CMS II-6: Transition-metal oxides, strong correlations, and LDA+U

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Outline

- Insufficiencies of LDA
- How to improve LDA
- Self-interaction correction (SIC)
- LDA + Hubbard U (LDA+U) method
- Applications of LDA+U on various transition-metal oxides

Insufficiencies of LDA (LDA, LSDA, GGA)

- LDA is successful for lots of systems such as metallic or weakly correlated materials
- BUT LDA has some problems:
- Gaps too small or no gap,
  PRB44, 943 (1991)
- Spin and orbital moment too small,
  PRB44, 943 (1991)
- Especially for transition metal oxides or strongly correlated systems

TABLE II. Experimental (expt) and calculated (LDA + U) spin moments (m, in μ_B) and energy gaps (E, in eV) of the late-3d-transition-metal monoxides. For comparison, we also show these quantities as calculated from LSDA (Ref. 1).

	E_{LSD}	$E_{\mathrm{LSD}+U}$	E_{expt}	m_{LSD}	$m_{\mathrm{LSD}+U}$	m_{expt}
$CaCuO_2$	0.0	2.1	1.5[a]	0.0	0.66	0.51[b]
CuO	0.0	1.9	1.4[c]	0.0	0.74	0.65[d]
NiO	0.2	3.1	4.3,[e]4.0[f]	1.0	1.59	1.77,[g]1.64,[h]1.90[i]
CoO	0.0	3.2	2.4[j,k]	2.3	2.63 (3.60)	3.35,[l]3.8[m]
FeO	0.0	3.2	2.4[n]	3.4	3.62 (4.59)	3.32[m]
MnO	0.8	3.5	3.6–3.8[o]	4.4	4.61	4.79,[g]4.58[i]

[a]Y. Tokura, T. Arima, S. Koshihara, T. Ido, S. Ishibasi, H. Takagi, and S. Uchida, *Proceedings of the Second International Symposium on Superconductivty,* Tsukuba (Springer, New York, in press).
[b]D. Vaknin, E. Couignol, P. K. Devies, J. E. Fischer, D. C. Johnson, and D. P. Goshorn, Phys. Rev. B **39**, 9122 (1989).
[c]F. P. Koffyberg and F. A. B
[d]J. B. Forsyth, P. J. Brown, a
[e]G. A. Sawatzky and J. W. A
[f]S. Hüfner, J. Osterwalder, T.
[g]B. E. F. Fender, A. J. Jacob
[h]H. A. Alperin, J. Phys. Soc.
[i]A. K. Cheetham and D. A. C
[j]J. van Elp *et al.* (unpublished).
[k]R. J. Powell and W. E. Spicer, Phys. Rev. B **2**, 2182 (1970).
[l]D. C. Kahn and R. A. Ericson, Phys. Rev. B **1**, 2243 (1970).
[m]W. L. Roth, Phys. Rev. **110**, 1333 (1958); D. Hermann-Ronzaud, P. Burlet, and J. Rossat Mignod, J. Phys. C **11**, 2123 (1978).
[n]H. K. Bowen, D. Adler, and B. H. Auker, J. Solid State Chem. **12**, 355 (1975).
[o]R. N. Iskenderov, I. A. Drabkin, L. T. Emel'yanova, and Ya. Ksendzov, Fiz. Tverd. Tela (Leningrad) **10**, 2573 (1968) [Sov. Phys.—Solid State **10**, 2031 (1969)]; L. Messick, W. C. Walker, and R. Glosser, Phys. Rev. B **6**, 3941 (1972).

Gaps too small or no gap

Spin and orbital moment too small

PRB 44 (1991) 943

Beyond LDA

- Self-interaction correction (SIC) PRB23(1981)5048, PRL65(1990)1148
- Optimized effective potential method (OEP)
- Hartree-Fock (HF) method, PRB48(1993)5058
- GW approximation (GWA), PRB46(1992)13051, PRL74(1995)3221
- Time-dependent density functional theory (TDDFT)
- Dynamical mean field theory (DMFT)
- Quantum Monte-Carlo method (QMC)
- LDA+Hubbard U (LDA+U) method, PRB44(1991)943, PRB48(1993)16929

Local density approximation (LDA)

Kohn-Sham scheme PR140(1965)A1133

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

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

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

Self-interaction correction (SIC)

Perdew and Zunger, PRB23(1981)5048

$$E_G^{SIC}[n] = E_G^{LDA}[n]$$

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

$$V_i^{SIC}(\vec{r}) = V^{LDA}(\vec{r}) - \int d^3r' \frac{n_i(\vec{r}')}{|\vec{r}-\vec{r}'|} - V_{xc}[n_i(\vec{r})]$$

Basic idea of LDA+U

PRB 44 (1991) 943, PRB 48 (1993) 169

- Delocalized s and p electrons : LDA
- Localized (strongly correlated) d or f electrons : +U

  using on-site d-d Coulomb interaction (Hubbard-like term)

  $$U \sum_{i \neq j} n_i n_j$$

  instead of averaged Coulomb energy

  $$UN(N-1)/2$$

When to use LDA+U

- Systems that LDA gives bad results
- Narrow band materials : $U \geqq W$
- Localized electron systems
- Transition-metal oxides
- Strongly correlated materials
- Insulators (for semiconductors: use GWA)
- …..

Where to find U and J

- PRB 44 (1991) 943 : 3d atoms
- PRB 50 (1994) 16861 : 3d, 4d, 5d atoms
- PRB 58 (1998) 1201 : 3d atoms
- PRB 44 (1991) 13319 : Fe(3d)
- PRB 54 (1996) 4387 : Fe(3d)
- PRL 80 (1998) 4305 : Cr(3d)
- PRB 58 (1998) 9752 : Yb(4f)

Notes on using LDA+U

- The magnitude of U is difficult to calculate and measure accurately, the deviation could be typically as large as $\pm$1eV
- For the same element, U depends also on the ionicity in different compounds: the higher ionicity, the larger U
- One thus varies U in a reasonable range to obtain better results
- One might varies U in a much larger range to see the effect of U (qualitatively)
- $\rightarrow$ Self-consistent LDA+U (much more difficult)

Various LDA+U methods

- Hubbard model in mean field approx. (HMF)
  LDA+U : PRB 44 (1991) 943 (WIEN2K, LMTO)
- Approximate self-interaction correction (SIC)
  LDA+U : PRB 48 (1993) 16929 (WIEN2K)
- Around the mean field (AMF) LDA+U :
  PRB 49 (1994) 14211 (WIEN2K)
- Rotationally invariant LDA+U :
  PRB 52 (1995) R5468 (VASP4.6, LMTO)
- Simplified rotationally invariant LDA+U :
  PRB 57 (1998) 1505 (VASP4.6, LMTO)

Rotationally invariant LDA+U: PRB52(1995)R5468

$$E = E^{LDA} - \frac{1}{2}Un(n-1) + \frac{1}{2}J[n^{\uparrow}(n^{\uparrow}-1) + n^{\downarrow}(n^{\downarrow}-1)]$$

$$+\frac{1}{2}\sum_{\{m\},\sigma}\{<mm''|V_{ee}|m'm'''>n^{\sigma}_{mm'}n^{-\sigma}_{m''m'''}$$

$$+(<mm''|V_{ee}|m'm'''>-<mm''|V_{ee}|m'''m'>)n^{\sigma}_{mm'}n^{\sigma}_{m''m'''}\}$$

$$V^{\sigma}_{mm'} = -U(n-\frac{1}{2}) + J(n^{\sigma}-\frac{1}{2}) + \sum_{m''m'''}\{<mm'|V_{ee}|m'm'''>n^{-\sigma}_{m''m'''}$$

$$+(<mm'|V_{ee}|m'm'''>-<mm'|V_{ee}|m'''m'>)n^{\sigma}_{m''m'''}\}$$

V_{ee}： Slater integral

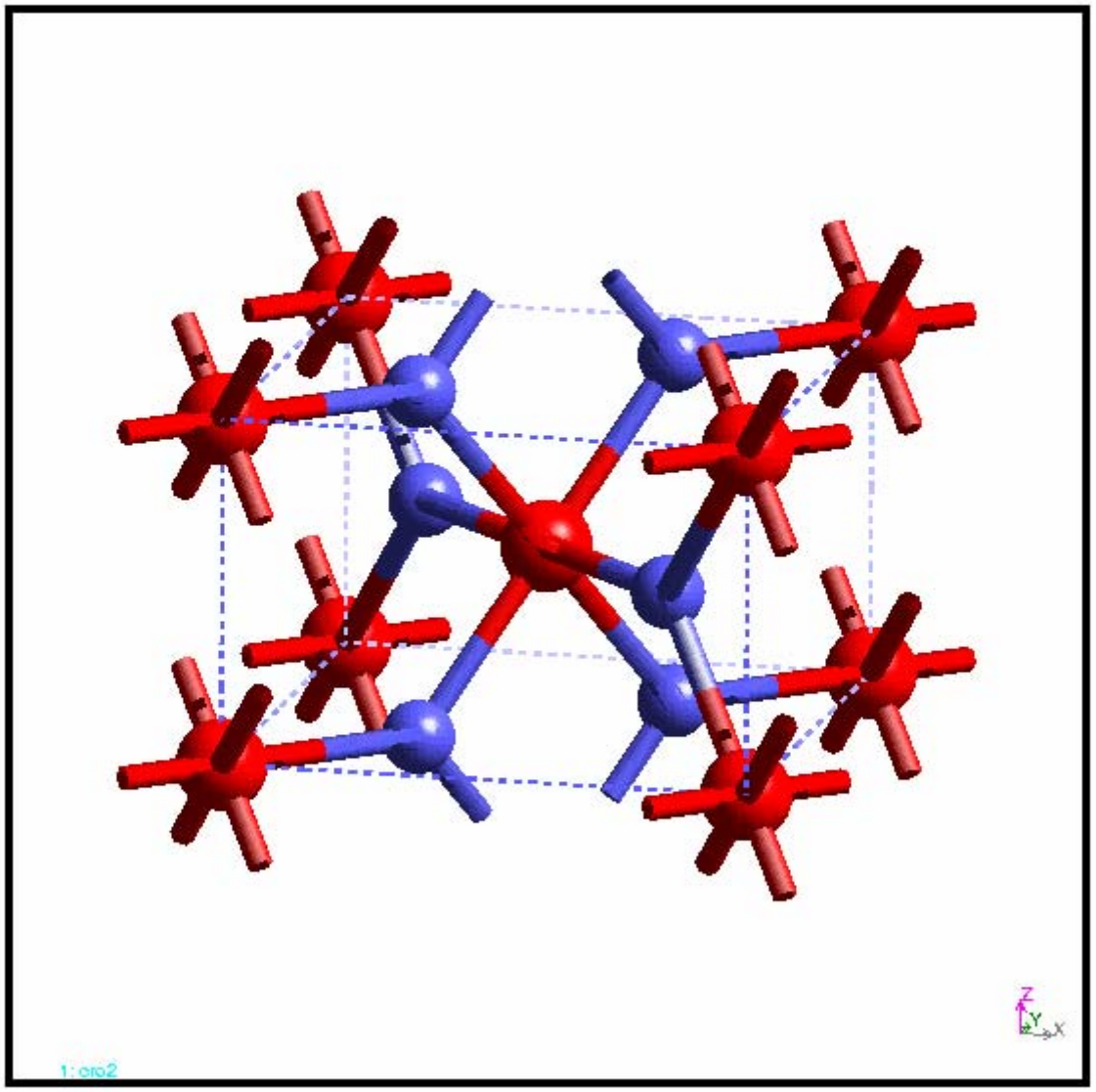
Applications of LDA+U on transition-metal oxides

- Rutile : CrO2 (FP-LMTO)
- Pyrochlore : Cd2Re2O7 (VASP)
- Double perovskite : Sr2FeMoO6, Sr2FeReO6, Sr2CrWO6 (FP-LMTO)
- Perovskite ruthenate SrRuO3 (VASP)
- Cubic inverse spinel : high-temperature magnetite (Fe3O4) (FP-LMTO)
- Low-temperature charge-orbital ordering Fe3O4 (VASP)

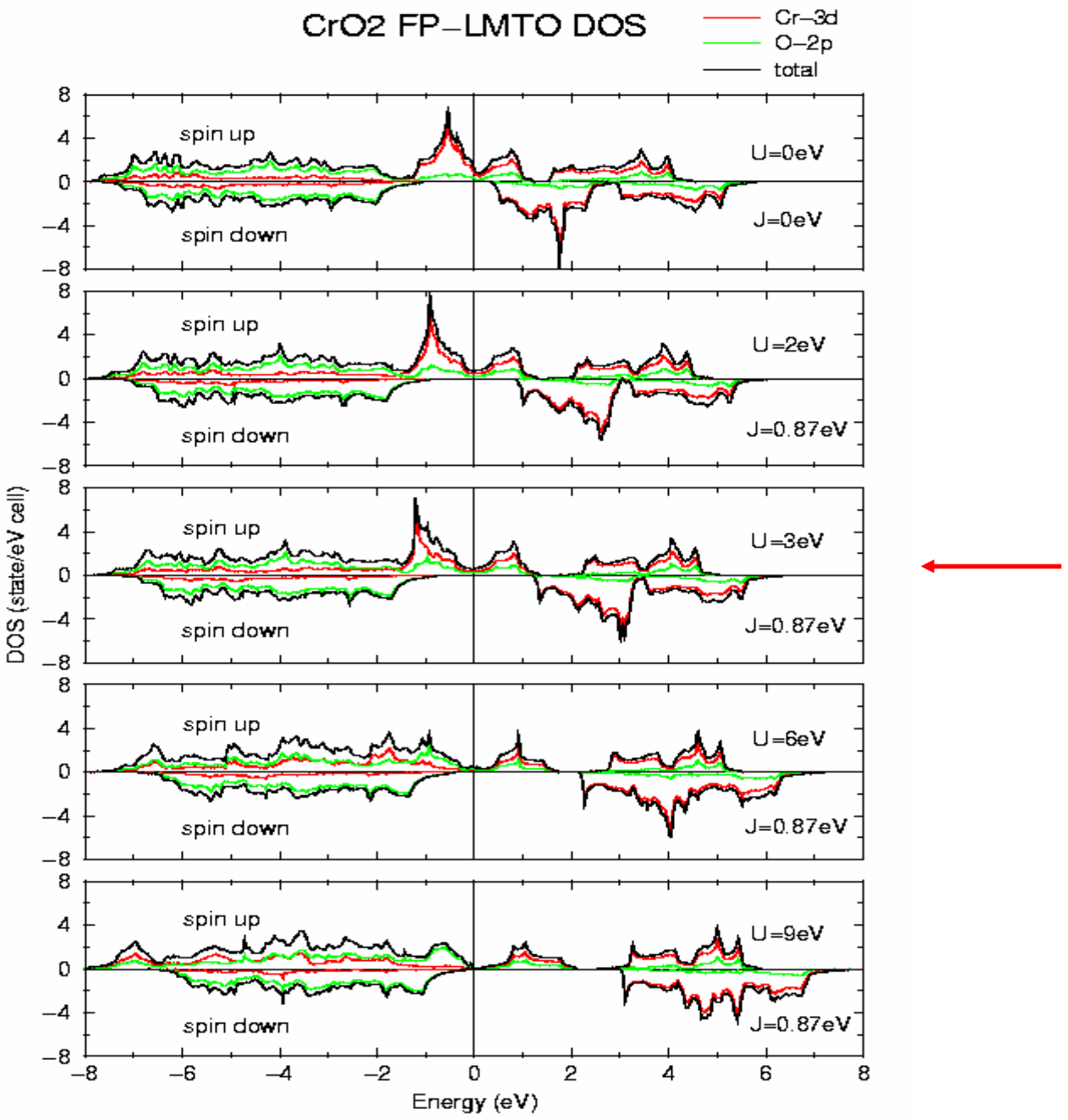
Rutile CrO2

- Half-metal, moment = 2 μ_B
- Lattice type : bct
- 6 atoms in bct unit cell
- Space group : $P4_2/mnm$
- a = 4.419A, c=2.912A, u=0.303
- Ionic model : $Cr^{+4}(3d^2)$, $O^{-2}(2p^6)$
- U = 3.0 eV, J = 0.87 eV

Rutile structure



Jeng et al
JAP (2002)



PRB 56 (1997) 15509

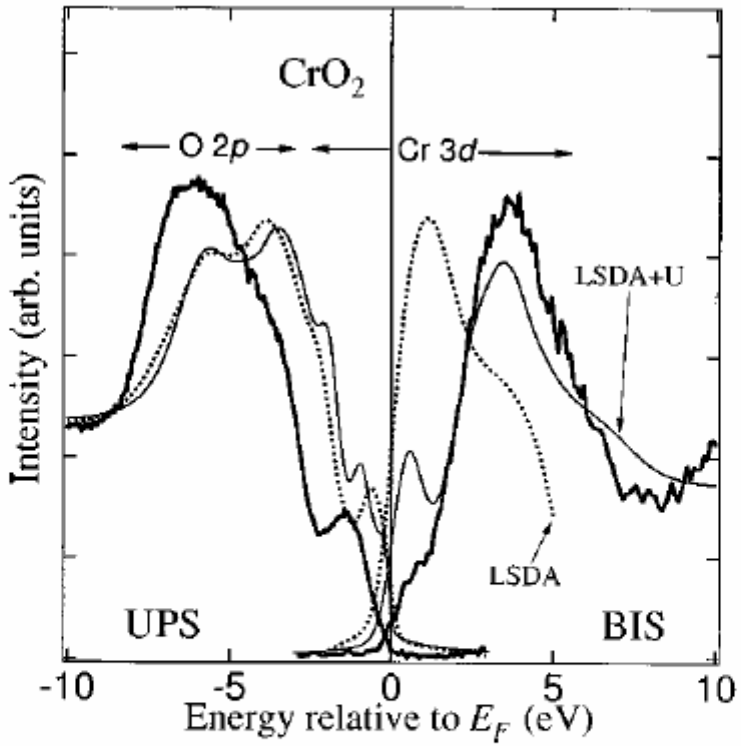


FIG. 4. UPS ($h\nu = 40.8$ eV) and BIS ($h\nu = 1486.6$ eV) spectra (solid curves) compared with theoretical spectra deduced from the LSDA (Ref. 3) and LSDA+U (Ref. 8) calculations (dashed curves).

Spin and orbital magnetic moments of CrO2
PRB66(2002)174440

(u_B)	Spin moment			Orbital moment	
	Cr	O	Total	Cr	O
LDA	1.89	-0.042	2.00	-0.037	-0.0011
LDA+U	1.99	-0.079	2.00	-0.051	-0.0025
Exp.			2	-0.05*	-0.003*

* D. J. Huang et al, SRRC

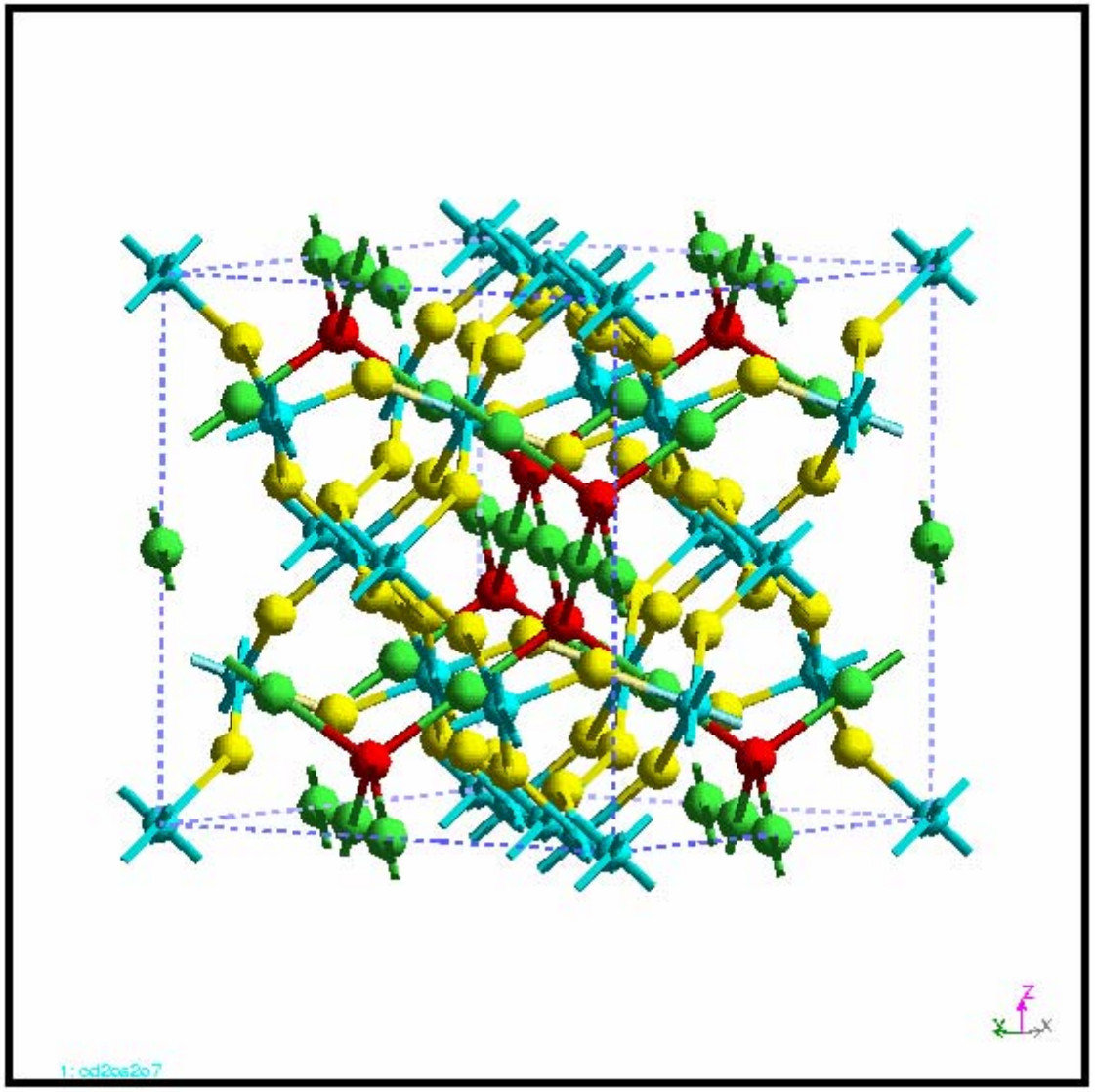
Rutile CrO2

- LDA+U enhances the gap and the exchange splitting at the Fermi level
- LDA+U also gives larger spin and orbital magnetic moment
- U∼W, orbital moment quenched, →stronger hybridization, stronger crystal field, → close to itinerant picture

Pyrochlore $Cd_2Re_2O_7$

- Lattice type : fcc
- 88 atoms in cubic unit cell
- Space group : Fd3m
- a = 10.219A, x=0.316
- Ionic model: $Cd^{+2}(4d^{10})$, $Re^{+5}(5d^{2})$, $O^{-2}(2p^{6})$
- U(Cd) = 5.5 eV, U(Re) = 3.0 eV
- J = 0 eV (no spin moment)

Pyrochlore structure



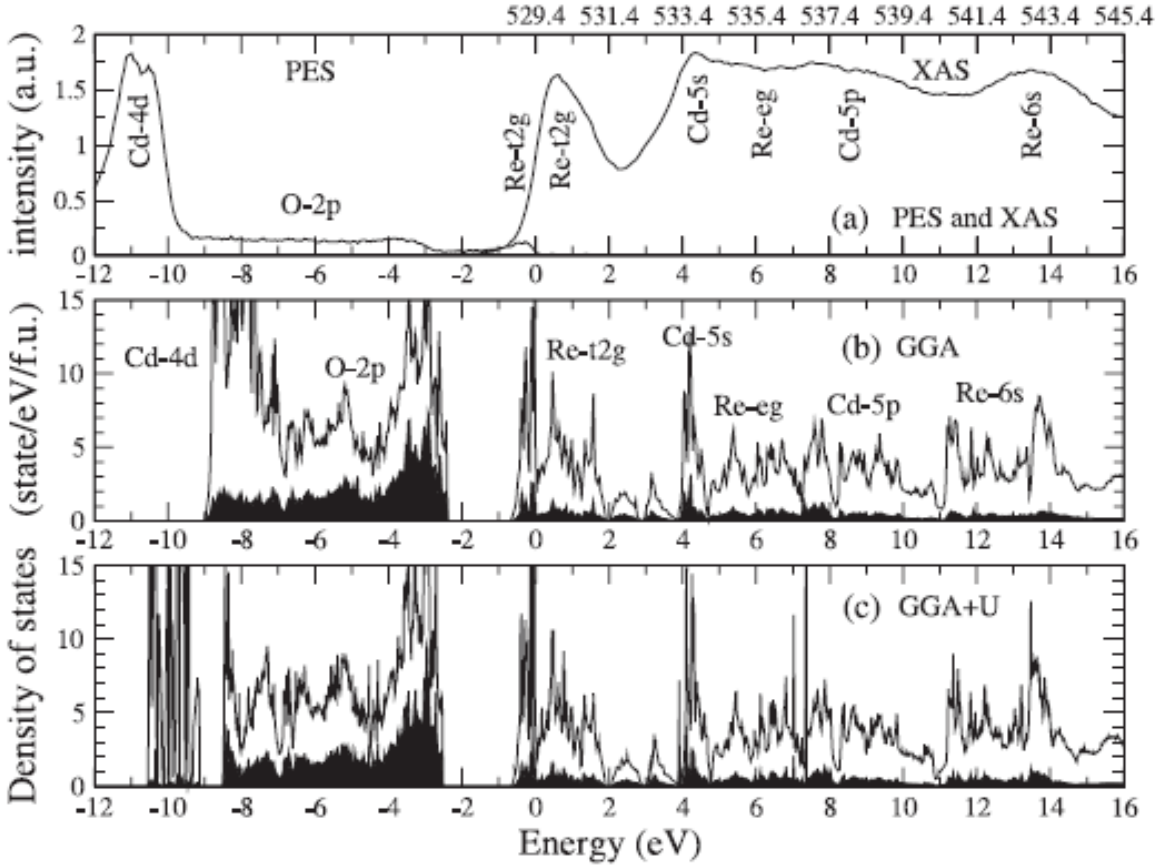


Figure 2. (a) PES [26] and O 1s XAS (this work) spectra of $Cd_2Re_2O_7$. The Fermi level of XAS is at 529.4 eV (reflection point method). (b) Total density of states from GGA (b) and GGA + U (c). The dark area in (b) and (c) are the contributions from O p states.

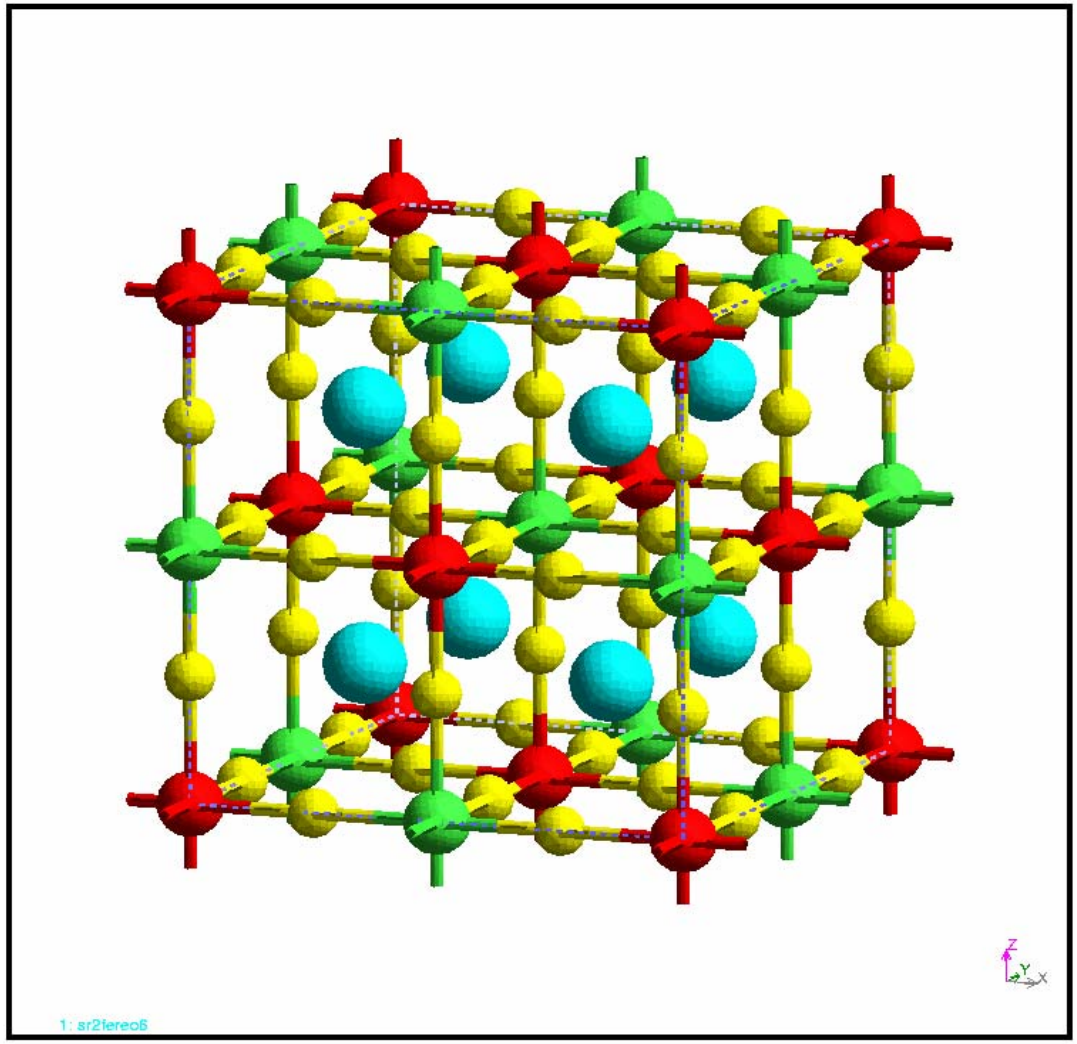
Pyrochlore $Cd_2Re_2O_7$

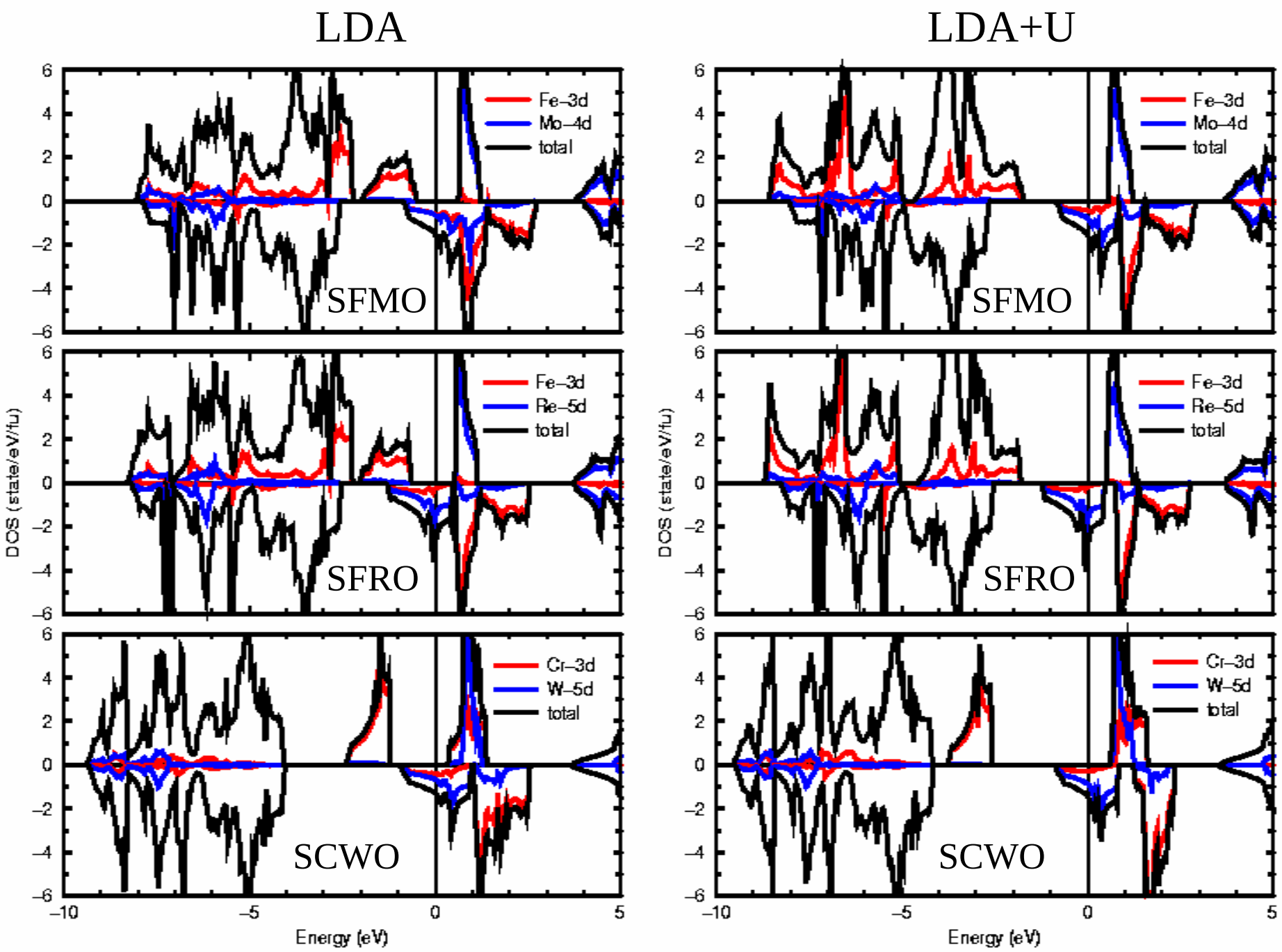
- LDA unoccupied DOS agree well with XAS data from K. D. Tsuei, SRRC
- Cd-4d band from LDA is ~3 eV higher than photo emission spectrum (PRB66(2002)1251)
- Cd-4d band from LDA+U agree well with photo emission spectrum (PRB66(2002)1251)
- Cd-4d orbital is close to localized electron picture, whereas the other orbitals are more or less itinerant

Double perovskites :
Sr2FeMoO6, Sr2FeReO6, Sr2CrWO6

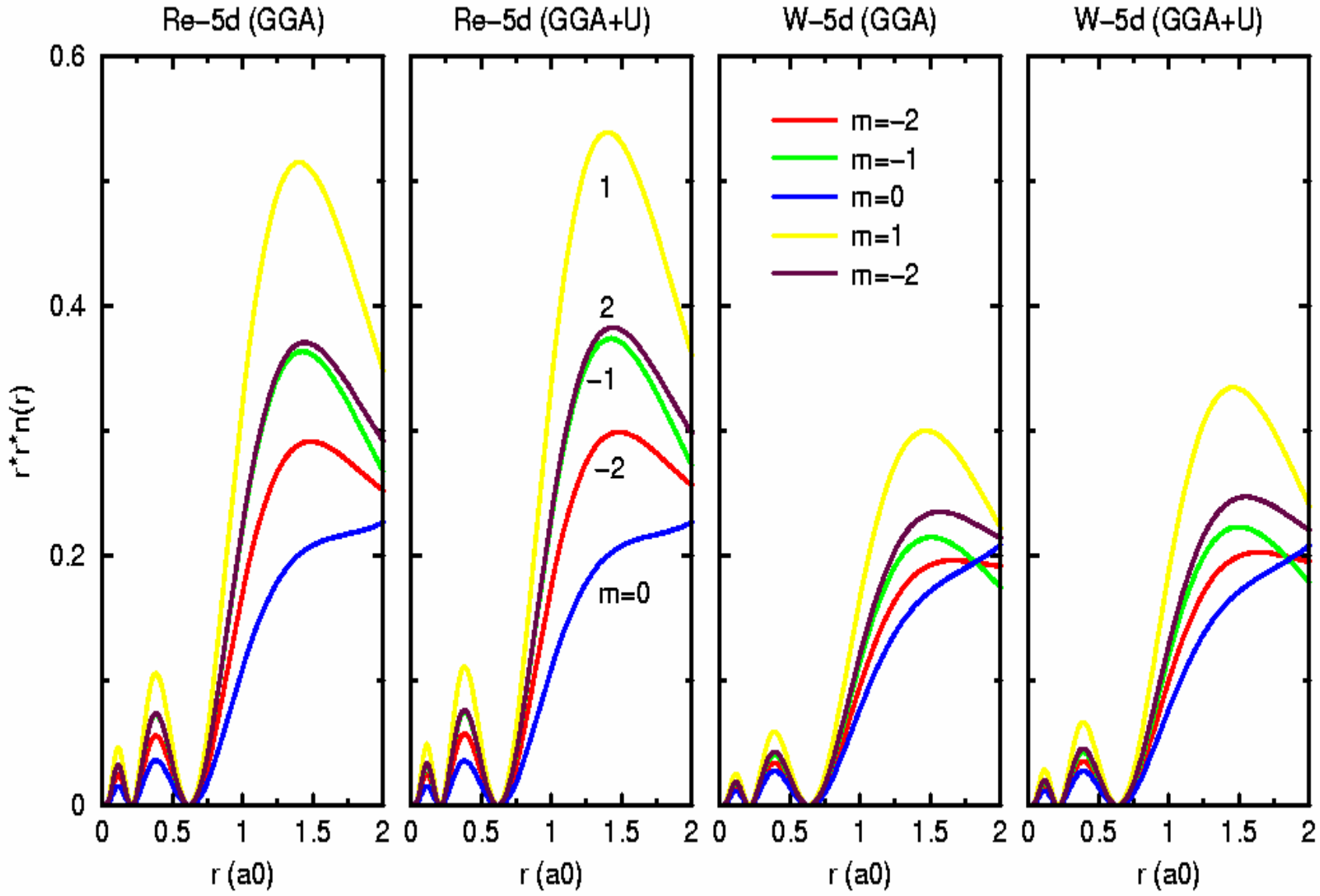
- Half-metal, moment = 4, 3, 2 μ_B
- Lattice type : tet, fcc, fcc
- 40 atoms in tet, fcc, fcc unit cell
- Space group : I4/mmm, Fm3m, Fm3m
- a = 7.89, 7.832, 7.878A, c/a=1.001, 1, 1
- Ionic model : $Fe^{+3}(3d^5)$, $Cr^{+3}(3d^3)$, $Mo^{+5}(4d^1)$, $Re^{+5}(5d^2)$, $W^{+5}(5d^1)$
- U(Fe,Cr) = 4,3 eV, J(Fe,Cr) = 0.89, 0.87 eV

Double perovskite structure




LDA
LDA+U
Fe–3d
Mo–4d
total
SFMO
Fe–3d
Re–5d
total
SFRO
Cr–3d
W–5d
total
SCWO
DOS (state/eV/fu)
Energy (eV)
6
4
2
0
–2
–4
–6
–10
–5
0
5

	spin moment			orbital moment	
Sr_2FeMoO_6	Fe	Mo	total	Fe	Mo
GGA	3.80	-0.33	4.00	0.043	0.032
GGA+U	3.96	-0.43	4.00	0.047	0.045
Sr_2FeReO_6	Fe	Re	total	Fe	Re
GGA	3.81	-0.85	3.00	0.070	0.23
GGA+U	3.98	-0.96	3.00	0.066	0.27
Sr_2CrWO_6	Cr	W	total	Cr	W
GGA	2.30	-0.33	2.00	-0.007	0.10
GGA+U	2.46	-0.45	2.00	-0.007	0.15



Jeng et al PRB (2003)

Double perovskites :
Sr2FeMoO6, Sr2FeReO6, Sr2CrWO6

- LDA+U has significant effects on DOS, but experimental data is not available
- Orbital moment of 3d and 4d elements are all quenched because of strong crystal field
- 5d elements exhibit large unquenched orbital moment because of strong spin-orbit interaction in 5d orbitals

$SrRuO_3$

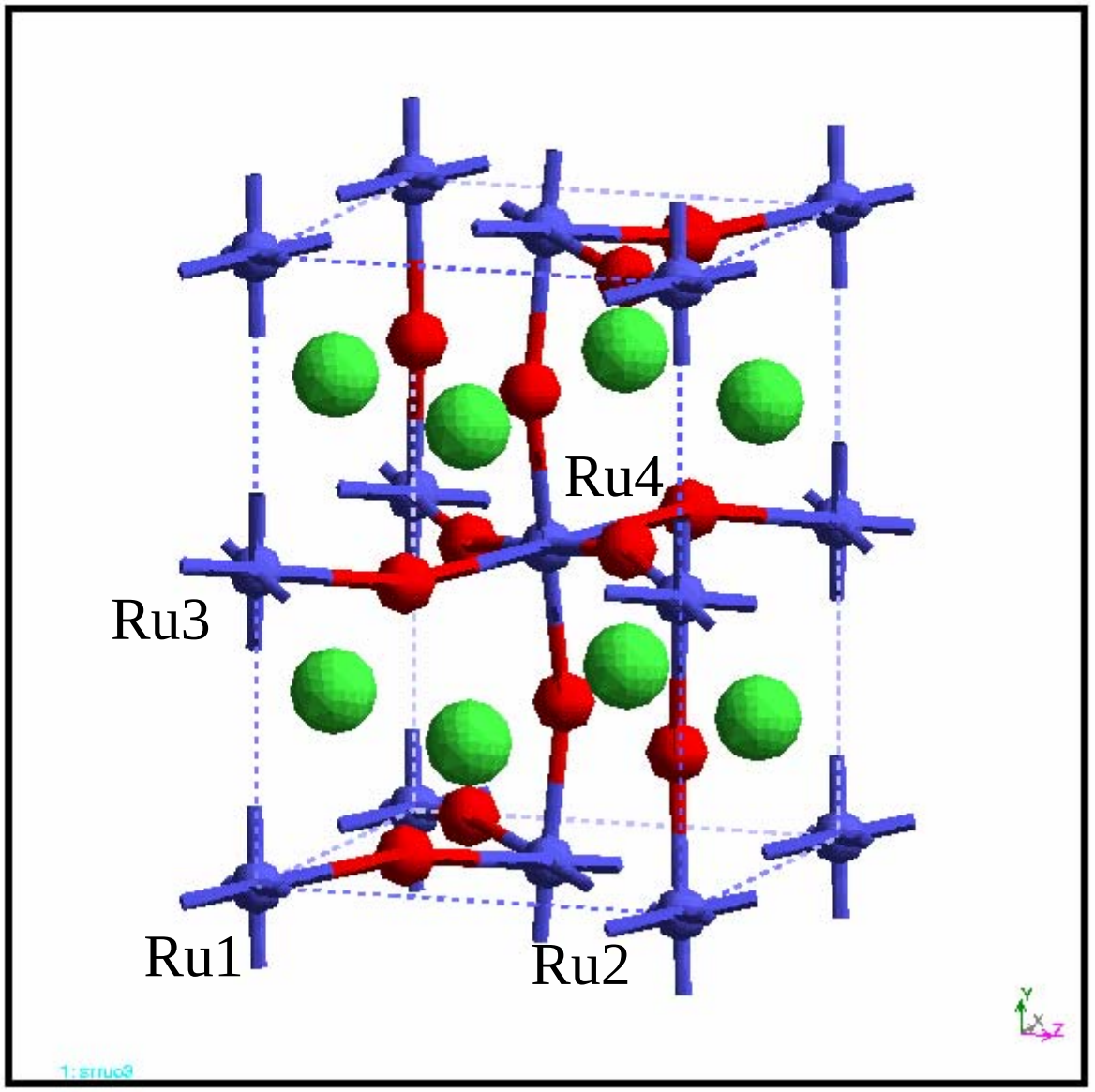
- The only ferromagnetic conductor of 4d oxides
- Lattice type : orthorhombic perovskite
- Space group : Pnma (No. 62)
- 20 atoms in orthorhombic unit cell
- a=5.5332 A, b=5.57169 A, c=7.8491 A
- Ionic model : $Ru^{4+}(4d^4, t2g^3 \uparrow, t2g^1 \downarrow)$
- U = 3.5 eV, J = 0.58 eV
- Pseudopotential, 100 k-point, 31360 plane wave, Cut-off energy = 400 eV

Orthorhombic perovskite $SrRuO_3$

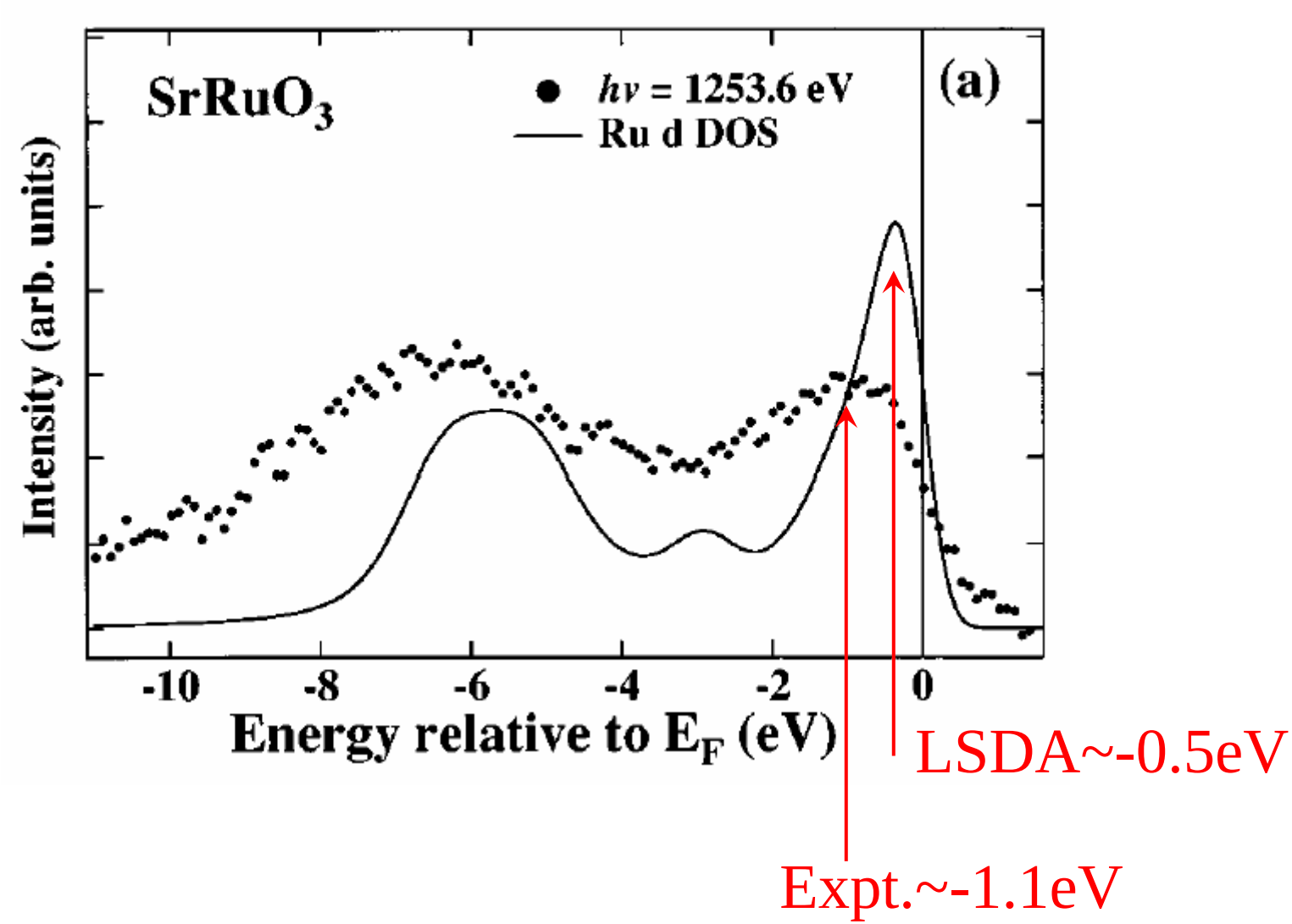
Sr

Ru

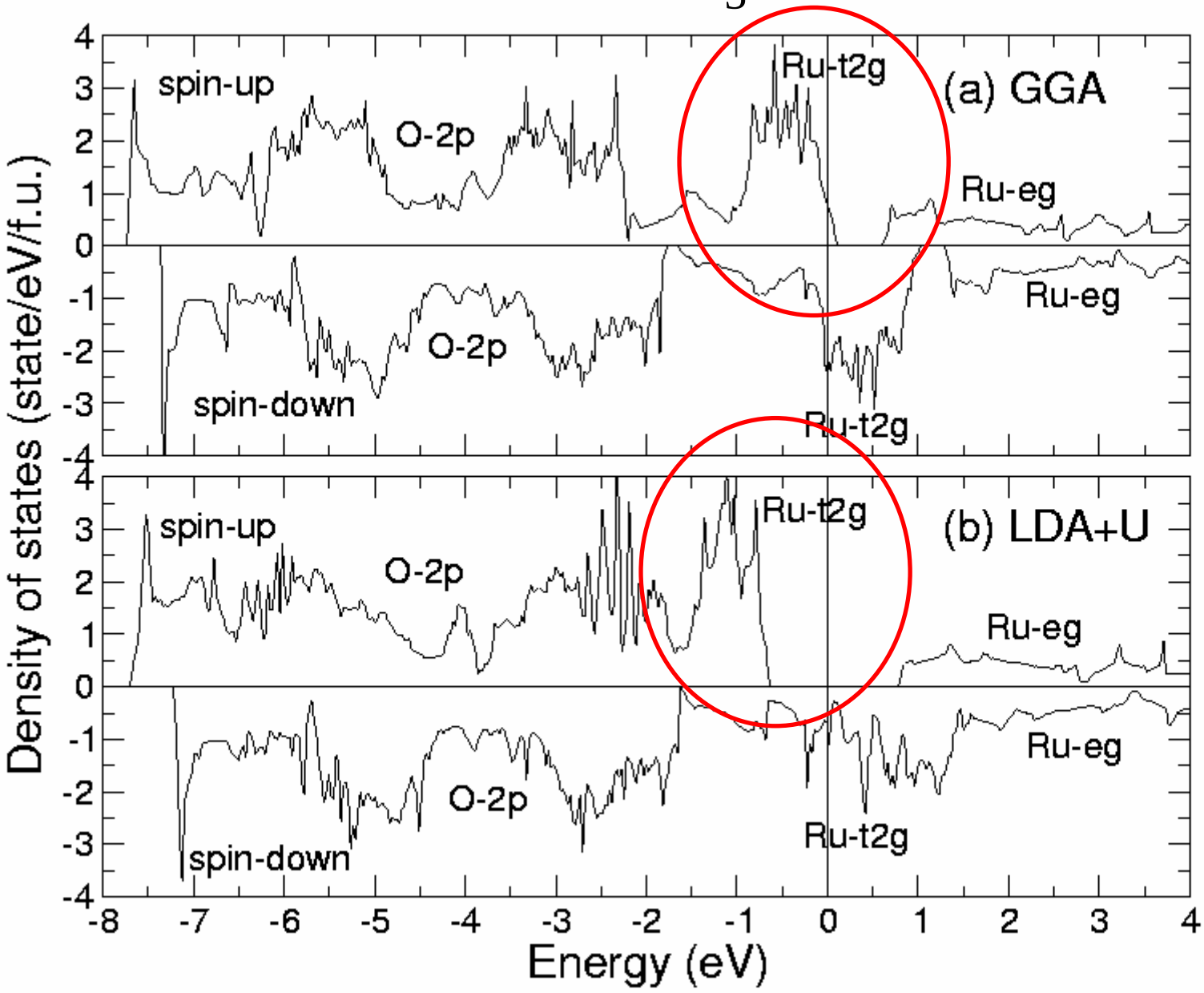
O



PRB56(1997)6380

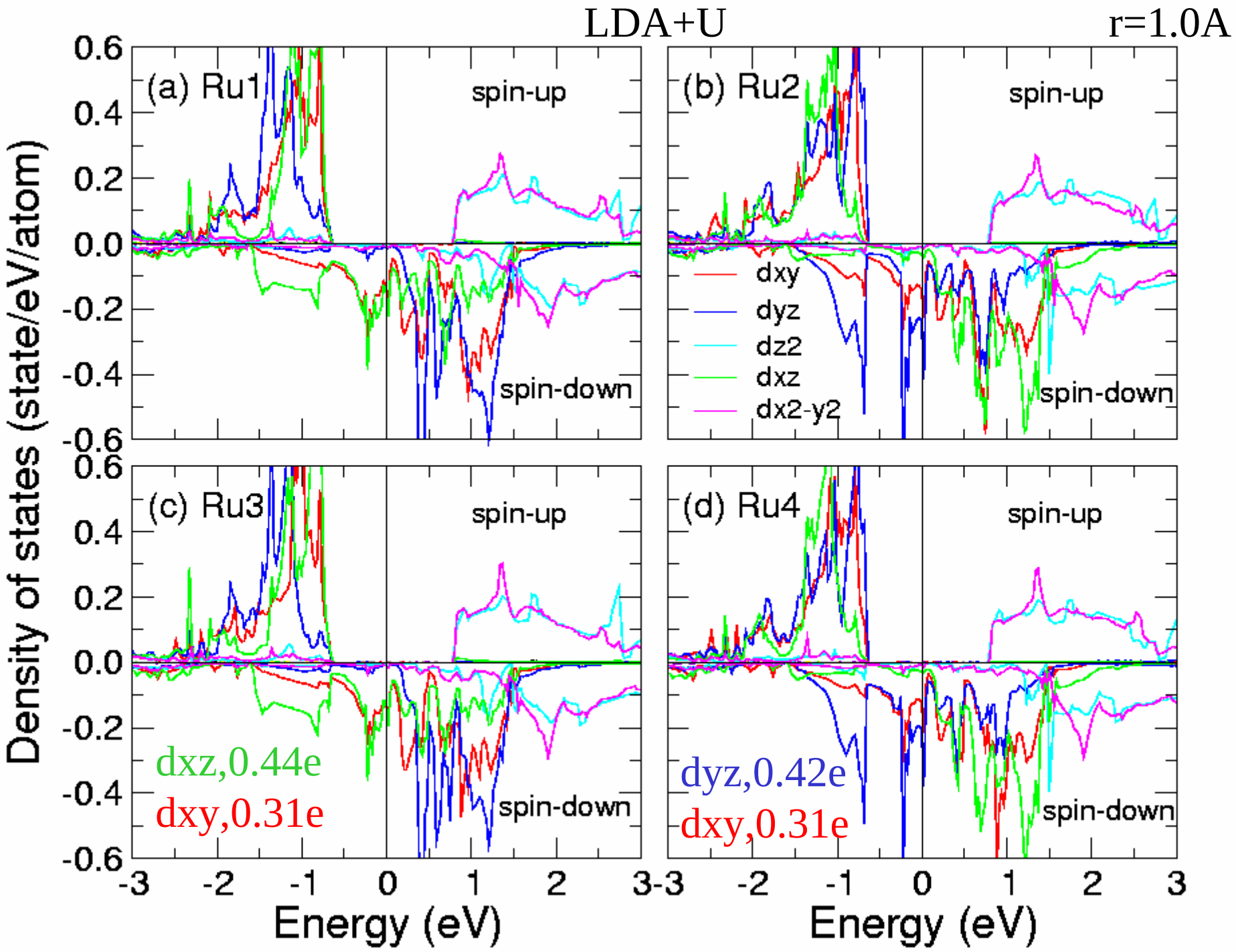


$SrRuO_3$

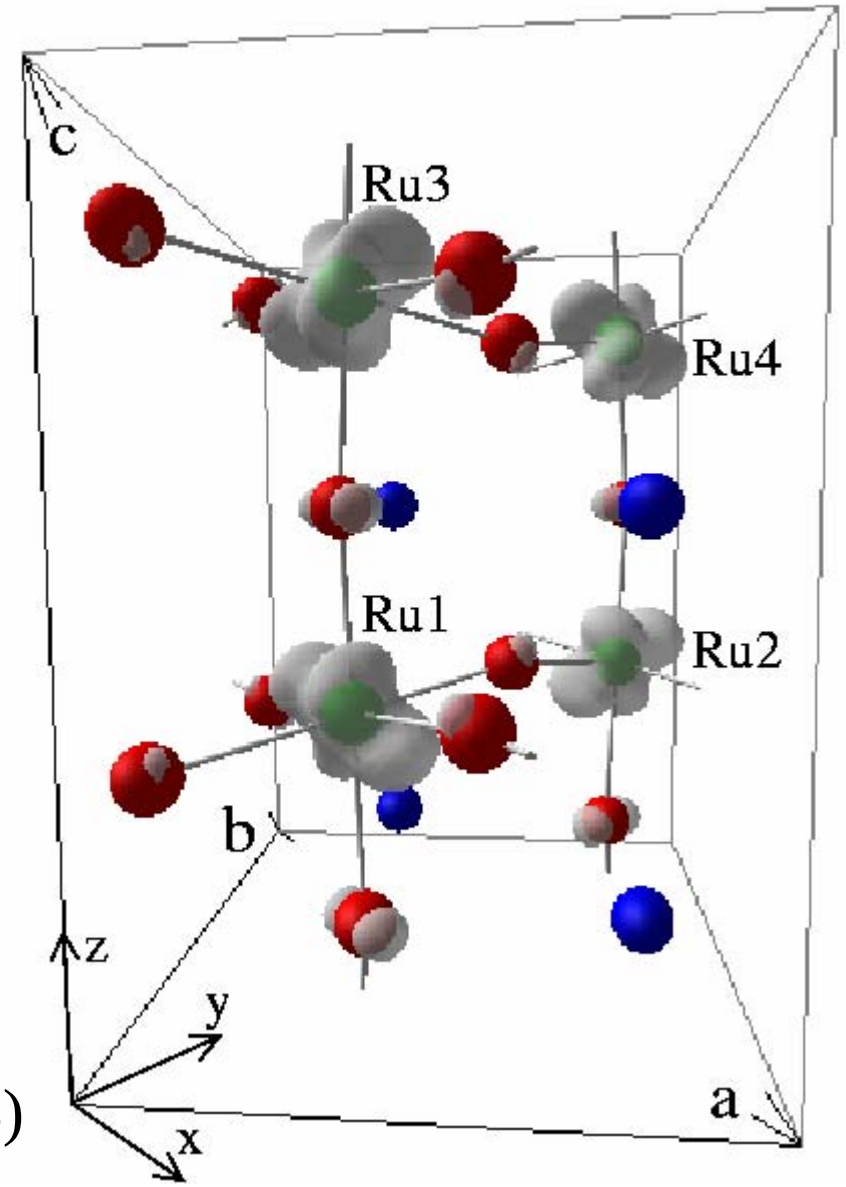


Metal

Half-metal


LDA+U
r=1.0A
(a) Ru1
spin-up
spin-down
(b) Ru2
spin-up
spin-down
dxy
dyz
dz2
dxz
dx2-y2
(c) Ru3
spin-up
spin-down
dxz,0.44e
dxy,0.31e
(d) Ru4
spin-up
spin-down
dyz,0.42e
dxy,0.31e
Density of states (state/eV/atom)
Energy (eV)
Energy (eV)
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
-3
-2
-1
0
1
2
3

$SrRuO_3$



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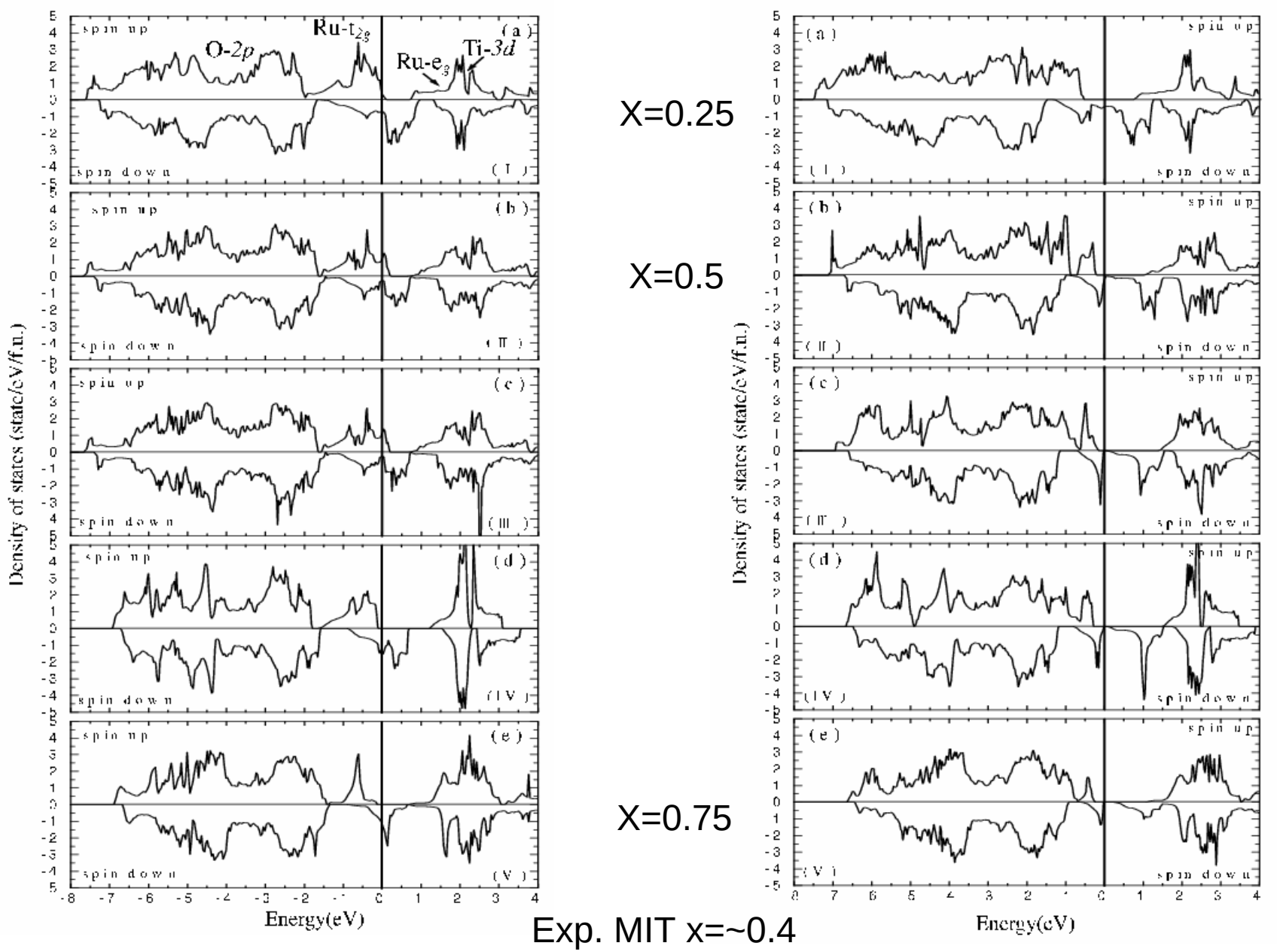
PRL97(200
6)67002

MIT in $SrRu_{1-x}Ti_xO3$

GGA

GGA+U



X=0.25

X=0.5

X=0.75

Exp. MIT x=~0.4

$SrRuO_3$

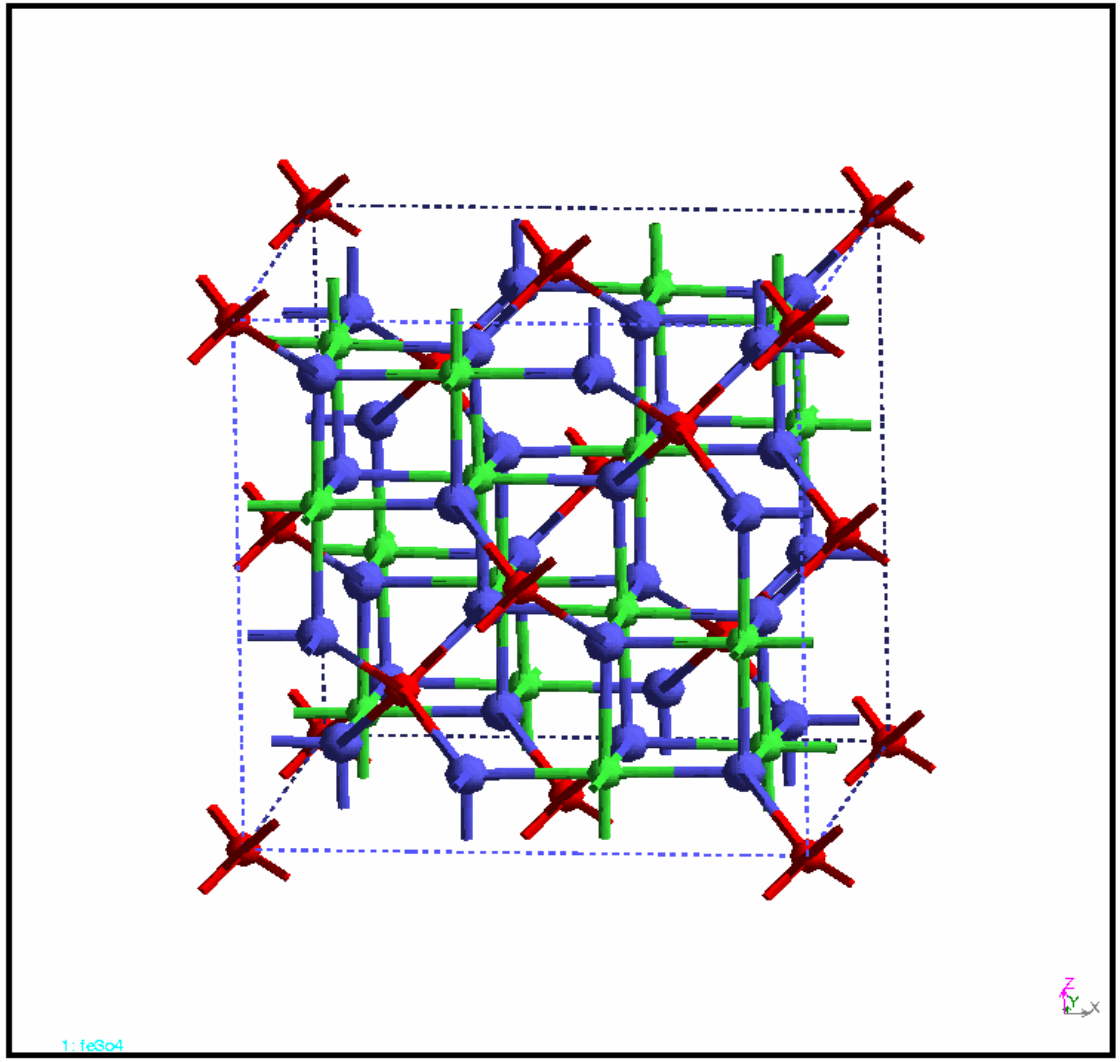
- GGA $\rightarrow$ $SrRuO_3$ is a normal metal without orbital ordering
- LDA+U $\rightarrow$ $SrRuO_3$ is a half-metal with $\downarrow$ 4d-t2g orbital ordering
- LDA+U successfully gives the metal-insulator transition upon doping Ti in SrRuO3, indicating the strong correlation is important in this system

High temperature magnetite (Fe3O4)

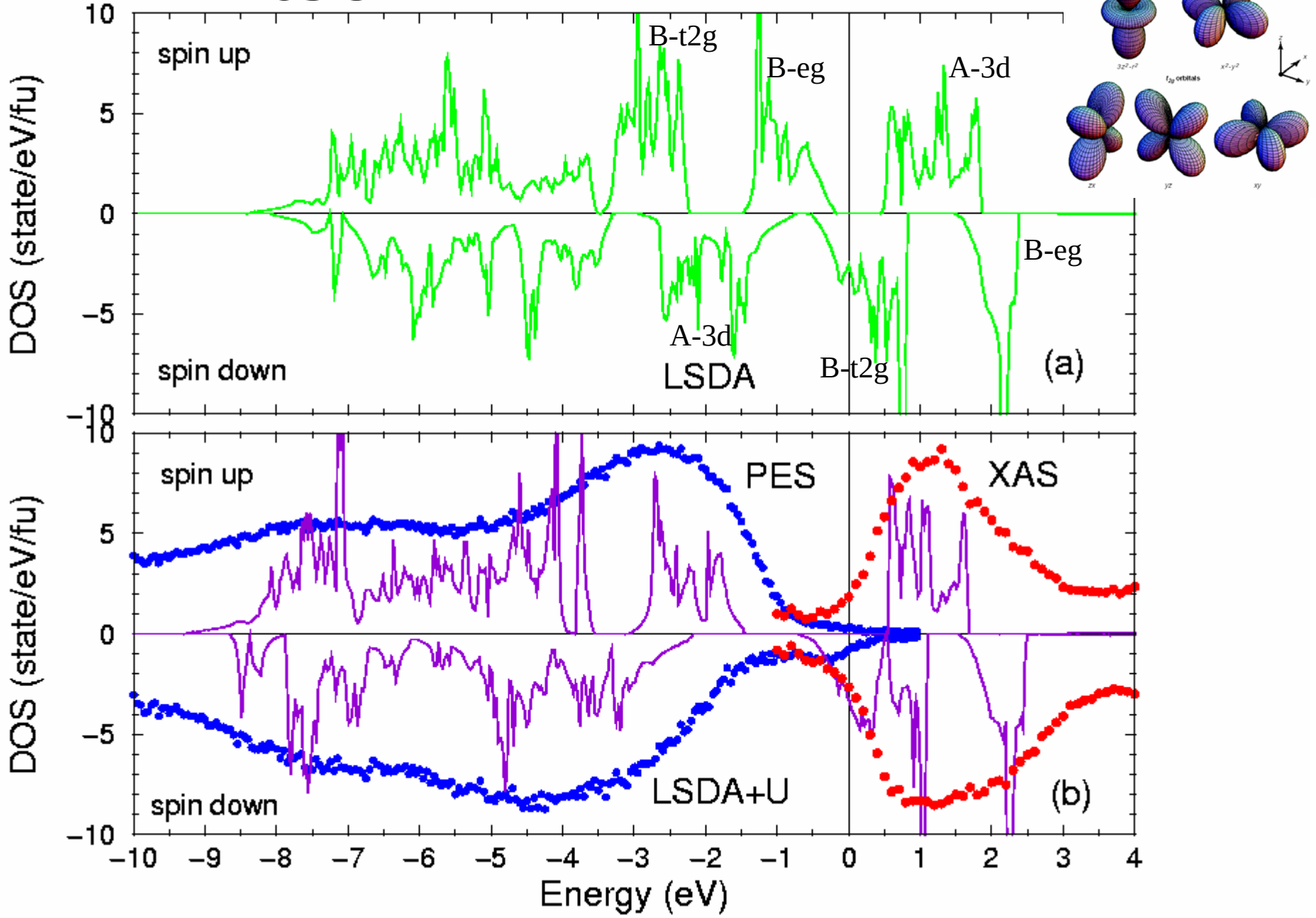
- Half-metal, insulator, moment = 4 μ_B
- Lattice type : fcc
- Space group : Fd3m
- 56 atoms in fcc unit cell
- a = 8.394, 8.383, 8.351 A
- Ionic model : $Fe^{+3}(3d^5)$, $Fe^{+2}(3d^6)$
- U(Fe^{+3},Fe^{+2})=4.5, 4.0eV
- J(Fe) = 0.89eV

Spinel structure

Author:
Date: Sun May 21 16:31:45 2000



Fe_3O_4 (PES, XAS: D.J. Huang, SRRC)

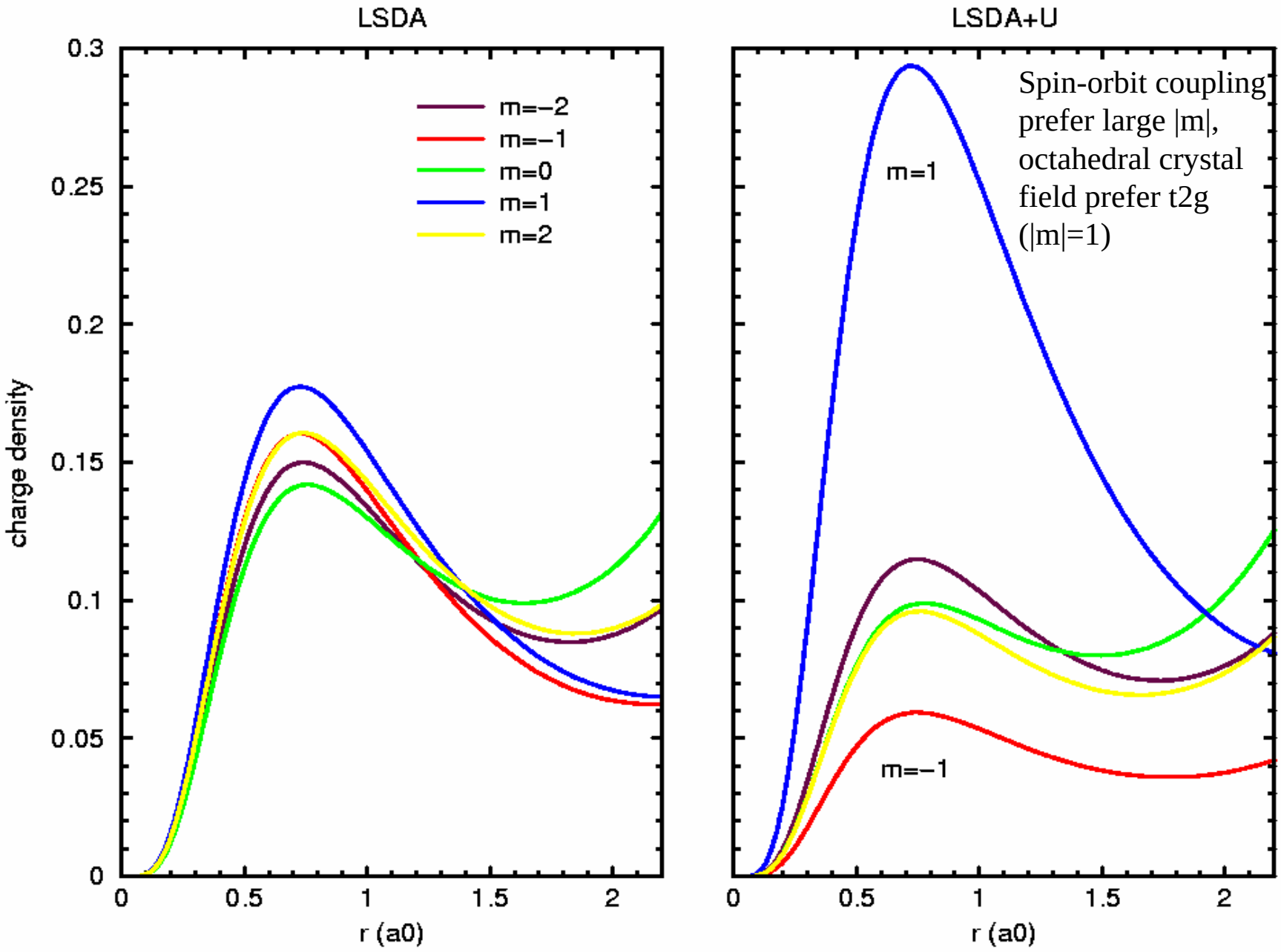


Spin and orbital magnetic moments of Fe_3O_4

(u_B)	Spin moment			Orbital moment	
	Fe(A)	Fe(B)	Total	Fe(A)	Fe(B)
LDA	-3.31	3.52	4.00	-0.018	0.039
GGA	-3.44	3.60	4.00	-0.016	0.038
LDA+U	-3.81	3.81	4.00	-0.014	0.21
Exp.	-3.8[+]		4.1		0.2~0.4[*]

[+]J. Phys. C 11 (1978) 4389 [*] D. J. Huang et al, SRRC

Fe_3O_4, PRL93(2004)77204



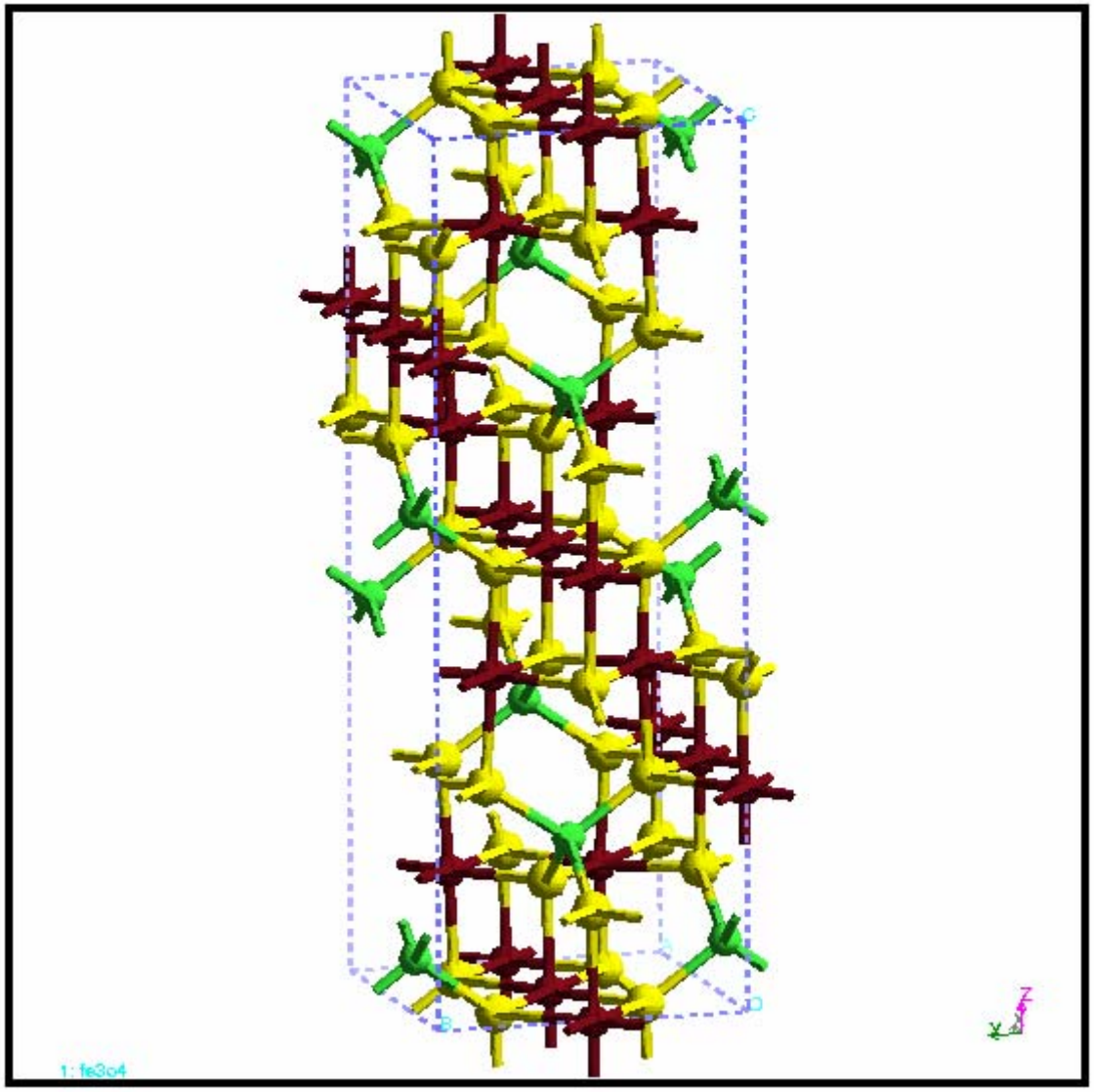
High temperature magnetite (Fe3O4)

- LDA+U gives better DOS for Fe3O4
- Spin moment of Fe3O4 from LDA+U agrees better with neutron scattering measurement
- On-site U gives large unquenched orbital magnetic moments for Fe(B) compatible with MCD results

Low-temperature Fe_3O_4

- Insulator
- Lattice type : monoclinic
- Space group : P2/c
- 56 atoms in monoclinic unit cell
- a = 5.9444 A, b=5.925 A, c=16.775 A
- β =90.2363^0
- Ionic model : $Fe^{+3}(3d^5)$, $Fe^{+2}(3d^6)$
- U=4.5 eV, J = 0.89 eV
- Pseudopotential (75600 plane wave up to 400eV)

P2/C structure (low-temperature magnetite)



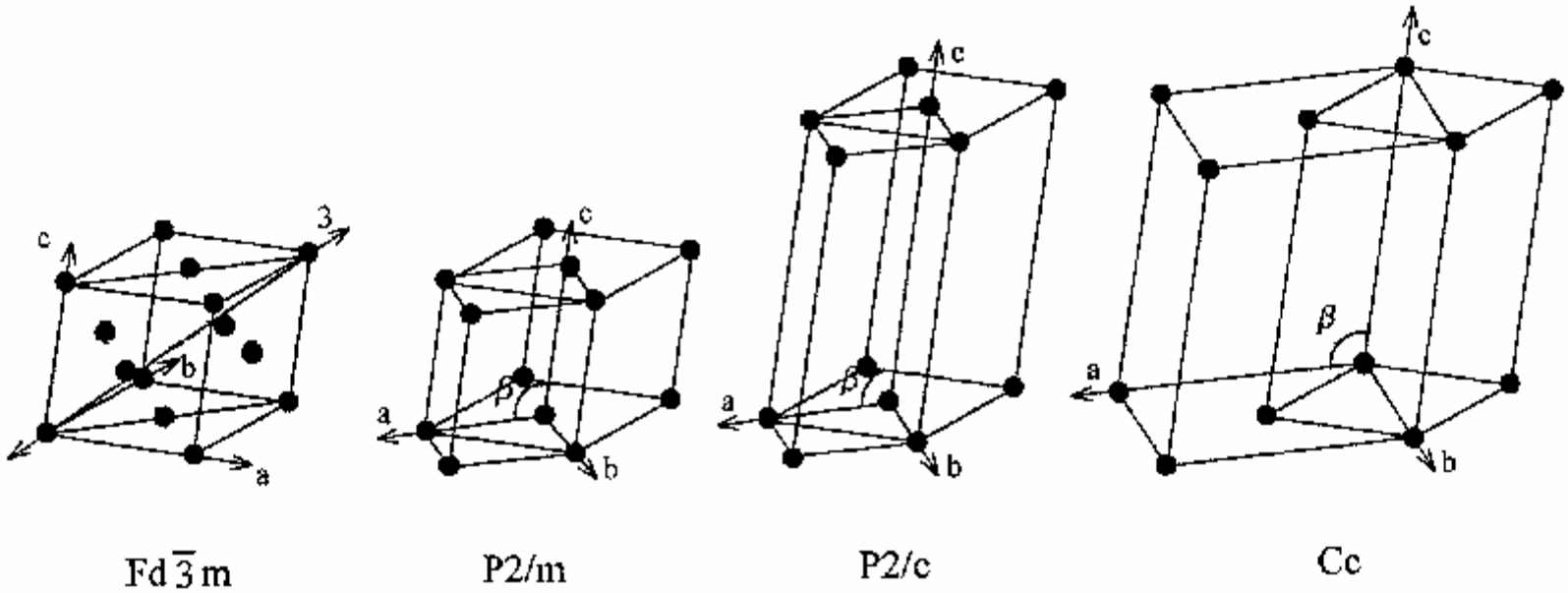


FIG. 2. Relationships between the unit cells referred to in the text.

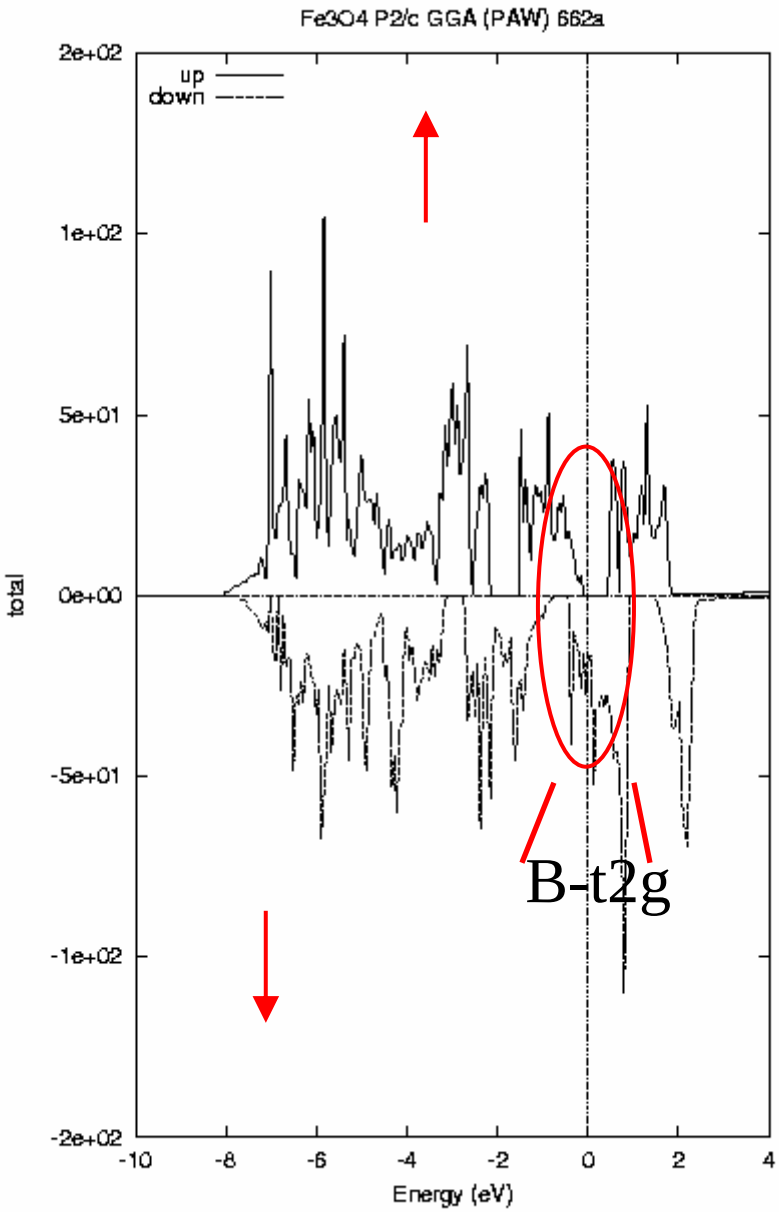
grown by the skull melter technique. A trace of Fe_2O_3 (0.8 wt % by Rietveld analysis), perhaps arising from surface oxidation of the powder during grinding, was found in the diffraction patterns for this sample. High-resolution neutron powder-diffraction data were collected at 90 and 130 K using the high-resolution neutron powder-diffractometer (HRPD) instrument at the ISIS spallation source, United Kingdom.[33] Approximately 10 g of sample was loaded into a vanadium sample can and mounted in a closed-cycle refrigerator to maintain temperature control while retaining a low instrumental background. Data were collected at 90 K for a total of

further distortions were required to account for the peak broadenings and splittings. Figure 2 shows the relationships between the unit cells in the low- and high-temperature phases.

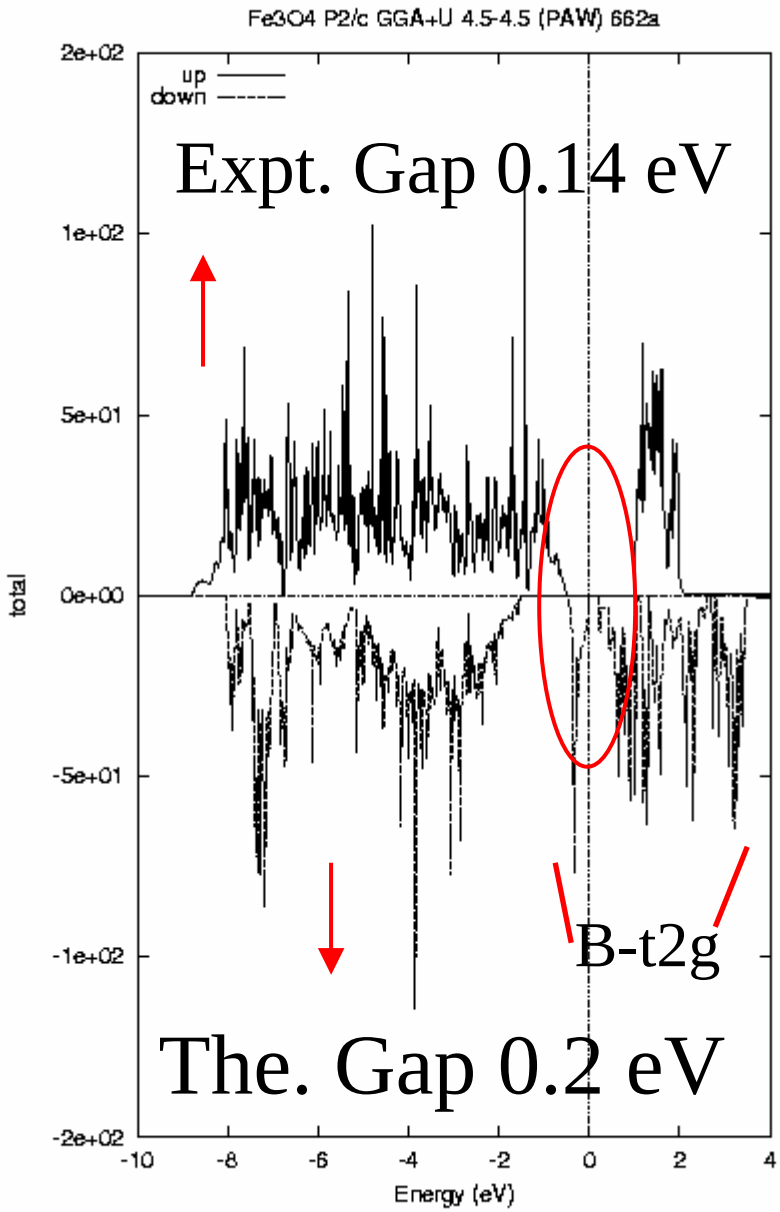
Numerous superstructure peaks were identified by comparing the 90 and 130 K profiles. All of these superstructure peaks were indexed on the monoclinic unit cell previously proposed,[8] which has *Cc* symmetry and axes;

$$\mathbf{a_m} = -(\mathbf{a_c} + \mathbf{b_c}),$$

LDA Half-metal



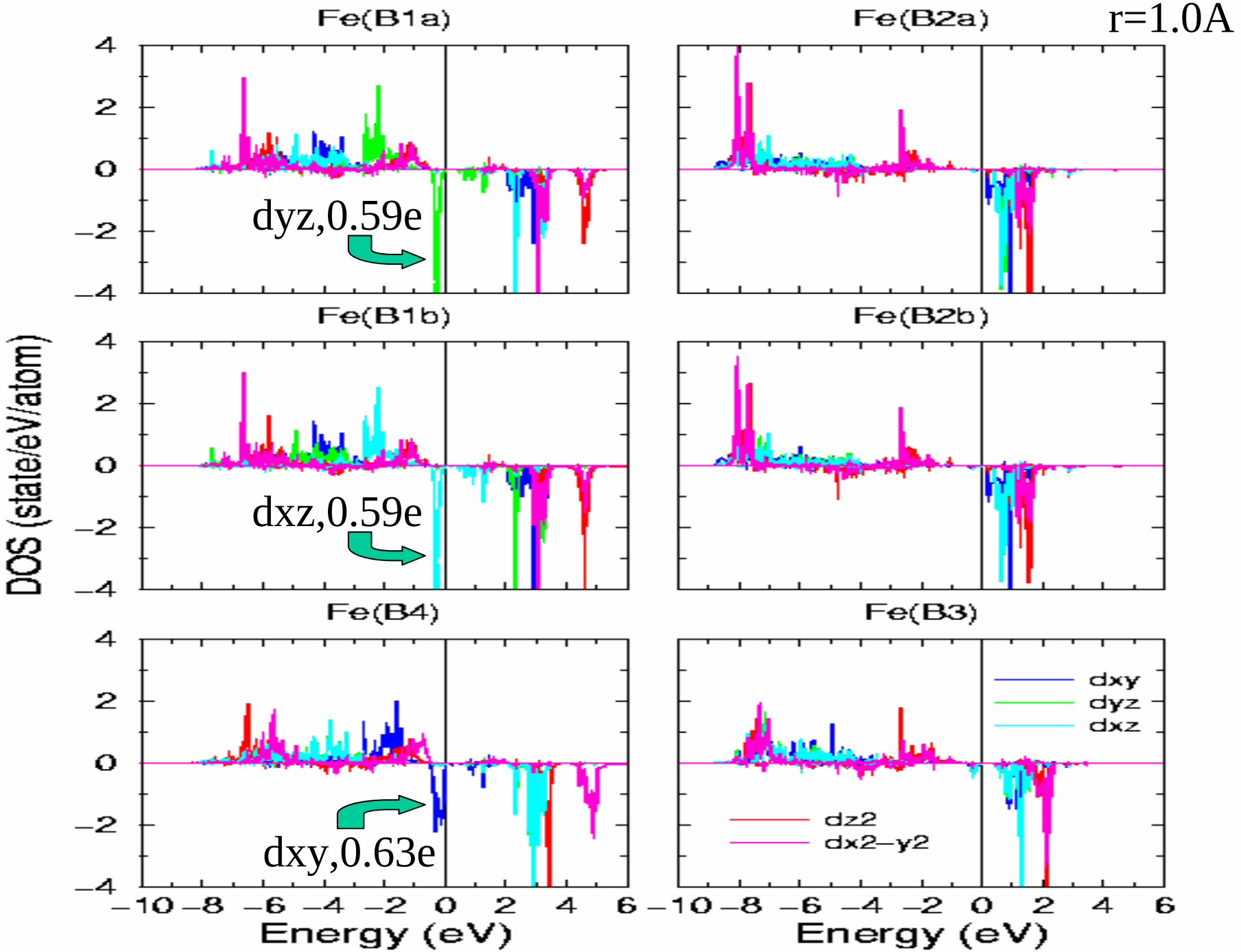
LDA+U Insulator

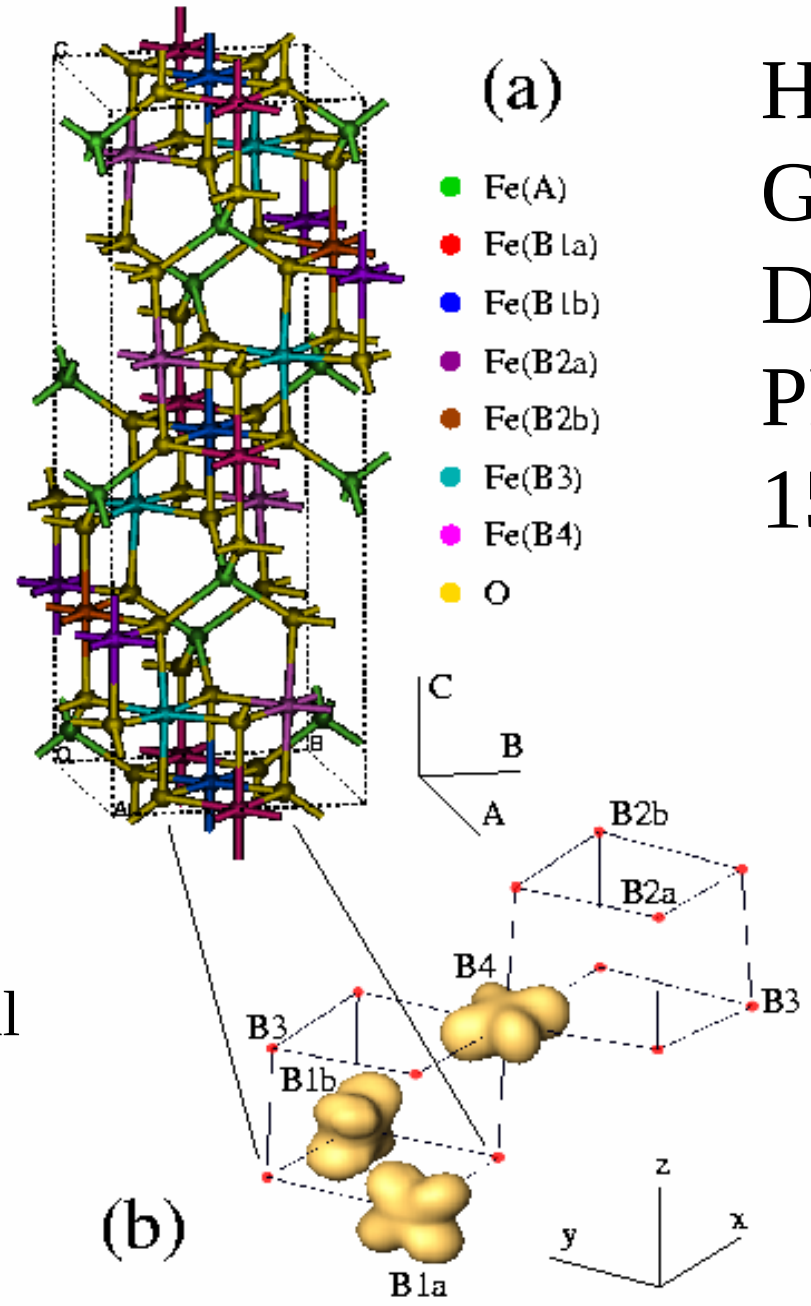


Charge and spin moment of Fe_3O_4 in low-temperature phase (r_{mt}= 1.0 A)

	LDA	LDA	Exp.*	LDA+ U	LDA+ U
	Spin	Charge	Charge	Charge	Spin
Fe(B1)	3.34	5.53	5.6	5.57	3.45
Fe(B2)	3.43	5.50	5.4	5.41	3.90
Fe(B3)	3.32	5.52	5.4	5.44	3.81
Fe(B4)	3.39	5.52	5.6	5.58	3.39

* PRL 87 (2001) 266401


r=1.0A
Fe(B1a)
Fe(B2a)
Fe(B1b)
Fe(B2b)
Fe(B4)
Fe(B3)
dyz,0.59e
dxz,0.59e
dxy,0.63e
dxy
dyz
dxz
dz2
dx2−y2
DOS (state/eV/atom)
Energy (eV)
Energy (eV)



H. T. Jeng,
G. Y. Guo,
D. J. Huang,
PRL93(2004)
156403,

3-1 charge-orbital ordering

Low-temperature Fe3O4

- LSDA + lattice distortion → half-metal, no charge ordering
- LSDA+U + lattice distortion → insulating ground state with charge-orbital ordering

Conclusions

- Transition-metal oxides
  → narrower bandwidth
  → closer to localized electron picture
  → more or less strongly correlated
  → LDA+U gives better result
  → the on-site Coulomb correlation U is important in these systems

CMS II-6 Hands-on: LDA+U, orbital decomposed DOS, and band decomposed charge distribution

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Working list

- Setup LDA+U bulk calculations for NiO(AFMII)
- Calculate orbital decomposed DOS for NiO(AFMII)
- Calculate band decomposed charge and spin density distribution for NiO(AFMII)

Setup LDA+U bulk calculations for NiO(AFMII)

INCAR:

SYSTEM = NiO FCC

DOS related values
LDAU = .TRUE.
LDAUTYPE = 1
LDAUL = 2 -1
LDAUU = 8.0 0.0
LDAUJ = 0.95 0.0
LMAXMIX = 4
LDAUPRINT = 2
ISMEAR = -5
ISPIN = 2
MAGMOM = 2 -2 2*0
GGA = 91
RWIGS = 1.2 0.8

KPOINTS, POSCAR, and POTCAR are the same

Switch on L(S)DA+U calculation
Setup rotationally invariant L(S)DA+U scheme
+U in d(l=2) orbital, no on-site U if -1
U=8 and 0eV for Ni and O, respectively
J=0.95 and 0eV for Ni and O, respectively
Expand charge in Ylm up to l=4 (for d orbital)
Output occupation matrix

*U and J must be specified for all atomic types

LDA+U controlling parameters

The L(S)DA+U in VASP is switched on by means of the following tags

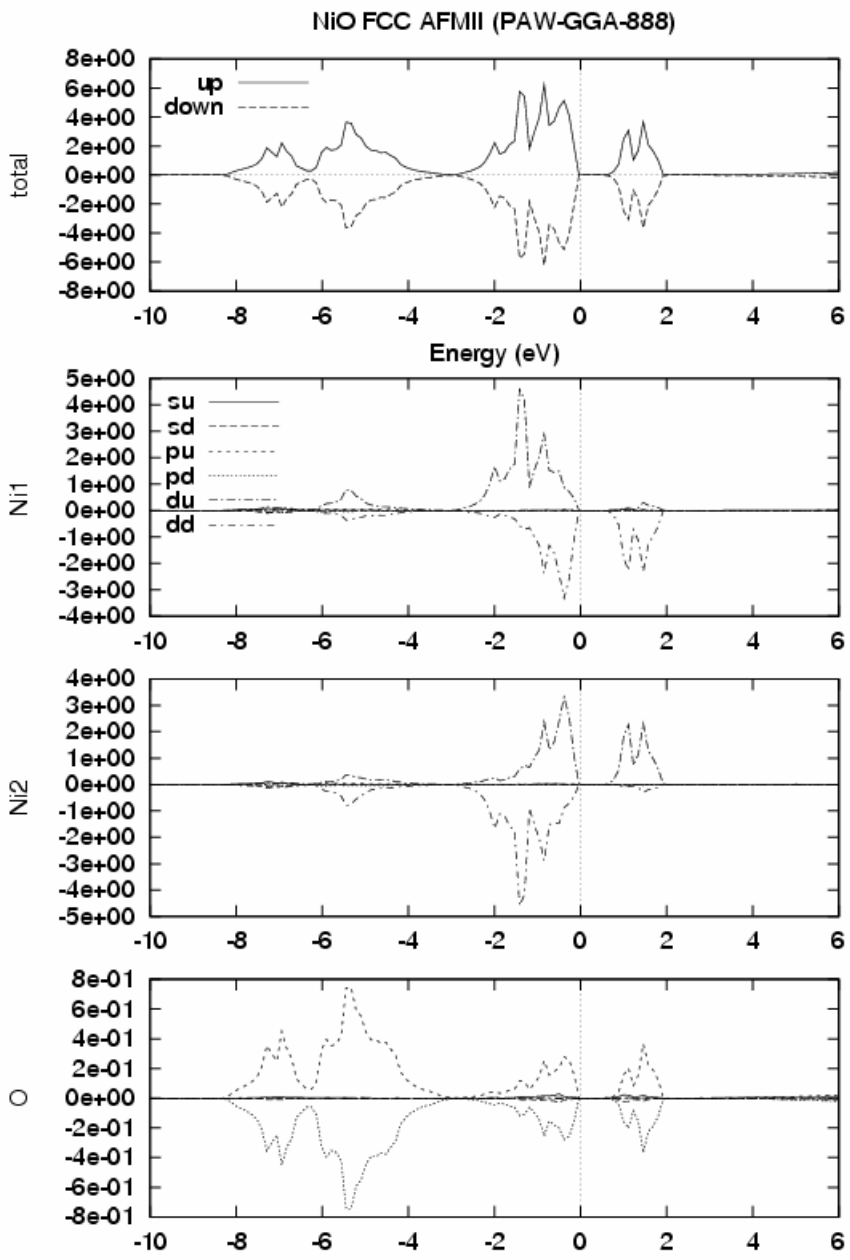
- `LDAU = .TRUE.` Switches on the L(S)DA+U.
- `LDAUTYPE = 1|2|4` Type of L(S)DA+U (Default: `LDAUTYPE = 2`)

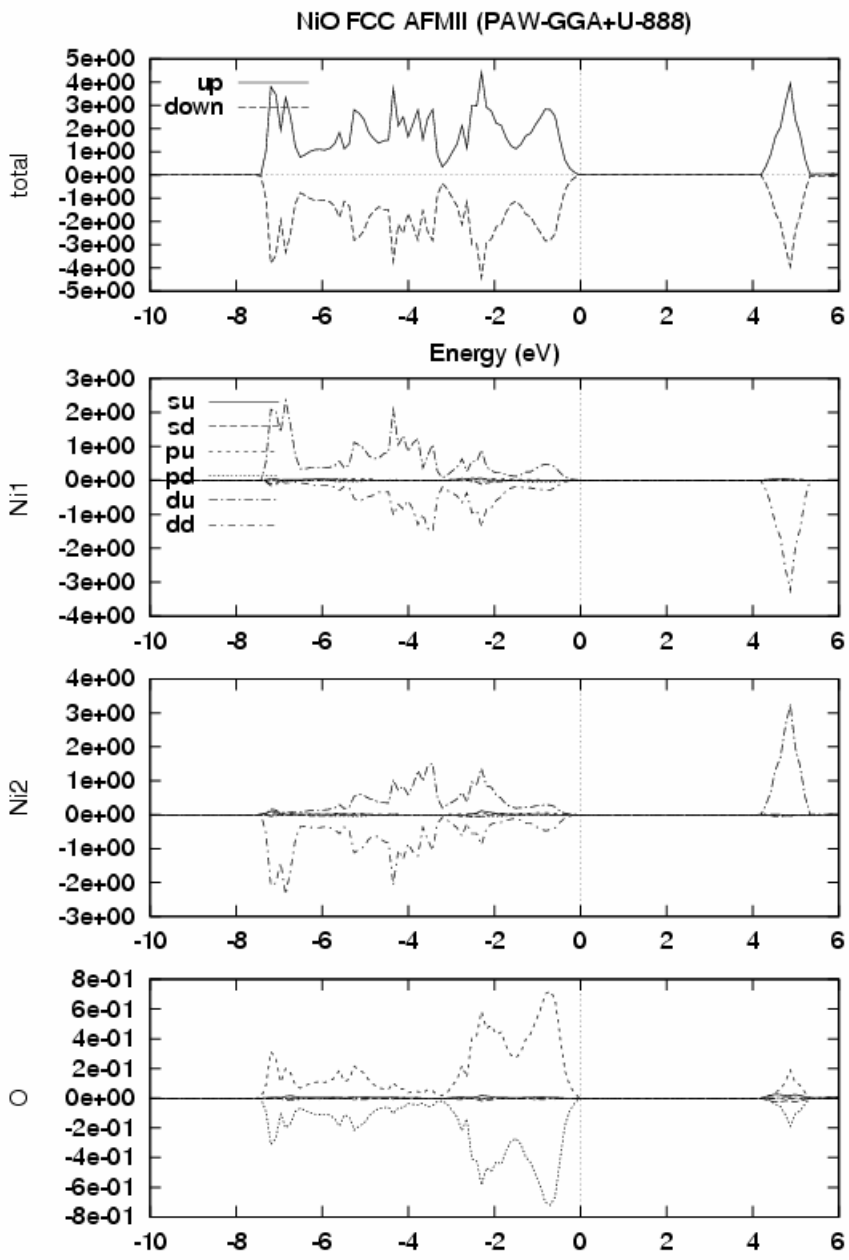
  1 Rotationally invariant LSDA+U according to Liechtenstein *et al.*

  4 Idem 1., but LDA+U instead of LSDA+U (i.e. no LSDA exchange splitting)

  2 Dudarev's approach to LSDA+U (Default)
- `LDAUL = L ..` l-quantum number for which the on site interaction is added
  (-1: no on site terms added, 1: p, 2: d, 3: f, Default: `LDAUL = 2`)
- `LDAUU = U ..` Effective on site Coulomb interaction parameter
- `LDAUJ = J ..` Effective on site Exchange interaction parameter
- `LDAUPRINT = 0|1|2` Controls verbosity of the L(S)DA+U module
  (0: silent, 1: Write occupancy matrix to OUTCAR, 2: idem 1., plus potential matrix dumped to stdout, Default: `LDAUPRINT = 0`)

NB: `LDAUL`, `LDAUU`, and `LDAUJ` must be specified for *all* atomic species!


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


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

Orbital decomposed DOS for NiO(AFMII)

INCAR:

SYSTEM = NiO FCC

DOS related values
LORBIT = 1
LDAU = .TRUE.
LDAUTYPE = 1
LDAUL = 2 -1
LDAUU = 8.0 0.0
LDAUJ = 0.95 0.0
LMAXMIX = 4
LDAUPRINT = 2
ISMEAR = -5
ISPIN = 2
MAGMOM = 2 -2 2*0
GGA = 91
RWIGS = 1.2 0.8

Switch on orbital decomposed DOS calculation

Total DOS

```
.....................
   17.428  0.0000E+00  0.0000E+00  0.2000E+02  0.2000E+02
   17.542  0.0000E+00  0.0000E+00  0.2000E+02  0.2000E+02
   17.656  0.0000E+00  0.0000E+00  0.2000E+02  0.2000E+02
   17.65555450   -16.50226769  301      4.12051746      1.00000000
  -16.502  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E
  -16.388  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E
  -16.275  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E
.....................
```

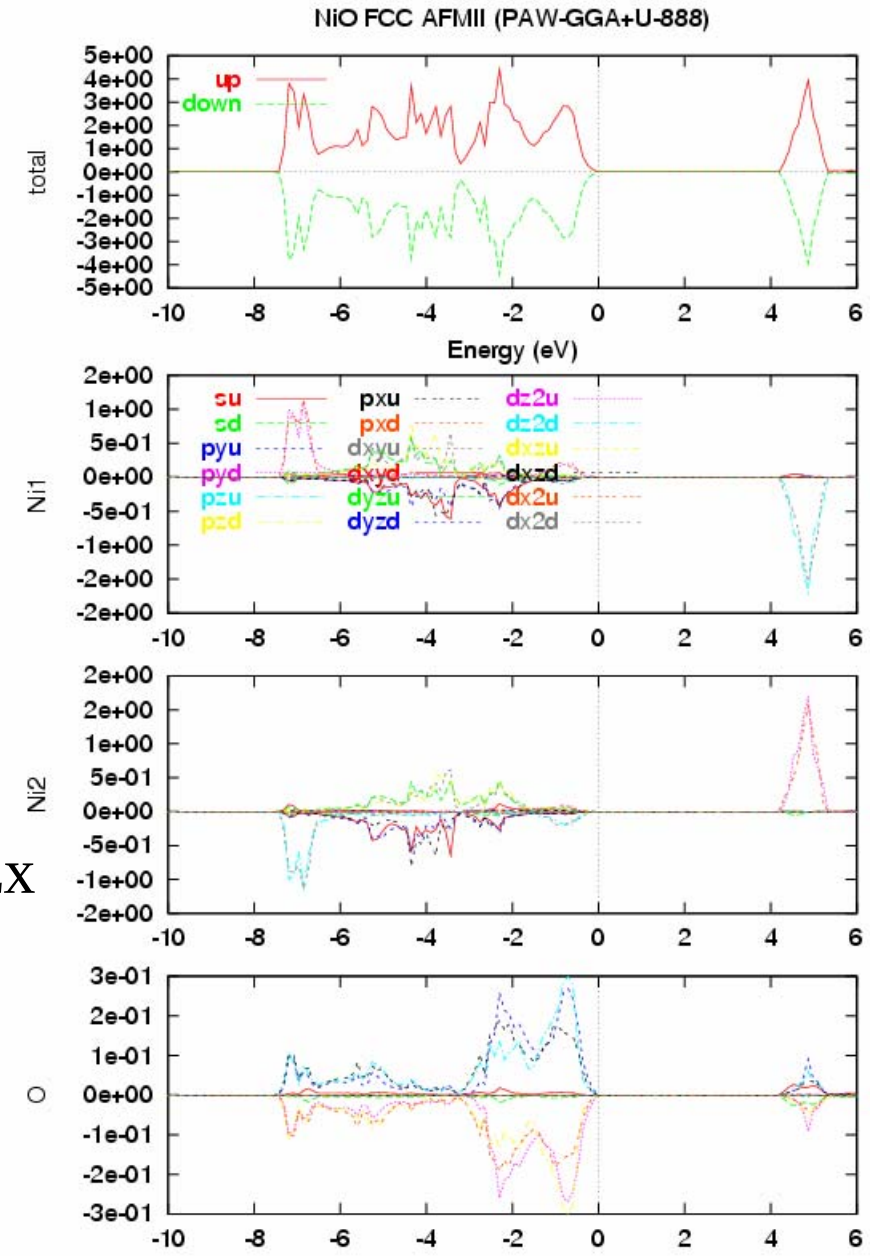
PDOS of the 1st atom in order of ((l=2)+1)^2=9 terms

s py pz px dxy dyz dz2 dxz dx2

u d u d u d u d u d u d u d u d u d

9*(u d)=18 terms

t2g: dxy, dyz, dzx



eg: dz2, dx2-y2

band decomposed charge and spin density distribution for NiO(AFMII)

INCAR:

SYSTEM = NiO FCC

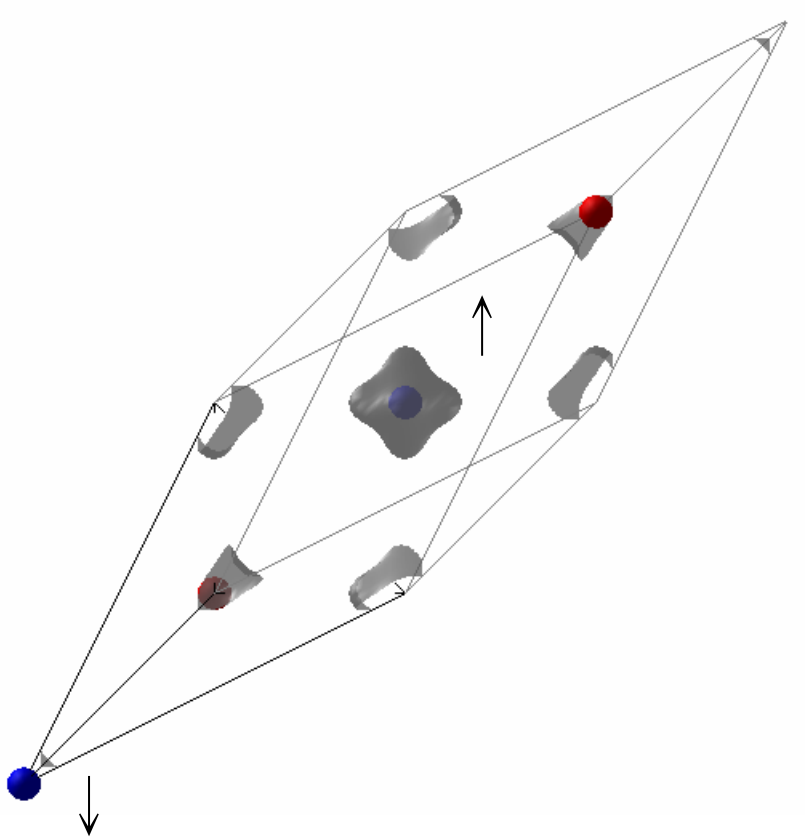
DOS related values
LPARD = .TRUE.
EINT = 4.0 6.0
NBMOD = -3
LDAU = .TRUE.
LDAUTYPE = 1
LDAUL = 2 -1
LDAUU = 8.0 0.0
LDAUJ = 0.95 0.0
LMAXMIX = 4
LDAUPRINT = 2
ISMEAR = -5
ISPIN = 2
MAGMOM = 5 -5 0 0
GGA = 91
RWIGS = 1.2 0.8

Switch on partial charge distribution calculation
From 4eV to 6eV
With respect to Fermi level

Note: You need to calculate a Convergent WAVECAR first!! Then use this WAVECAR to do this calculation

LDA+U NiO AFMII eg band: 4~6eV charge distribution

vaspview PARCHG



Homework

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

- Calculate and plot LDA+U DOS of CrO2, NiO, CoO, and FeO (U=3,8,7.8,4.5eV, J=0.87, 0.95, 0.92, 0.89eV for Cr, Ni, Co, and Fe, respectively)
- Calculate and plot orbital decomposed LDA+U DOS of NiO, CoO, and FeO
- Calculate and plot (vaspview) the charge density distribution of the unoccupied eg band of NiO, CoO, and FeO from LDA+U
- Make a list of the magnetic moment (total and individual) of FeO, CoO, NiO, and CrO2 from LDA and LDA+U