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

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June 07, 2007
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, BUT
• Poor eigenvalues, PRB23, 5048 (1981)
• Lack of derivative discontinuity at integer N, PRL49, 1691 (1982)
• 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 $\mu_B$) 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).

<table>
<thead>
<tr>
<th>Species</th>
<th>$E_{\text{LSD}}$</th>
<th>$E_{\text{LSD} + U}$</th>
<th>$E_{\text{expt}}$</th>
<th>$m_{\text{LSD}}$</th>
<th>$m_{\text{LSD} + U}$</th>
<th>$m_{\text{expt}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CaCuO$_2$</td>
<td>0.0</td>
<td>2.1</td>
<td>1.5</td>
<td>0.0</td>
<td>0.66</td>
<td>0.51</td>
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<tr>
<td>CuO</td>
<td>0.0</td>
<td>1.9</td>
<td>1.4</td>
<td>0.0</td>
<td>0.74</td>
<td>0.65</td>
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<tr>
<td>NiO</td>
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<td>3.1</td>
<td>4.3</td>
<td>1.0</td>
<td>1.59</td>
<td>1.77</td>
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<tr>
<td>CoO</td>
<td>0.0</td>
<td>3.2</td>
<td>2.4</td>
<td>2.3</td>
<td>2.63 (3.60)</td>
<td>3.35</td>
</tr>
<tr>
<td>FeO</td>
<td>0.0</td>
<td>3.0</td>
<td>3.4</td>
<td>4.4</td>
<td>4.61</td>
<td>4.79</td>
</tr>
<tr>
<td>MnO</td>
<td>0.8</td>
<td>3.5</td>
<td>3.6–3.8</td>
<td>4.4</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>


$^c$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


$^i$A. K. Cheetham and D. A. C

$^j$J. van Elp et al. (unpublished).


Gaps too small or no gap
Spin and orbital moment too small
PRB 44 (1991) 943
Beyond LDA

- Self-interaction correction (SIC)
- Optimized effective potential method (OEP)
- Hartree-Fock (HF) method, PRB48(1993)5058
- Time-dependent density functional theory (TDDFT)
- Dynamical mean field theory (DMFT)
- Quantum Monte-Carlo method (QMC)
- LDA+Hubbard U (LDA+U) method,
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

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

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

\[ V_i^{SIC}(\vec{r}) = V_i^{LDA}(\vec{r}) - \int d^3 r' \frac{n_i(\vec{r}')}{|\vec{r} - \vec{r}'|} - V_{xc}[n_i(\vec{r})] \]
Basic idea of LDA+U

• 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: $U \geq W$
- 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 $\pm 1\text{eV}$
- 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)
- 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'' \mid V_{ee} \mid m' m''' > n_{mm}^\sigma n_{m''m'''}^{-\sigma} \}

\[ + ( < mm'' \mid V_{ee} \mid m' m''' > - < mm'' \mid V_{ee} \mid m''' m' > ) n_{mm}^\sigma n_{m''m'''}^\sigma \}

\[ V_{mni}^\sigma = -U(n - \frac{1}{2}) + J(n^\sigma - \frac{1}{2}) + \sum_{m''} \{ < mni' \mid V_{ee} \mid m' m''' > n_{m''m'''}^{-\sigma} \}

\[ + ( < mni' \mid V_{ee} \mid m' m''' > - < mni' \mid V_{ee} \mid m''' m' > ) n_{m''m'''}^\sigma \}

\[ V_{ee} : \text{ Slater integral} \]
Applications of LDA+U on transition-metal oxides

- Pyrochlore: Cd2Re2O7 (VASP)
- Rutile: CrO2 (FP-LMTO)
- 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)
Pyrochlore Cd2Re2O7

- Lattice type: fcc
- 88 atoms in cubic unit cell
- Space group: Fd3m
- $a = 10.219\text{Å}$, $x=0.316$
- Ionic model: $\text{Cd}^{+2}(4d^{10})$, $\text{Re}^{+5}(5d^2)$, $\text{O}^{-2}(2p^6)$
- $U(\text{Cd}) = 5.5$ eV, $U(\text{Re}) = 3.0$ eV
- $J = 0$ eV (no spin moment)
Pyrochlore structure
FIG. 1. (a) Valence-band spectrum of Cd$_2$Re$_2$O$_7$ measured 800 eV photon energy at 300 K compared with a broadened calculated density of states and (b) measured using He I$_\alpha$ at 5.3 eV.
FIG. 1. (a) Valence-band spectrum of Cd$_2$Re$_2$O$_7$ measured 800 eV photon energy at 300 K compared with a broadened calculated density of states and (b) measured using He Iα at 5.3 eV.
Pyrochlore Cd2Re2O7

- 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
Rutile CrO2

• Half-metal, moment = 2 μ_B
• Lattice type : bct
• 6 atoms in bct unit cell
• Space group : P4_2/mnm
• a = 4.419Å, c=2.912Å, 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)
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

<table>
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<tr>
<th>(u_B)</th>
<th>Spin moment</th>
<th>Orbital moment</th>
</tr>
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<td></td>
<td>Cr</td>
<td>O</td>
</tr>
<tr>
<td>LDA</td>
<td>1.89</td>
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</tr>
<tr>
<td>LDA+U</td>
<td>1.99</td>
<td>-0.079</td>
</tr>
<tr>
<td>Exp.</td>
<td></td>
<td>2</td>
</tr>
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* D. J. Huang et al, SRRC
Rutile CrO$_2$

- LDA+U enhances the gap and the exchange splitting at the Fermi level
- LDA+U also gives larger spin and orbital magnetic moment
- $U \lesssim W$, orbital moment quenched,
  - stronger hybridization, stronger crystal field, close to itinerant picture
Double perovskites: 
Sr$_2$FeMoO$_6$, Sr$_2$FeReO$_6$, Sr$_2$CrWO$_6$

- Half-metal, moment = 4, 3, 2 $\mu_B$
- Lattice type: tet, fcc, fcc
- 40 atoms in tet, fcc, fcc unit cell
- Space group: I4/mmm, Fm3m, Fm3m
- $a = 7.89, 7.832, 7.878$Å, $c/a = 1.001, 1, 1$
- Ionic model: Fe$^{+3}(3d^5)$, Cr$^{+3}(3d^3)$, Mo$^{+5}(4d^1)$, Re$^{+5}(5d^2)$, W$^{+5}(5d^1)$
- $U(\text{Fe,Cr}) = 4.3$ eV, $J(\text{Fe,Cr}) = 0.89, 0.87$ eV
Double perovskite structure
<table>
<thead>
<tr>
<th>Material</th>
<th>Spin moment</th>
<th>Orbital moment</th>
</tr>
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<tbody>
<tr>
<td></td>
<td></td>
<td>spin moment</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Fe</td>
</tr>
<tr>
<td>(\text{Sr}_2\text{FeMoO}_6)</td>
<td>GGA</td>
<td>3.80</td>
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<td>GGA+U</td>
<td>3.96</td>
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<tr>
<td>(\text{Sr}_2\text{FeReO}_6)</td>
<td>GGA</td>
<td>3.81</td>
</tr>
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<td></td>
<td>GGA+U</td>
<td>3.98</td>
</tr>
<tr>
<td>(\text{Sr}_2\text{CrWO}_6)</td>
<td>GGA</td>
<td>2.30</td>
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<td></td>
<td>GGA+U</td>
<td>2.46</td>
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</tbody>
</table>
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
- \(a=5.5332\ \text{Å},\ b=5.57169\ \text{Å},\ c=7.8491\ \text{Å}\)
- Ionic model: Ru$^{4+}(4d^4, t2g^3\uparrow, t2g^1\downarrow)$
- \(U = 3.5\ \text{eV},\ J = 0.58\ \text{eV}\)
- Pseudopotential, 100 k-point, 31360 plane wave, Cut-off energy = 400 eV
Orthorhombic perovskite SrRuO$_3$
LSDA~$-0.5\text{eV}$

Expt.~$-1.1\text{eV}$
LDA+U

Energy (eV)

Density of states (state/eV/atom)

dxz, 0.44e

dxy, 0.31e

dyz, 0.42e

dxy, 0.31e

dxz, 0.44e

dyz, 0.42e

dxy, 0.31e
SrRuO$_3$

H. T. Jeng,
S. H. Lin,
C. S. Hsue
PRL97(2006)67002

(-1/3, -1/3, -1/3)
• GGA  SrRuO$_3$ is a normal metal without orbital ordering
• LDA+U  SrRuO$_3$ is a half-metal with 4d-t$_2$g orbital ordering
• The half-metallic orbital ordering ground state is robust upon varying U, lattice relaxation, and spin-orbit interaction
High temperature magnetite (Fe$_3$O$_4$)

- Half-metal, insulator, moment = 4 $\mu_B$
- Lattice type: fcc
- Space group: Fd3m
- 56 atoms in fcc unit cell
- $a = 8.394, 8.383, 8.351$ Å
- Ionic model: Fe$^{3+}$(3d$^5$), Fe$^{2+}$(3d$^6$)
- $U(\text{Fe}^{3+},\text{Fe}^{2+})=4.5, 4.0$ eV
- $J(\text{Fe}) = 0.89$ eV
Spinel structure
Fe$_3$O$_4$  (PES, XAS: D.J. Huang, SRRC)
## Spin and orbital magnetic moments of Fe₃O₄

<table>
<thead>
<tr>
<th>(uₜ)</th>
<th>Spin moment</th>
<th>Orbital moment</th>
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<tr>
<td></td>
<td>Fe(A)</td>
<td>Fe(B)</td>
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<tr>
<td></td>
<td>Total</td>
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<tr>
<td>LDA</td>
<td>-3.31</td>
<td>3.52</td>
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<tr>
<td>GGA</td>
<td>-3.44</td>
<td>3.60</td>
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<td>LDA+U</td>
<td>-3.81</td>
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<tr>
<td>Exp.</td>
<td>-3.8⁺</td>
<td>4.10</td>
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</table>

*J. Phys. C 11 (1978) 4389  * D. J. Huang et al, SRRC
Fe$_3$O$_4$, 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$_3$O$_4$

- Insulator
- Lattice type: monoclinic
- Space group: P2/c
- 56 atoms in monoclinic unit cell
- $a = 5.9444$ Å, $b=5.925$ Å, $c=16.775$ Å
- $\beta = 90.2363^0$
- 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)
LDA      Half-metal

Expt. Gap 0.14 eV

B-t2g

The. Gap 0.2 eV

LDA+U    Insulator

Expt. Gap 0.14 eV

B-t2g
Charge and spin moment of Fe$_3$O$_4$

in low-temperature phase ($r_{mt}=1.0$ A)

<table>
<thead>
<tr>
<th></th>
<th>LDA</th>
<th>LDA</th>
<th>Exp.*</th>
<th>LDA+ U</th>
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<td>Charge</td>
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<tr>
<td>Fe(B1)</td>
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<td>Fe(B2)</td>
<td>3.43</td>
<td>5.50</td>
<td>5.4</td>
<td>5.41</td>
<td>3.90</td>
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<td>Fe(B3)</td>
<td>3.32</td>
<td>5.52</td>
<td>5.4</td>
<td>5.44</td>
<td>3.81</td>
</tr>
<tr>
<td>Fe(B4)</td>
<td>3.39</td>
<td>5.52</td>
<td>5.6</td>
<td>5.58</td>
<td>3.39</td>
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</table>

* PRL 87 (2001) 266401
dyz, 0.59e

dxz, 0.59e

dxy, 0.63e

Fe(B1a)  Fe(B2a)  r = 1.0 Å

Fe(B1b)  Fe(B2b)

Fe(B4)  Fe(B3)
3-1 charge-orbital ordering

H. T. Jeng,
G. Y. Guo,
D. J. Huang,
PRL93(2004)
156403,
Low-temperature Fe$_3$O$_4$

- 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

Horng-Tay Jeng
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June 07, 2007
Work 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(AFMI11)

**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.
- **LDAU_TYPE = 1|2|4** Type of L(S)DA+U (Default: LDAU_TYPE = 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!
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

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<th>p</th>
<th>d</th>
<th>E</th>
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<td>17.542</td>
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<td>17.656</td>
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<td>0.2000E+02</td>
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Total DOS

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<th>p</th>
<th>d</th>
<th>E</th>
<th>p</th>
<th>d</th>
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PDOS of the 1st atom in order of 
((l=2)+1)^2=9 terms

s   py   pz   px   dxy   dyz   dz2   dxz   dx2
u   u   d   u   u   d   u   u   u   d   u   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 the calculation
LDA+U NiO AFMII eg band: 4~6eV charge distribution
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
• Make a list of the magnetic moment (total and individual) of FeO, CoO, NiO, and CrO2 from LDA and LDA+U