm\varepsilon}\rangle c_{lm\varepsilon} + \sum |\phi_{lm\varepsilon}\rangle c_{lm\varepsilon}$



AE pseudo pseudo-onsite AE-onsite

- same trick works for
  - wavefunctions
  - charge density
  - kinetic energy
  - exchange correlation energy
  - Hartree energy

LDA vs LSDA

LDA

$$E_G[n(\vec{r})] = T_S[n] + \int n(\vec{r}) V_{ext}(\vec{r})\, d^3r$$

$$+ \frac{1}{2}\int \frac{n(\vec{r})\, n(\vec{r}\,')}{|\vec{r} - \vec{r}\,'|} d^3r\, d^3r' + E_{xc}[n]$$

$$V(\vec{r}) = V_{ext}(\vec{r}) + \int d^3r' \frac{n(\vec{r}\,')}{|\vec{r} - \vec{r}\,'|} + V_{xc}[n(\vec{r})]$$

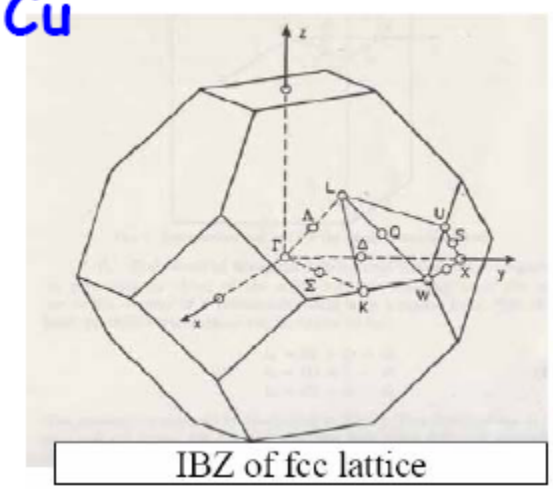
LSDA

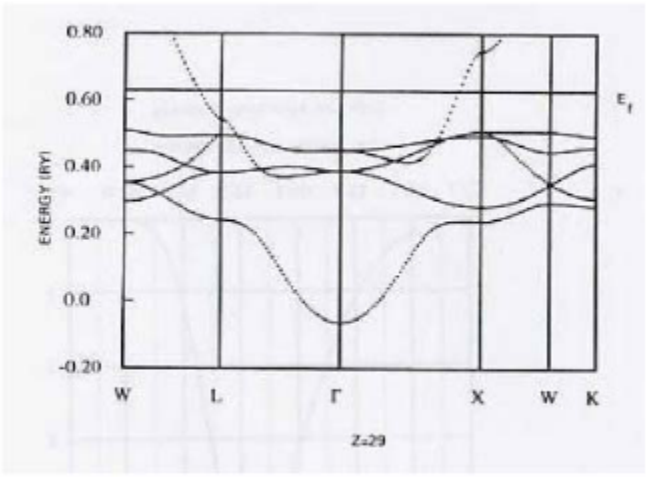
$$E_G = T_0[n] + \int d^3r n(\vec{r}) v(\vec{r}) + \frac{1}{2}\int d^3r d^3r' \frac{n(\vec{r}) n(\vec{r'})}{|\vec{r} - \vec{r'}|} + E_{xc}[n_+, n_-]$$

$$v^{\sigma}_{\text{eff}}(\vec{r}) = v(\vec{r}) + \int d^3r' \frac{n(\vec{r'})}{|\vec{r} - \vec{r'}|} + v^{\sigma}_{xc}([n_+, n_-]; \vec{r})$$

LDA vs LSDA

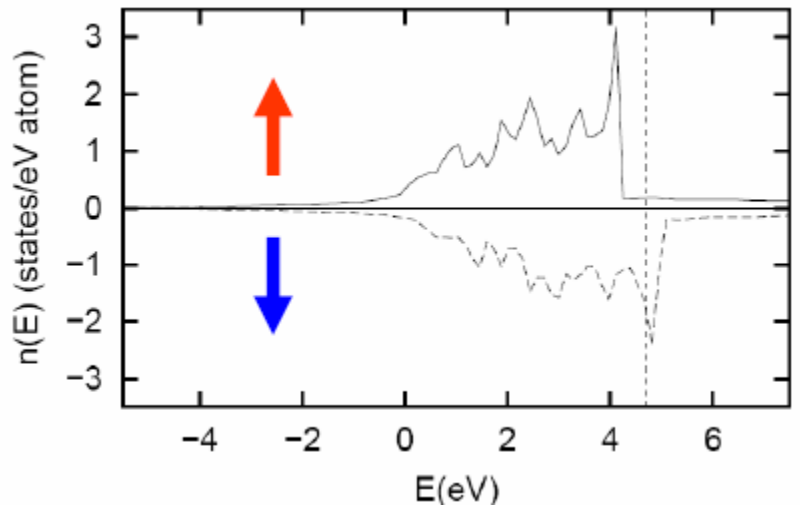
FCC- Cu



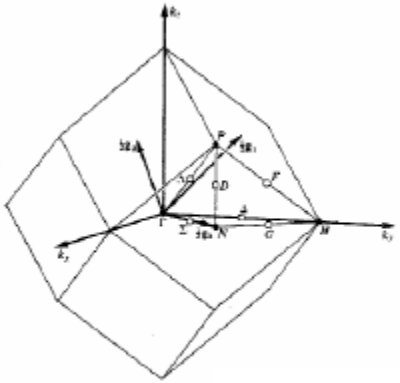


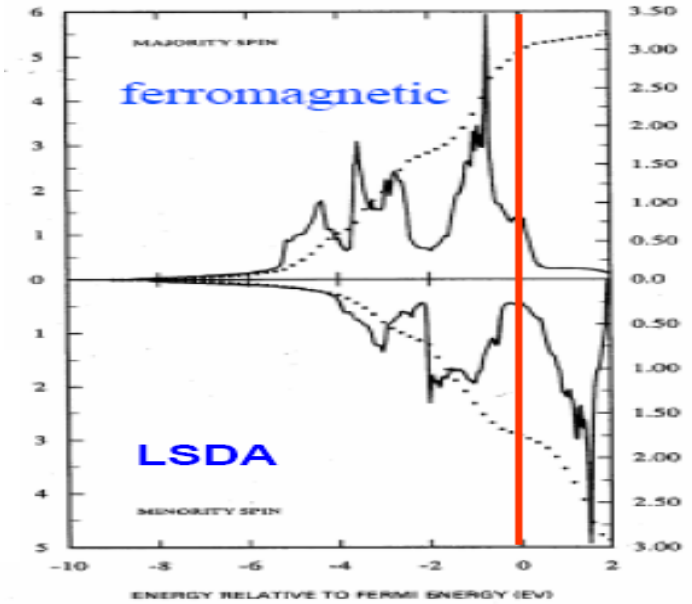
FCC-Ni

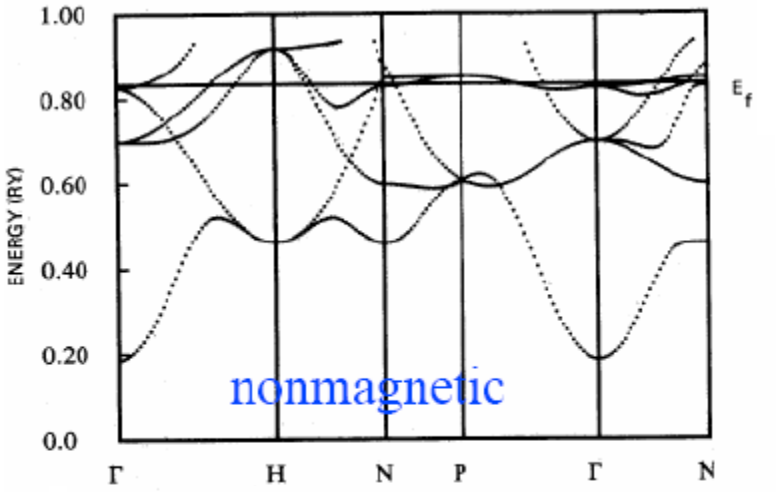
fcc Ni

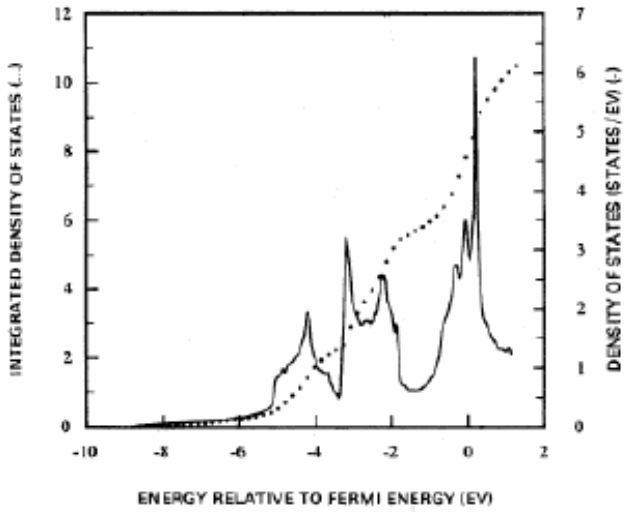


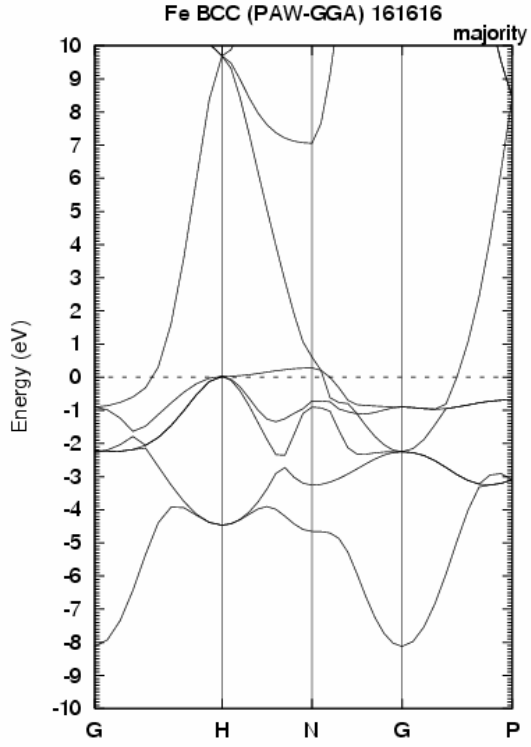
Fe(BCC)

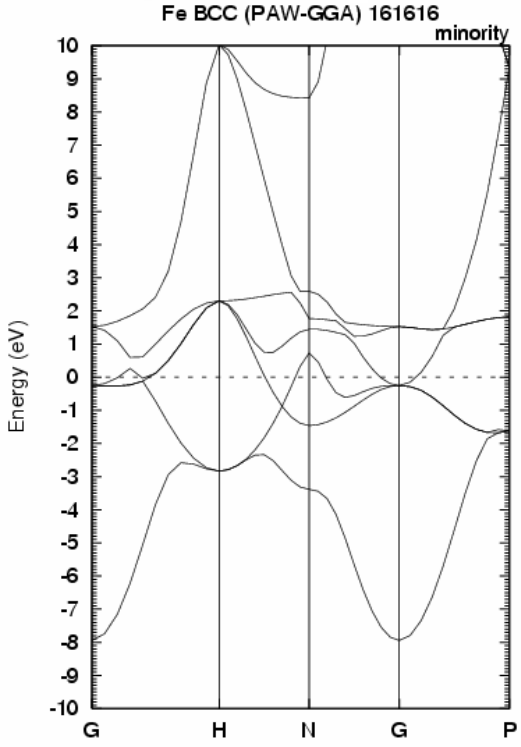



MAJORITY SPIN
ferromagnetic
LSDA
MINORITY SPIN
ENERGY RELATIVE TO FERMI ENERGY (EV)

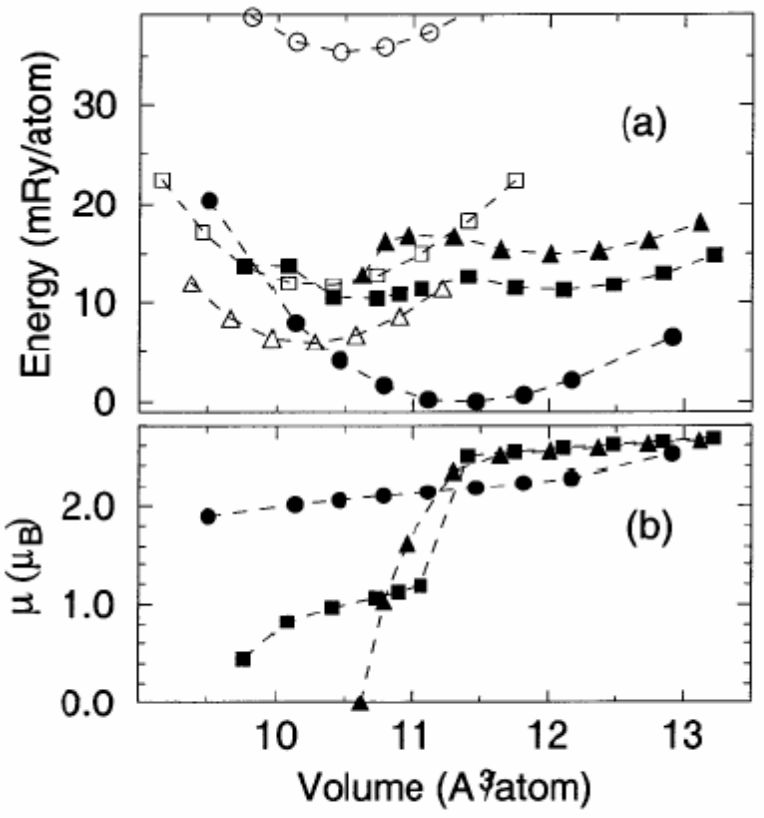

ENERGY (RY)
E_f
nonmagnetic
Γ H N P Γ N


INTEGRATED DENSITY OF STATES (..)
DENSITY OF STATES (STATES / EV) (-)
ENERGY RELATIVE TO FERMI ENERGY (EV)


Fe BCC (PAW-GGA) 161616
majority
Energy (eV)
G H N G P


Fe BCC (PAW-GGA) 161616
minority
Energy (eV)
G H N G P

Fe energy: GGA vs LSDA



GGA
- FCC
- HCP
- BCC

LDA
- FCC
- HCP
- BCC

G.Y. Guo and H.H.Wang CJP (2000)

Half-metal

CrO2

Jeng et al, JAP (2002)

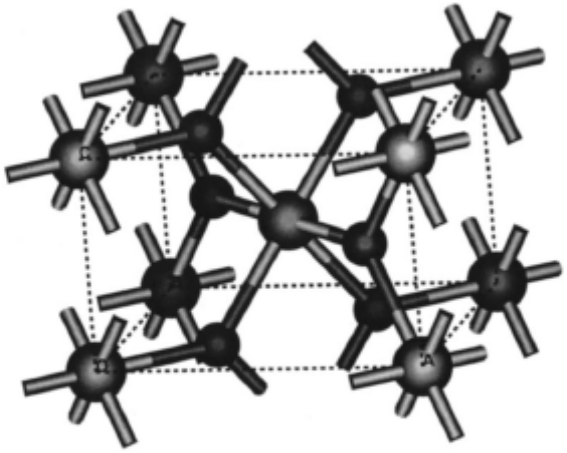
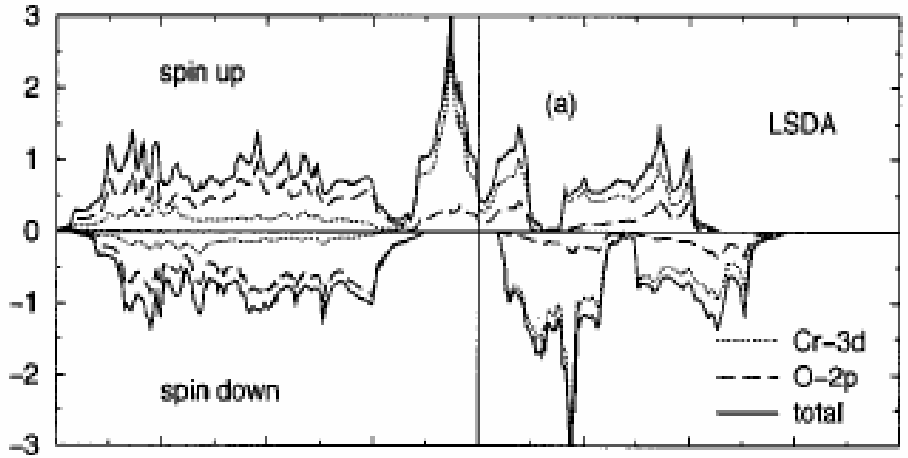


FIG. 1. Rutile structure of CrO_2. Big light balls denote Cr atoms and small dark balls denote O atoms.



Double perovskite

Jeng et al, PRB (2003)

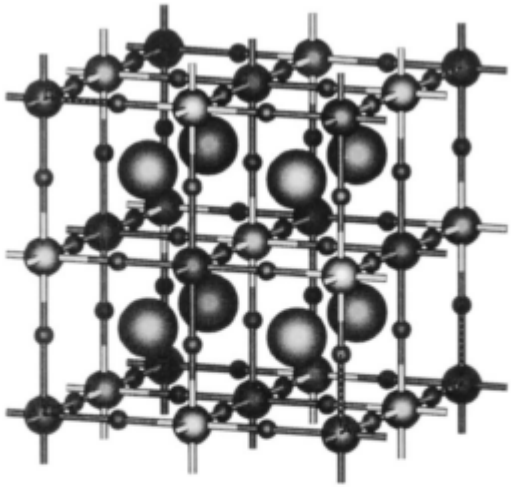


FIG. 1. Crystal structure of double perovskite. Big and small balls denote Sr and O, respectively. Middle light and middle dark balls denote the two different transition-metal atoms, respectively.

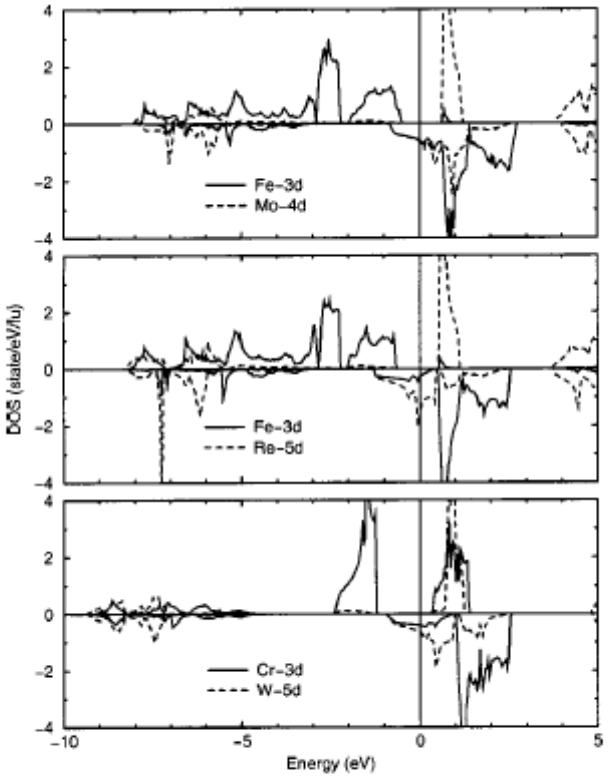


FIG. 2. Density of states of Sr_2FeMoO_6 (upper panel), Sr_2FeReO_6 (middle panel), and Sr_2CrWO_6 (lower panel) from the GGA. The Fermi level is at zero energy.

Magnetite

Jeng et al, PRB (2002)

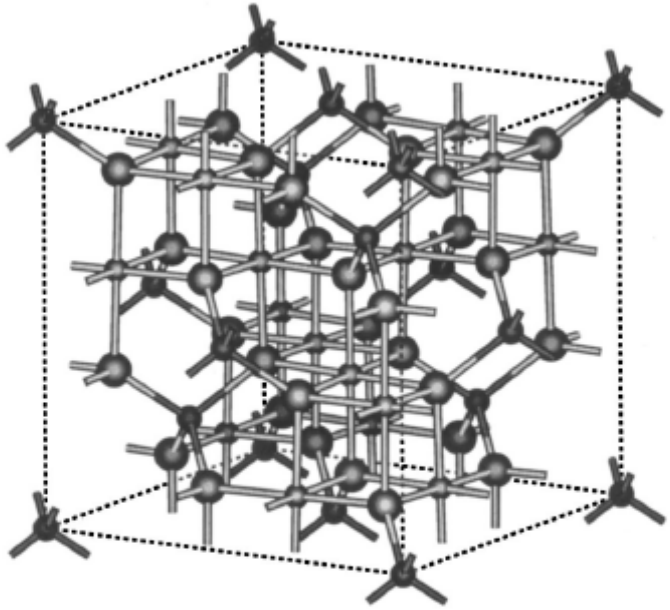


FIG. 1. Crystal structure of Fe_3O_4. Big balls denote oxyge atoms, small dark balls denote A-site (tetrahedral) iron atoms, an small light balls denote B-site (octahedral) iron atoms.

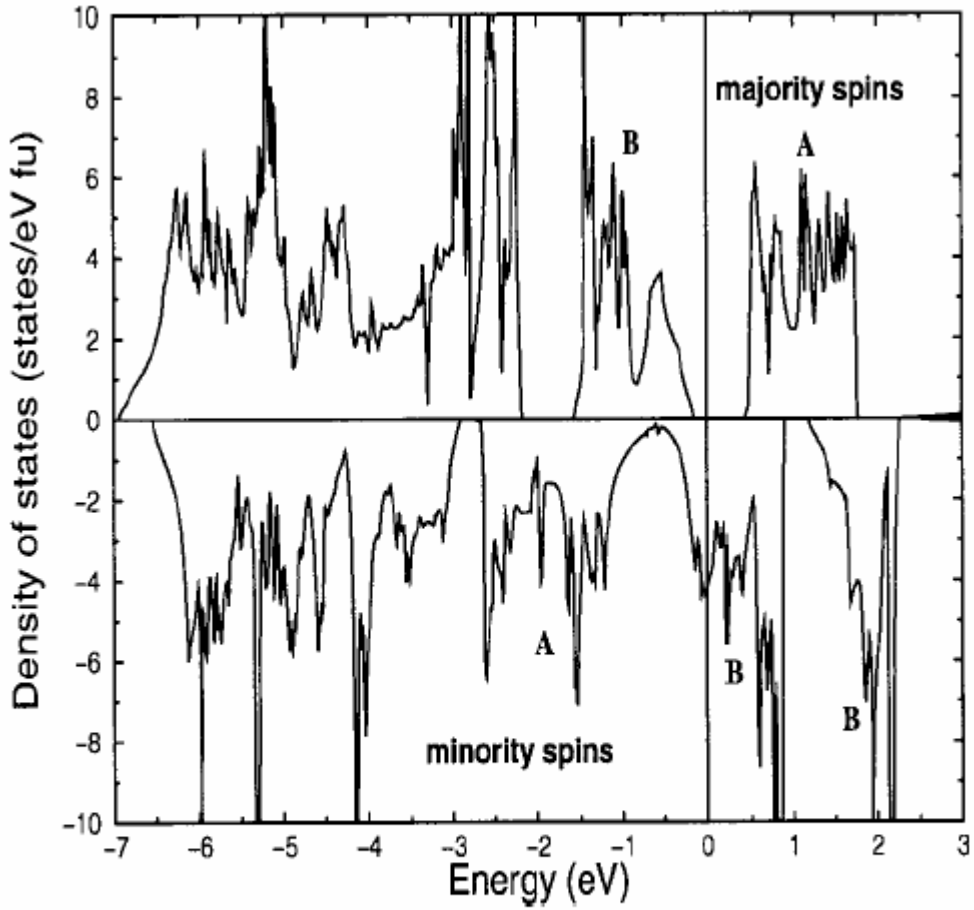


FIG. 3. Spin-decomposed densities of states for unstrained cubic Fe_3O_4. A and B indicate Fe(A) and Fe(B) $3d$ dominant bands, respectively. The Fermi level is at zero energy.

CMS II-5 Hands-on: spin polarized DOS and BS calculation

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Working list

- Spin polarized DOS and BS calculation of ferromagnetic transition metal Fe(BCC)
- Plot spin polarized DOS and BS
- Half-metallic oxide CrO2
- Antiferromagnetic oxide NiO

Spin polarized DOS calculation of Fe(BCC)

INCAR:

SYSTEM = Fe BCC

DOS related values
ISMEAR = -5
ISPIN = 2
MAGMOM = 5
GGA = 91
RWIGS = 1.3

KPOINTS:

Fe
0
Monkhorst-Pack
16 16 16
0 0 0

POTCAR:

potpaw_GGA

POSCAR:

Fe BCC
2.87
-0.5 0.5 0.5
0.5 -0.5 0.5
0.5 0.5 -0.5
1
direct
0.0 0.0 0.0 ! Fe

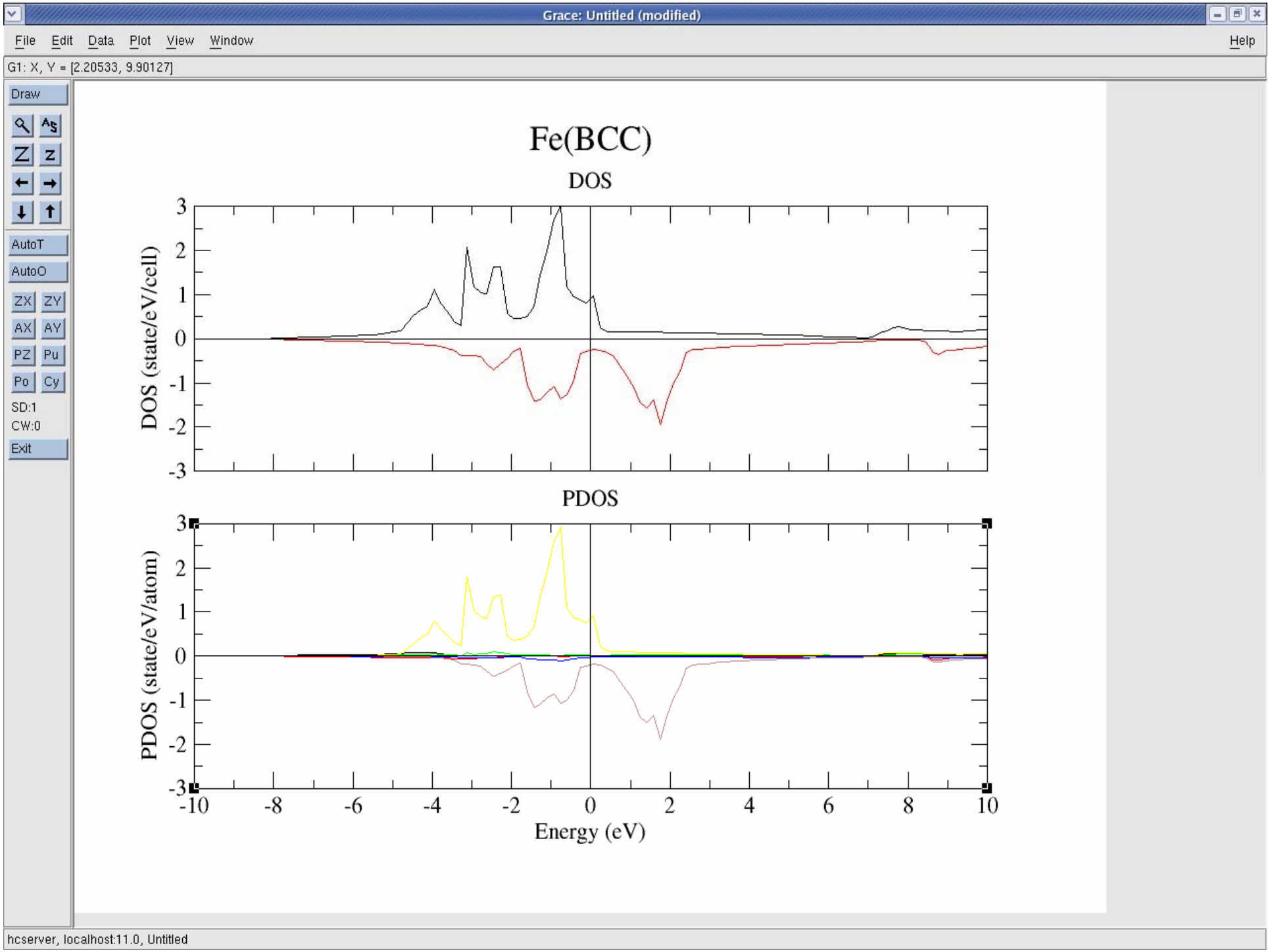
Spin polarized density of state

DOSCAR:

```
1   1   1   0
  0.1181995E+02  0.2485493E-09  0.2485493E-09  0.2485493E-09  0.5000000E-15
   1.000000000000000E-004
  CAR
 Fe BCC
    45.37866545     -4.96186562  301      5.37395808      1.00000000
    -4.962  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
    -4.794  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
    -4.626  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
……..
    45.043  0.0000E+00  0.0000E+00  0.1100E+02  0.1100E+02
    45.211  0.0000E+00  0.0000E+00  0.1100E+02  0.1100E+02
    45.379  0.0000E+00  0.0000E+00  0.1100E+02  0.1100E+02
    45.37866545     -4.96186562  301      5.37395808      1.00000000
    -4.962  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
    -4.794  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
    -4.626  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
……..
```

E Du Dd iDu iDd

E su sd pu pd du dd


Grace: Untitled (modified)
File Edit Data Plot View Window Help
G1: X, Y = [2.20533, 9.90127]
Draw
AutoT
AutoO
ZX ZY
AX AY
PZ Pu
Po Cy
SD:1
CW:0
Exit
Fe(BCC)
DOS
DOS (state/eV/cell)
PDOS
PDOS (state/eV/atom)
Energy (eV)
hcserver, localhost:11.0, Untitled

Spin polarized BS calculation of Fe(BCC)

INCAR:

```
SYSTEM = Fe BCC

DOS related values
 ICHARG = 11
 ISMEAR = 0
 ISPIN = 2
 MAGMOM = 5
 GGA = 91
 RWIGS = 1.3
```

POTCAR:

```
potpaw_GGA
```

POSCAR:

```
Fe BCC
 2.87
-0.5  0.5  0.5
 0.5 -0.5  0.5
 0.5  0.5 -0.5
 1
direct
 0.0        0.0        0.0        ! Fe
```

KPOINTS:

```
Fe(BCC)
11
Line-mode
Cartesian
0.0   0.0  0.0   ! G
0.0   1.0  0.0   ! H

0.0   1.0  0.0   ! H
0.5   0.5  0.0   ! N

0.5   0.5  0.0   ! N
0.0   0.0  0.0   ! G

0.0   0.0  0.0   ! G
0.5   0.5  0.5   ! P
```

Extract SP BS data using tool: bndace

```
EIGENVAL:
1    1    1    2
 0.1181995E+02  0.2485493E-09  0.2485493E-09  0.2485493E-09  0.5000000E-15
  1.0000000000000000E-004
 CAR
Fe BCC
    8   44   11
 0.0000000E+00  0.0000000E+00  0.0000000E+00  0.2272727E-01
  1      -2.7530    -2.5693
  2       3.1210     5.1225
  3       3.1211     5.1225
  4       3.1212     5.1229
  5       4.4740     6.9008
  6       4.4740     6.9008
  7      30.0813    29.8967
  8      30.0813    29.8968
  9      30.0814    29.8968
 10      35.0443    35.0632
 11      35.0443    35.0633
 0.5000000E-01 -0.5000000E-01  0.5000000E-01  0.2272727E-01
  1      -2.5523    -2.3677
  2       3.1207     5.1147
  3       3.1208     5.1149
 ……..
```

44 k-points, 11bands(eigenvalues)

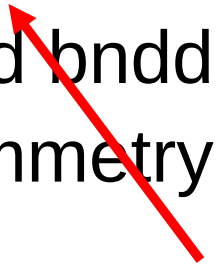
coordinates of the 1st k-point

the 11 spin up and spin down eigenvalues of the 1st k-point

the 2nd k-point …

How to use bndace

- Execute bndace and input Ef
  %~/tool/bndace
  Input Fermi level 5.37395808
- Output: bnd.kp, bndup.dat, and bnddn.dat
- bnd.kp: distances of high symmetry points
  0.0000: G
  0.5000: H
  0.8536: N
  1.2071: G
  1.6401: P



Note!!!
Ef should be from SCF calculation!!!

bndup.dat (for xmgrace):

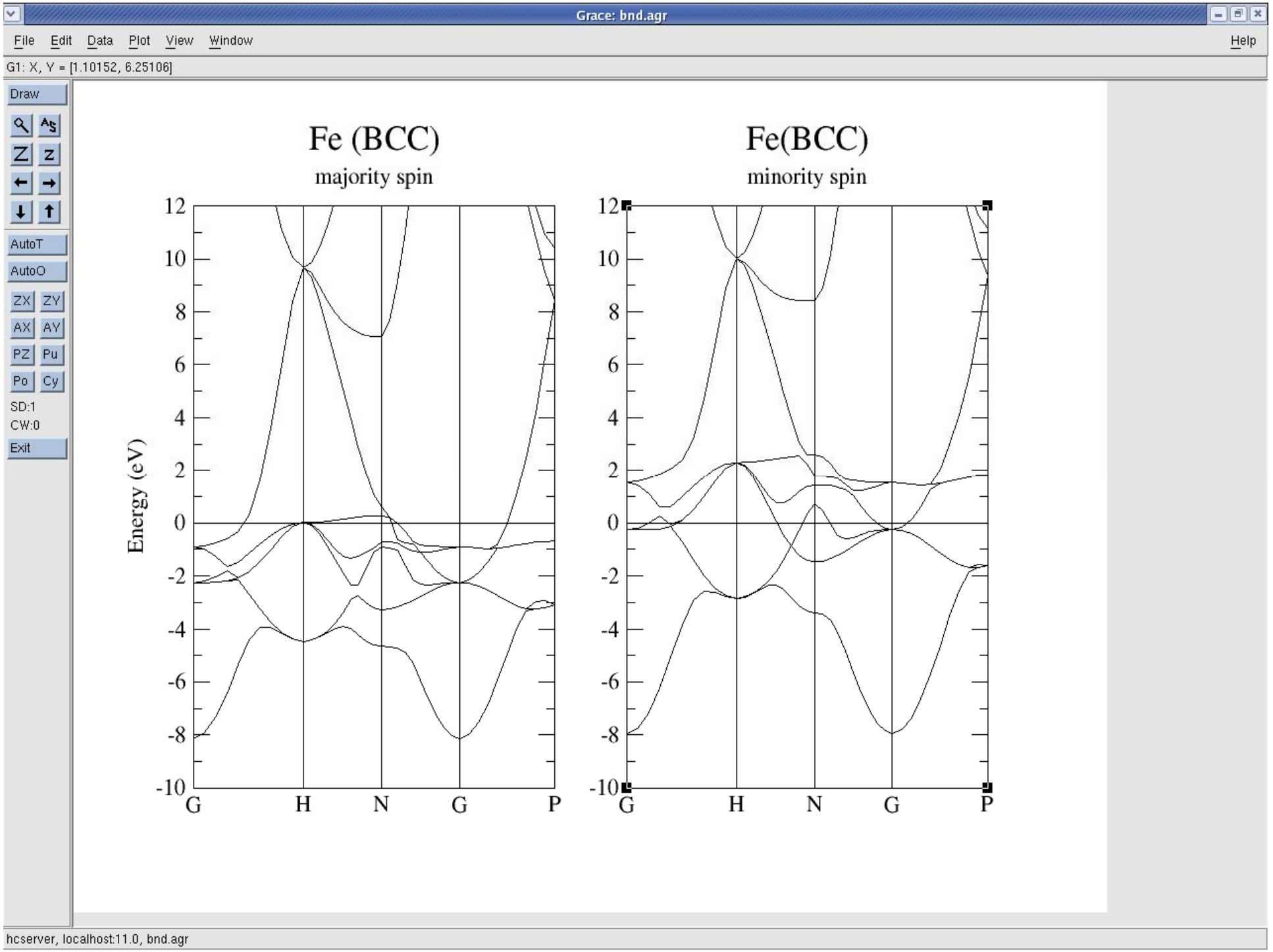
	k length	eig1	eig2	eig3	…						
G	0.0000	-8.1270	-2.2530	-2.2529	-2.2528	-0.9000	-0.9000	24.7073	24.7073	24.7074	29.6703	29.6703
	0.0500	-7.9263	-2.2533	-2.2532	-2.1994	-0.9871	-0.8652	23.4936	24.4557	24.4558	27.8662	29.4998
	0.1000	-7.3418	-2.2364	-2.2364	-2.0417	-1.2377	-0.7656	21.5602	23.3032	23.3033	25.3249	28.8301
	0.1500	-6.4354	-2.1855	-2.1855	-1.7892	-1.6366	-0.6026	19.8250	21.2336	21.2337	22.9489	29.5923
	0.2000	-5.3510	-2.1420	-2.0575	-2.0575	-1.4805	-0.3191	18.4262	18.9098	18.9099	20.9687	31.1533
	0.2500	-4.3918	-2.7003	-1.8226	-1.8226	-1.1334	0.3028	16.6242	16.6243	17.3641	19.4867	33.3546
	0.3000	-3.9236	-3.2540	-1.4646	-1.4646	-0.7792	1.6053	14.5081	14.5082	16.5949	18.4961	30.8687
	0.3500	-3.9377	-3.7497	-1.0155	-1.0154	-0.4590	3.5890	12.6255	12.6256	16.0517	17.8880	26.7202
	0.4000	-4.1675	-4.1374	-0.5342	-0.5341	-0.2023	5.9694	11.0942	11.0943	15.7053	17.3357	23.0796
	0.4500	-4.3837	-4.3836	-0.1373	-0.1372	-0.0364	8.3780	10.0615	10.0616	15.5140	16.3652	20.6589
H	0.5000	-4.4681	-4.4681	0.0208	0.0209	0.0211	9.6899	9.6901	9.6902	15.4527	15.4528	19.9476
H	0.5000	-4.4681	-4.4681	0.0208	0.0209	0.0211	9.6899	9.6901	9.6902	15.4527	15.4528	19.9476
	0.5354	-4.4259	-4.4246	-0.0945	-0.0610	0.0272	9.3210	9.4784	9.8773	15.6197	15.9179	20.2696
	0.5707	-4.3078	-4.2942	-0.4111	-0.2937	0.0450	8.4411	8.9846	10.4106	15.9722	17.0879	21.2303

……

bnddn.dat (for xmgrace):

	k length	eig1	eig2	eig3	…							
G	0.0000	-7.9433	-0.2515	-0.2515	-0.2511	1.5268	1.5268	24.5227	24.5228	24.5228	29.6892	29.6893
	0.0500	-7.7417	-0.2593	-0.2591	-0.1919	1.4165	1.5699	23.4004	24.3841	24.3842	28.1535	30.3530
	0.1000	-7.1518	-0.2632	-0.2630	-0.0173	1.0983	1.6880	21.5908	23.5828	23.5829	25.6756	29.3977
	0.1500	-6.2225	-0.2346	-0.2344	0.2616	0.5974	1.8538	19.9899	21.7950	21.7951	23.2984	29.9564
	0.2000	-5.0551	-0.1214	-0.1212	-0.0314	0.6074	2.0627	18.7345	19.5832	19.5834	21.3189	31.4773
	0.2500	-3.8498	-0.7183	0.1161	0.1163	0.9972	2.4093	17.3235	17.3237	17.8137	19.8701	33.5451
	0.3000	-2.9422	-1.3907	0.5007	0.5009	1.3954	3.1951	15.1816	15.1817	17.1719	18.9500	31.5025
	0.3500	-2.5794	-1.9842	1.0106	1.0108	1.7575	4.6826	13.2333	13.2334	16.7354	18.4277	27.4279
	0.4000	-2.6196	-2.4440	1.5874	1.5877	2.0484	6.7262	11.6003	11.6003	16.4661	17.9506	23.9027
	0.4500	-2.7654	-2.7341	2.0912	2.0915	2.2368	8.8824	10.4558	10.4558	16.3213	17.0657	21.6050
H	0.5000	-2.8332	-2.8332	2.3018	2.3019	2.3024	10.0298	10.0301	10.0303	16.2756	16.2757	20.9281
H	0.5000	-2.8332	-2.8332	2.3018	2.3019	2.3024	10.0298	10.0301	10.0303	16.2756	16.2757	20.9281
	0.5354	-2.7936	-2.7876	2.1544	2.1915	2.3091	9.7331	9.8824	10.2455	16.4143	16.6700	21.2377
	0.5707	-2.6745	-2.6616	1.7604	1.8829	2.3292	8.9947	9.5412	10.8450	16.7115	17.7025	22.1633

……


Grace: bnd.agr
File Edit Data Plot View Window Help
G1: X, Y = [1.10152, 6.25106]
Draw
AutoT
AutoO
ZX ZY
AX AY
PZ Pu
Po Cy
SD:1
CW:0
Exit
Fe (BCC)
majority spin
Fe(BCC)
minority spin
Energy (eV)
12
10
8
6
4
2
0
-2
-4
-6
-8
-10
G H N G P
hcserver, localhost:11.0, bnd.agr

Spin density distribution

vaspview

```
Fe BCC
   2.870000000000000
   -0.500000    0.500000    0.500000
    0.500000   -0.500000    0.500000
    0.500000    0.500000   -0.500000
  1
Direct
  0.000000  0.000000  0.000000

  18   18   18
0.10025339985E+03 0.92955633606E+02 0.74221060063E+02 0.51128363739E+02 0.30267430390E+02
0.15431178869E+02 0.75270158027E+01 0.48409528846E+01 0.40552510209E+01 0.38045919133E+01
0.40552510209E+01 0.48409528846E+01 0.75270158027E+01 0.15431178869E+02 0.30267430390E+02
.....
.....
18   18   18
0.43760763886E+02 0.40510865442E+02 0.31845872865E+02 0.20742791723E+02 0.10839185688E+02
0.44317302429E+01 0.14625111504E+01 0.48650442792E+00 0.16535915972E+00 0.69399174197E-01
0.16535915972E+00 0.48650442792E+00 0.14625111504E+01 0.44317302429E+01 0.10839185688E+02
.....
.....
```

Charge density

Spin density

Exchange charge and spin block, use vaspview to see spin density distribution

Magnetic moment

OSZICAR:

```
N       E                     dE             d eps      ncg     rms         rms(c)
DAV:   1    -0.171929423743E+02   -0.17193E+02   -0.71425E+02  7891   0.255E+02    0.270E+01
DAV:   2    -0.949680815166E+01    0.76961E+01   -0.19021E+02  7320   0.114E+02    0.101E+01
DAV:   3    -0.775005799055E+01    0.17468E+01   -0.12928E+01  6991   0.404E+01    0.485E+00
DAV:   4    -0.796148916414E+01   -0.21143E+00   -0.23930E-01  7276   0.405E+00    0.415E+00
DAV:   5    -0.798034989774E+01   -0.18861E-01   -0.13094E+00  7047   0.919E+00    0.480E+00
DAV:   6    -0.811689680787E+01   -0.13655E+00   -0.84602E-02  6630   0.218E+00    0.174E+00
DAV:   7    -0.814864724012E+01   -0.31750E-01   -0.47481E-02  7027   0.200E+00    0.369E-01
DAV:   8    -0.814990546628E+01   -0.12582E-02   -0.18405E-03  6675   0.313E-01    0.311E-01
DAV:   9    -0.815090027140E+01   -0.99481E-03   -0.11541E-03  5446   0.263E-01    0.468E-02
DAV:  10    -0.815096963218E+01   -0.69361E-04   -0.20415E-04  3532   0.119E-01

   1 F= -.81509696E+01 E0= -.81509696E+01  d E =0.000000E+00 mag=     2.2328
```

total moment (unit cell)

OUTCAR:

```
 ……..
total charge

# of ion     s       p       d       tot
------------------------------------------
  1        0.394   0.409   6.148   6.951

 magnetization (x)

# of ion     s       p       d       tot
------------------------------------------
  1       -0.008  -0.041   2.307   2.259
```

atomic moment (within RWGS)

Half-metallic CrO2(Rutile)

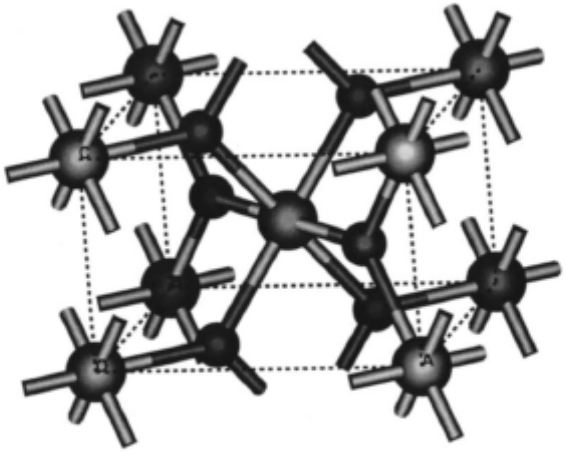


FIG. 1. Rutile structure of CrO_2. Big light balls denote Cr atoms and small dark balls denote O atoms.

KPOINTS:

```
CrO2
 0
Monkhorst-Pack
 6 6 9
 0 0 0
```

INCAR:

```
SYSTEM = CrO2

DOS related values
 ISMEAR = -5
 ISPIN = 2
 MAGMOM = 2*3 4*0
 GGA = 91
 RWIGS = 1.1 0.8
```

POSCAR:

```
CrO2 Rutile
 4.419
 1.0     0.0     0.0
 0.0     1.0     0.0
 0.0     0.0     0.659
 2 4
direct
 0.0     0.0     0.0     ! Cr
 0.5     0.5     0.5     ! Cr
 0.303   0.303   0.0     ! O
 0.697   0.697   0.0     ! O
 0.803   0.197   0.5     ! O
 0.197   0.803   0.5     ! O
```

POTCAR: potpaw_GGA

POTCAR(Cr)
POTCAR(O)

Rocksalt FeO, CoO, and NiO antiferro type II

INCAR:

```
SYSTEM = NiO FCC

DOS related values
 ISMEAR = -5
 ISPIN = 2
 MAGMOM = 2 -2 2*0
 GGA = 91
 RWIGS = 1.2 0.8
```

KPOINTS:

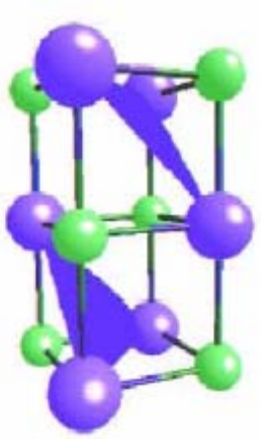
```
NiO
 0
Monkhorst-Pack
 8 8 8
 0 0 0
```

POSCAR:

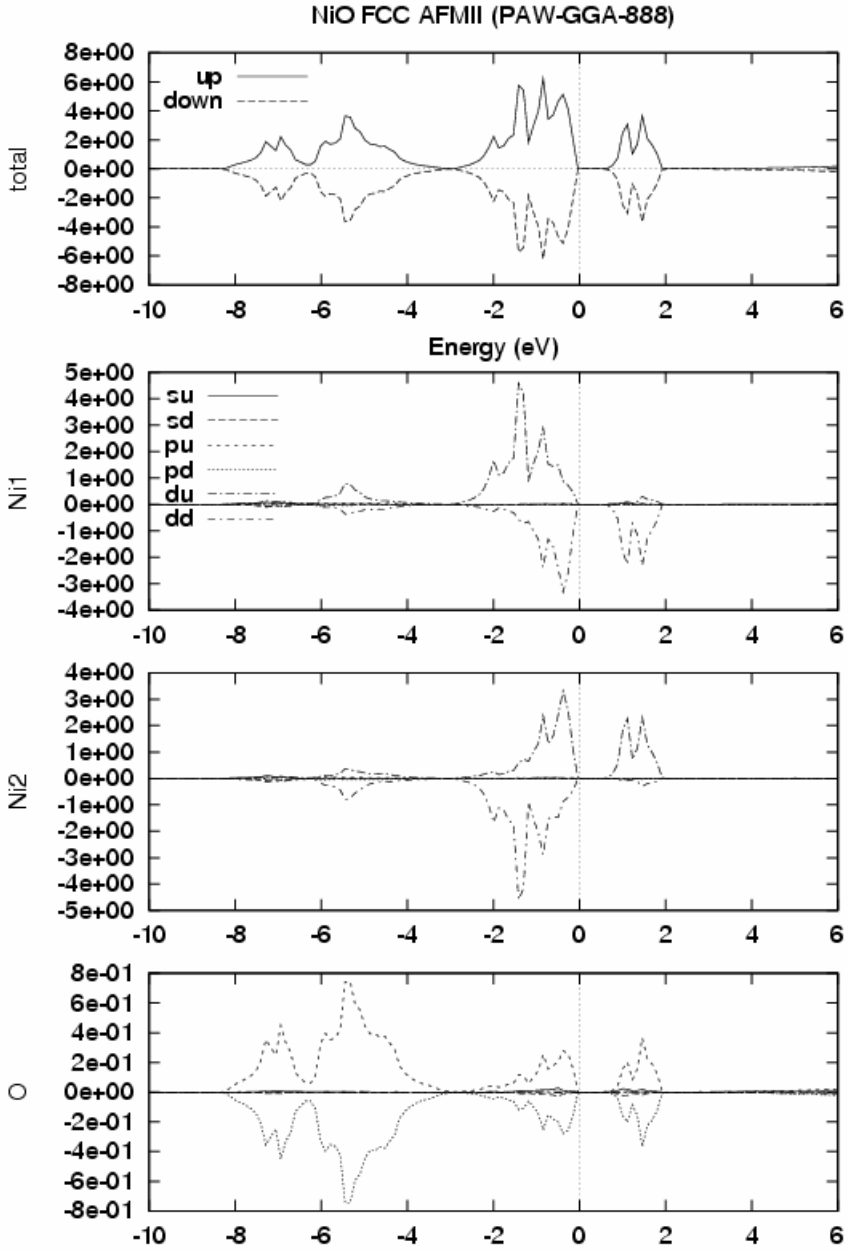
```
NiO FCC
 4.18
 1.0      0.5      0.5
 0.5      1.0      0.5
 0.5      0.5      1.0
 2 2
Cartesian
0.0       0.0      0.0      ! Ni
1.0       1.0      1.0      ! Ni
0.5       0.5      0.5      ! O
1.5       1.5      1.5      ! O
```

POTCAR:

potpaw_GGA(Ni,O)



FeO: a=4.33A
CoO: a=4.26A


NiO FCC AFMII (PAW-GGA-888)
total
up
down
Ni1
su
sd
pu
pd
du
dd
Ni2
O
Energy (eV)

Homework

please Email to jeng@phys.sinica.edu.tw

- Calculate and plot GGA spin polarized DOS and BS along high symmetry lines LGXWKG, GHNGP, GMKGA, for Ni(FCC), Fe(BCC), and Co(HCP), respectively
- Calculate and plot GGA spin polarized DOS of FeO, CoO, NiO, and CrO2
- Make a list of the GGA magnetic moment of Fe(BCC), Co(HCP), Ni(FCC), FeO, CoO, NiO, and CrO2