MAR09-2008-006217

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Sorting Category: 05.5 (C)

Electronic Properties of Rocksalt Copper Monoxide

PAUL MICHAEL GRANT, W2AGZ Technologies — Rocksalt copper monoxide, although not yet synthetically realized in bulk form, can be studied computationally as a proxy for the family of layered HTSC copper oxides. We report results for a series of tetragonal CuO rocksalt structures with c/a lattice parameter ratios ranging from 1.0 to 1.5, employing the plane-wave pseudopotential method with exchange/correlation LDA+U. As expected, we obtain a metallic state for U = 0 at all values of c/a given that the nominal valence electron configuration for Cu in copper monoxides is $3d^9$ yielding a partially occupied conduction band. However, completely unexpected was our finding similar metallic properties in rocksalt CuO for all physically plausible values of U (up to 10 eV) and c/a between 1.0 to approximately 1.2. Only for c/a > 1.2 do our calculations reveal the opening of a Mott-Hubbard charge-transfer gap. We interpret our results[1] as supporting the original motivations of Bednorz and Mueller that high temperature superconductivity in the layered copper oxide perovskites may begin with their tendency to exhibit Jahn-Teller strong electron-phonon coupling[2].

[1]P. M. Grant, J. Phys: CS **129** (2008) 01242.
[2]J. G. Bednorz and K. A. Mueller, Rev. Mod. Phys. **60** (1988) 585.

Paul Michael Grant
w2agz@pacbell.net
W2AGZ Technologies

[X] Prefer Oral Session
[ ] Prefer Poster Session

Date submitted: 21 Nov 2008 Electronic form version 1.4

Electronic Structure of Rocksalt Copper Monoxide: A Proxy for High Temperature Superconductivity

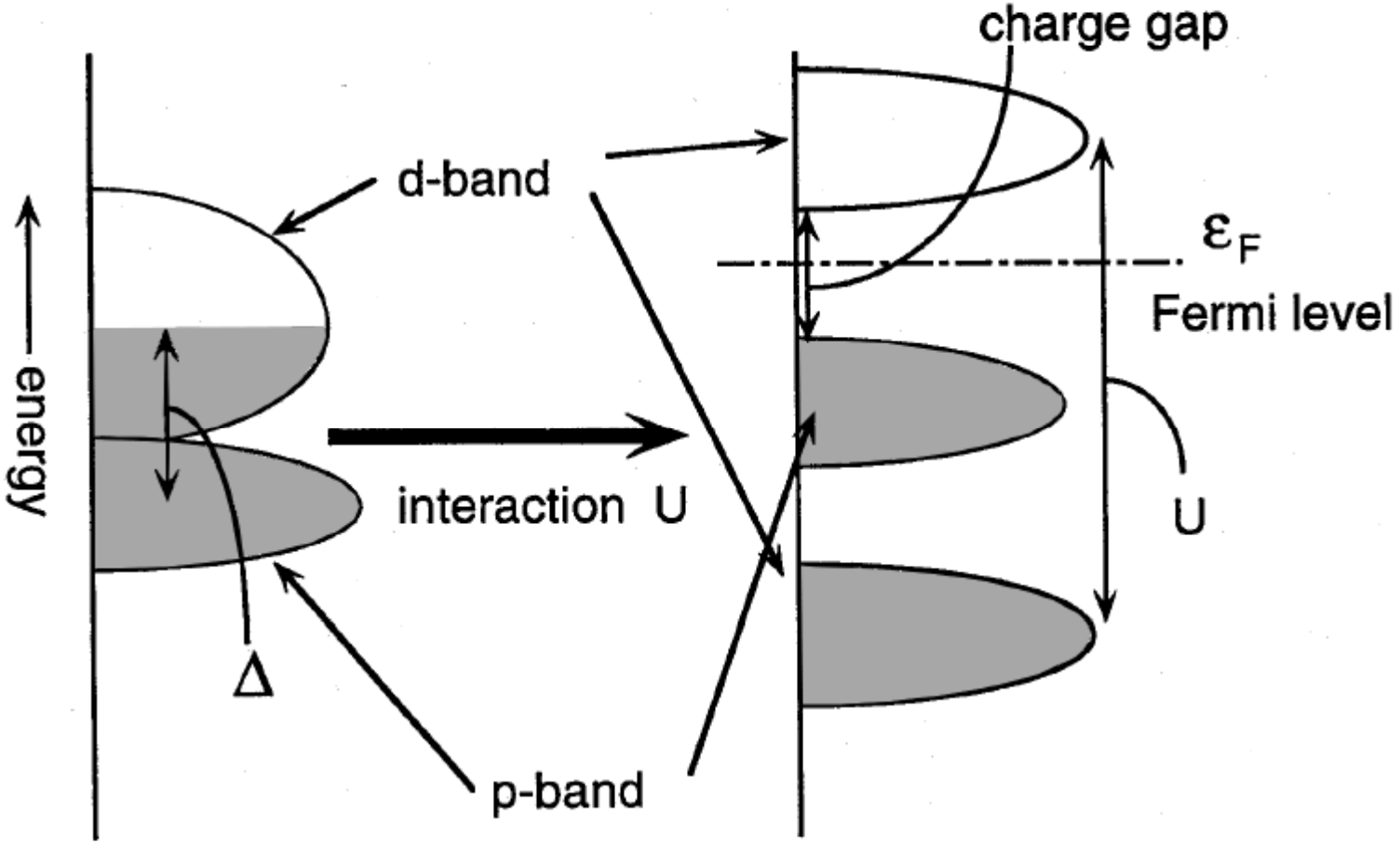
Paul M. Grant

W2AGZ Technologies
Visiting Scholar, Stanford University (2005-2008)

Aging IBM Pensioner

Financial Support From:
IBM Retiree Pension Fund Prior to 1990

Transition Metal Oxides
"Should be Metals, But Aren't"
(Charge Transfer Insulators, Instead)



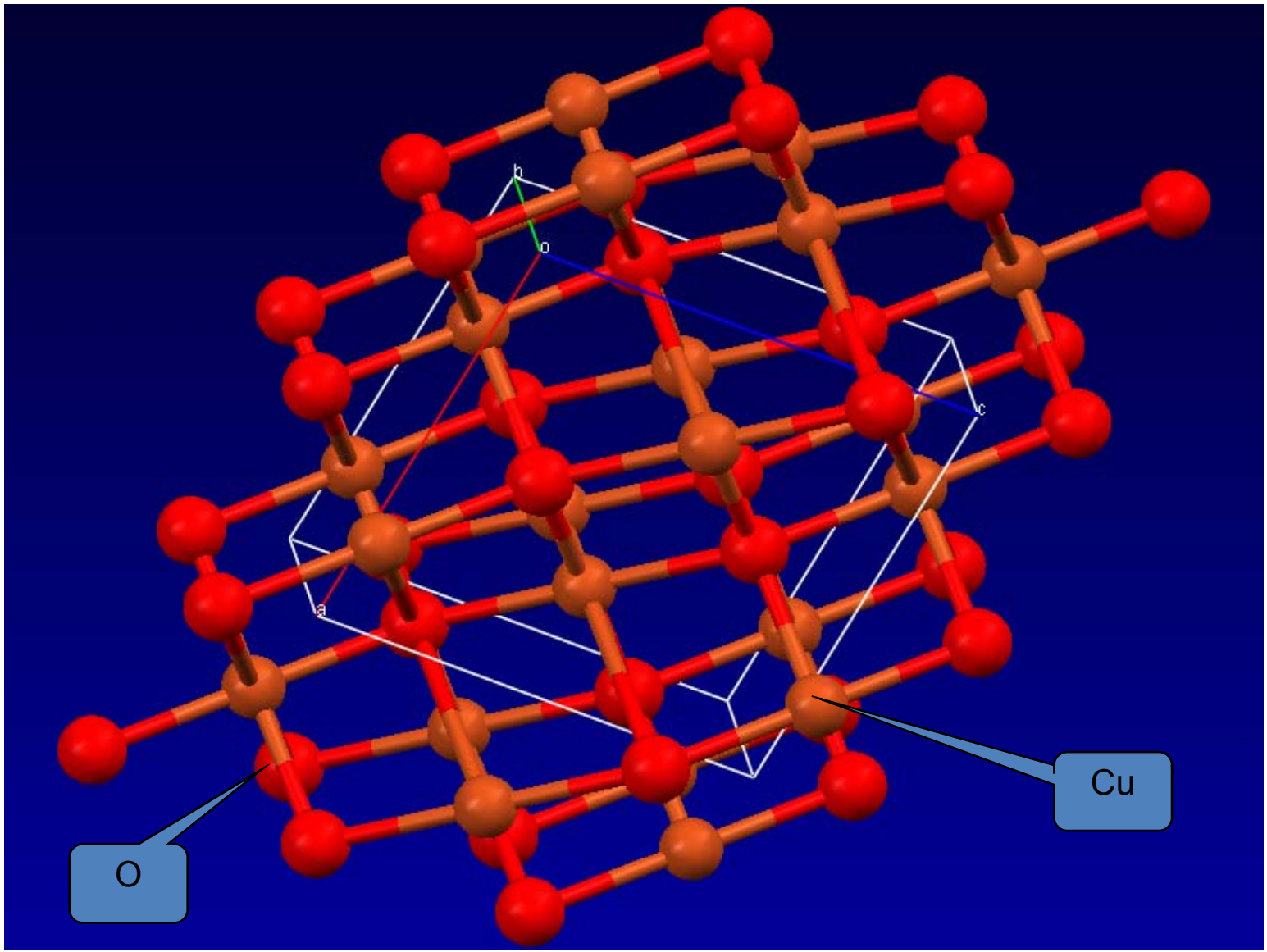
After Imada, et al, RMP 70, 1039 (1998)

Cubic Rocksalt Divalent TMOs

TMO	3d Config	Properties
MnO	5	MH-CTI (5.6)
FeO	6	MH-CTI (5.9)
CoO	7	MH-CTI (6.3)
NiO	8	MH-CTI (6.5)
CuO	9	***XX Doesn't Exist!***

See Imada, Fujimore,
Tokura, RPM 70 (1988)

Tenorite (Monoclinic CuO)



Experimental Equipment (Software)

- QUANTUM-ESPRESSO Suit of Codes
  - DFT (LDA+U) plus electron-phonon
  - Graphics by Tone Kolalj (XCrysDen)
  - www.quantum-espresso.org
- "Dial-in" Parameters
  - G^2 = 40 Ry ρ = 320 Ry
  - Convergence ≤ 10^{-6} Ry
  - "Smearing" = Methfessel-Paxton
  - Psuedopotentials: Ultrasoft, XC = Perdew-Zunger
    Cu: $3d^9 4s^2$ O: $2s^2 2p^4$

Experimental Equipment (Hardware)

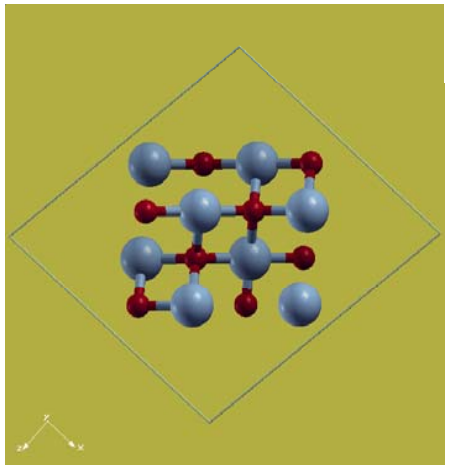
3-Cluster Home Network: AMD64 dual 3.5 GHz, 12 GB + IBM-X41 +…

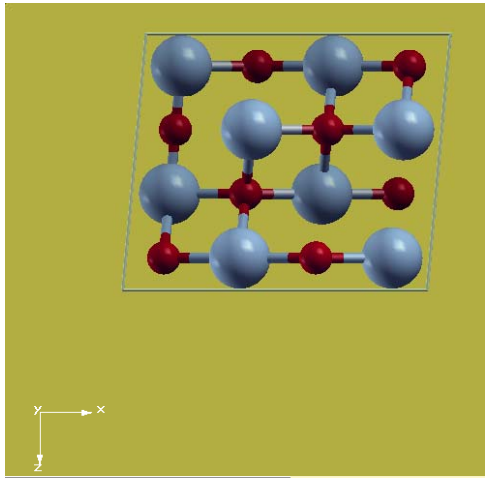
Diego Grant's Sony Playstation 3

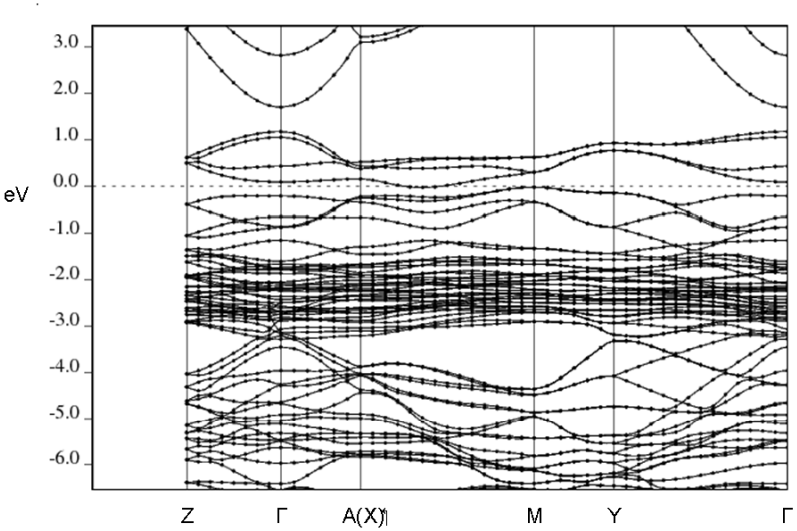
Tenorite “Test”

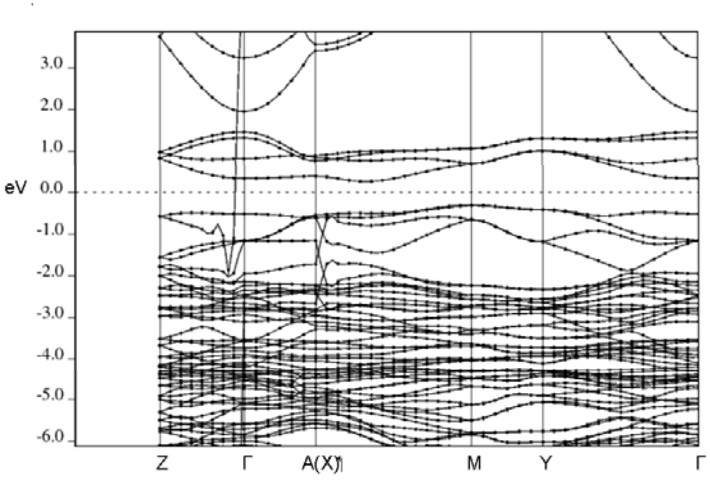
Chemical: U=0

AF: U=6

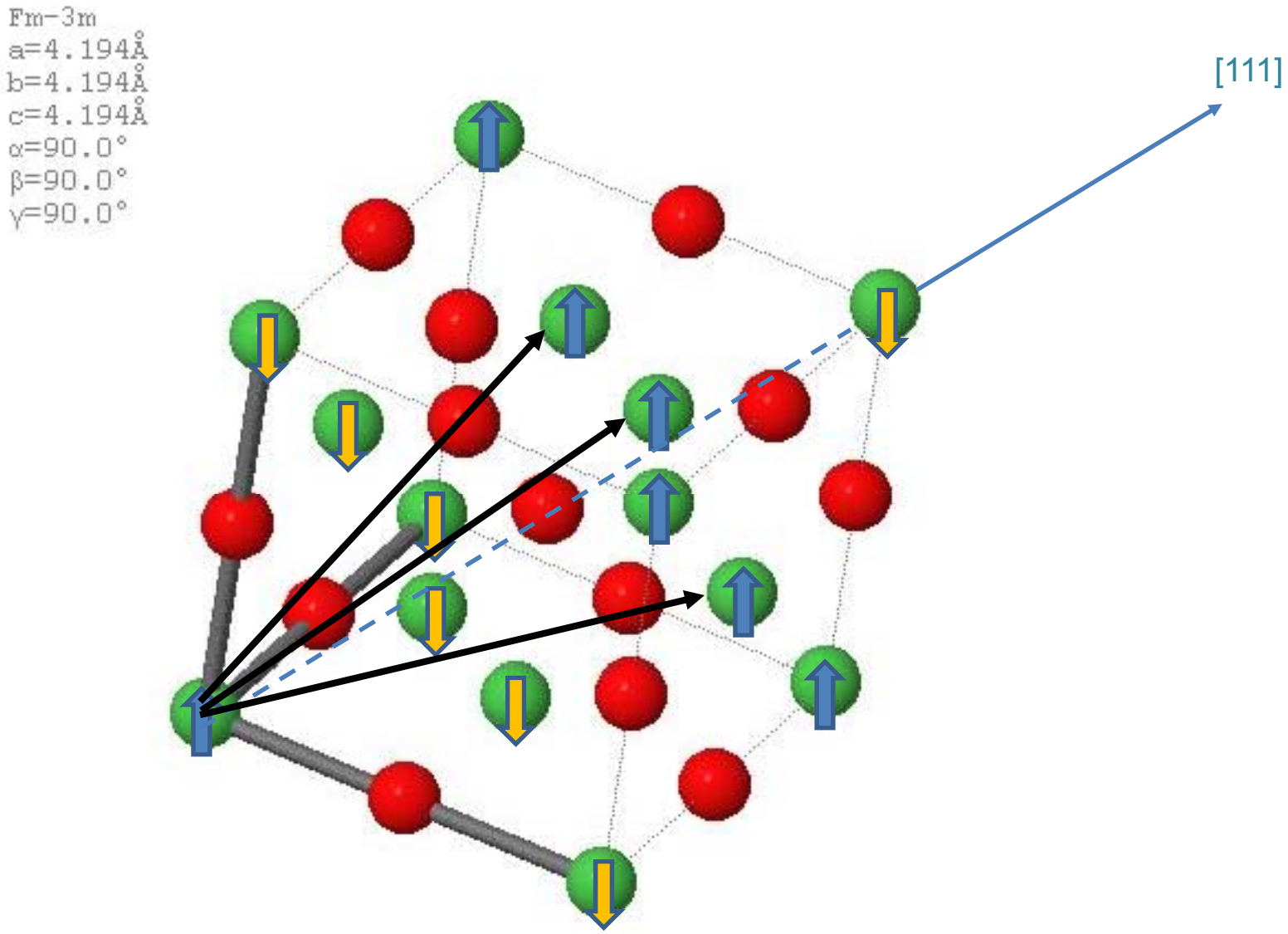




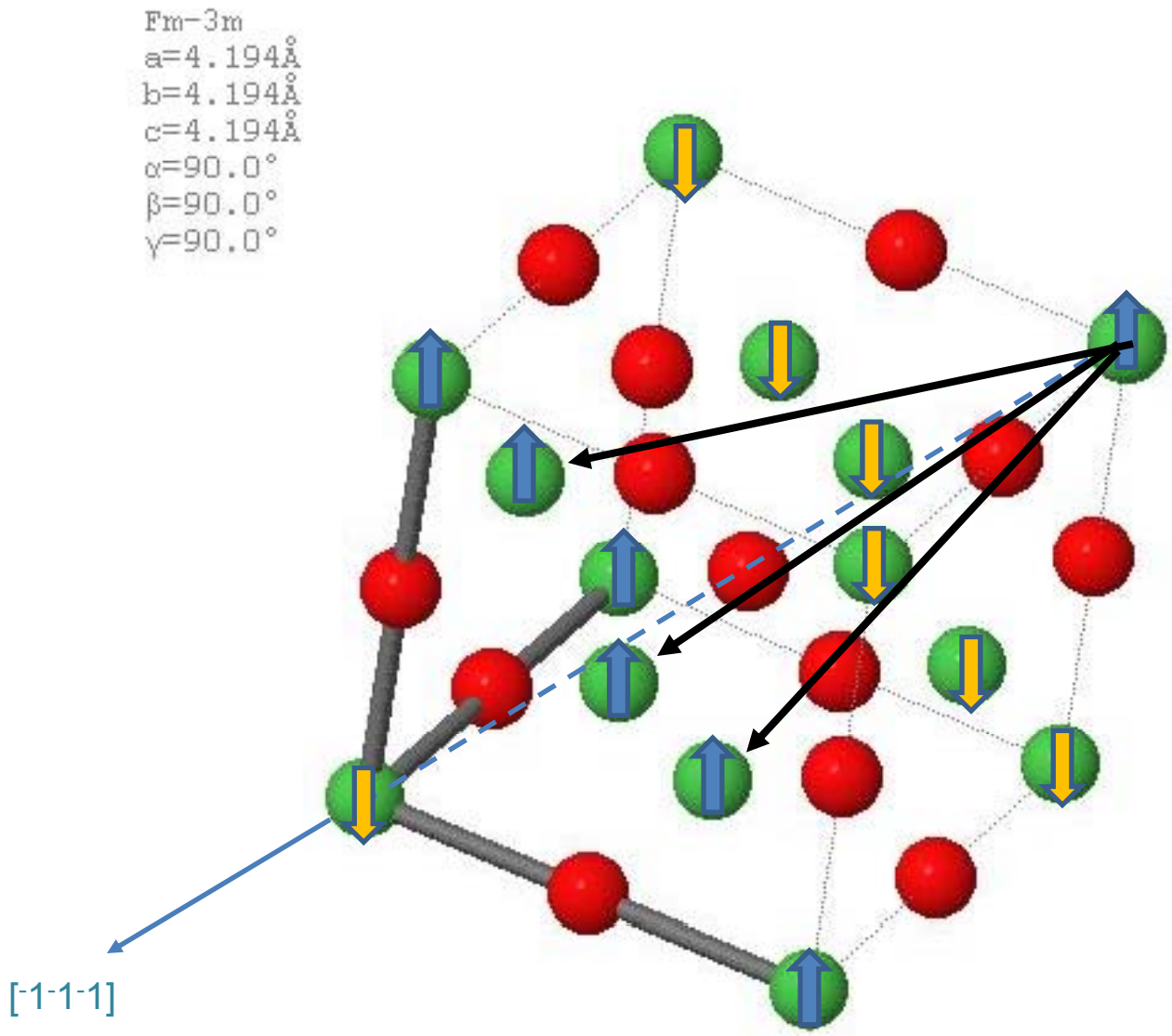




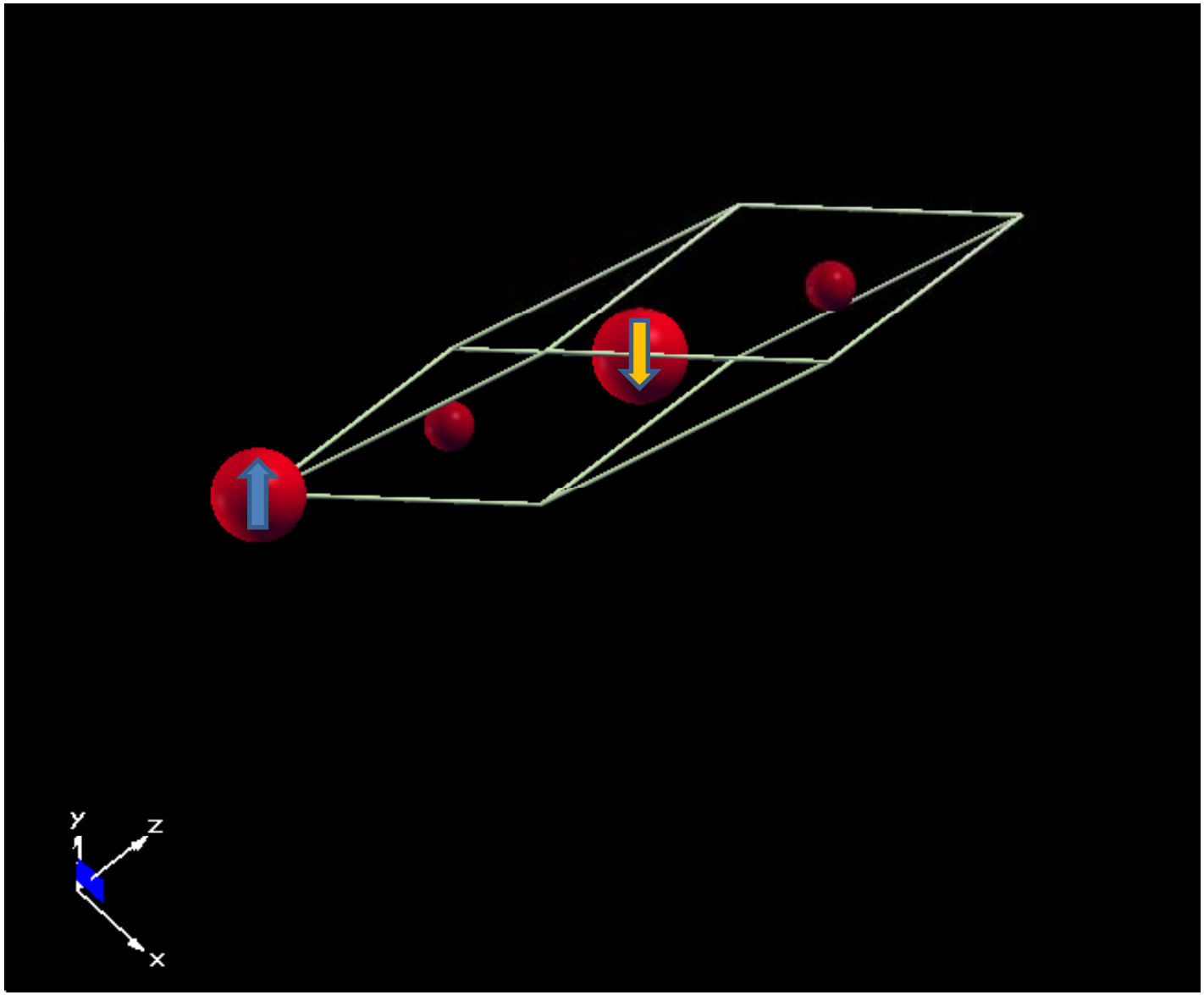
Proto-TMO AF Rock Salt

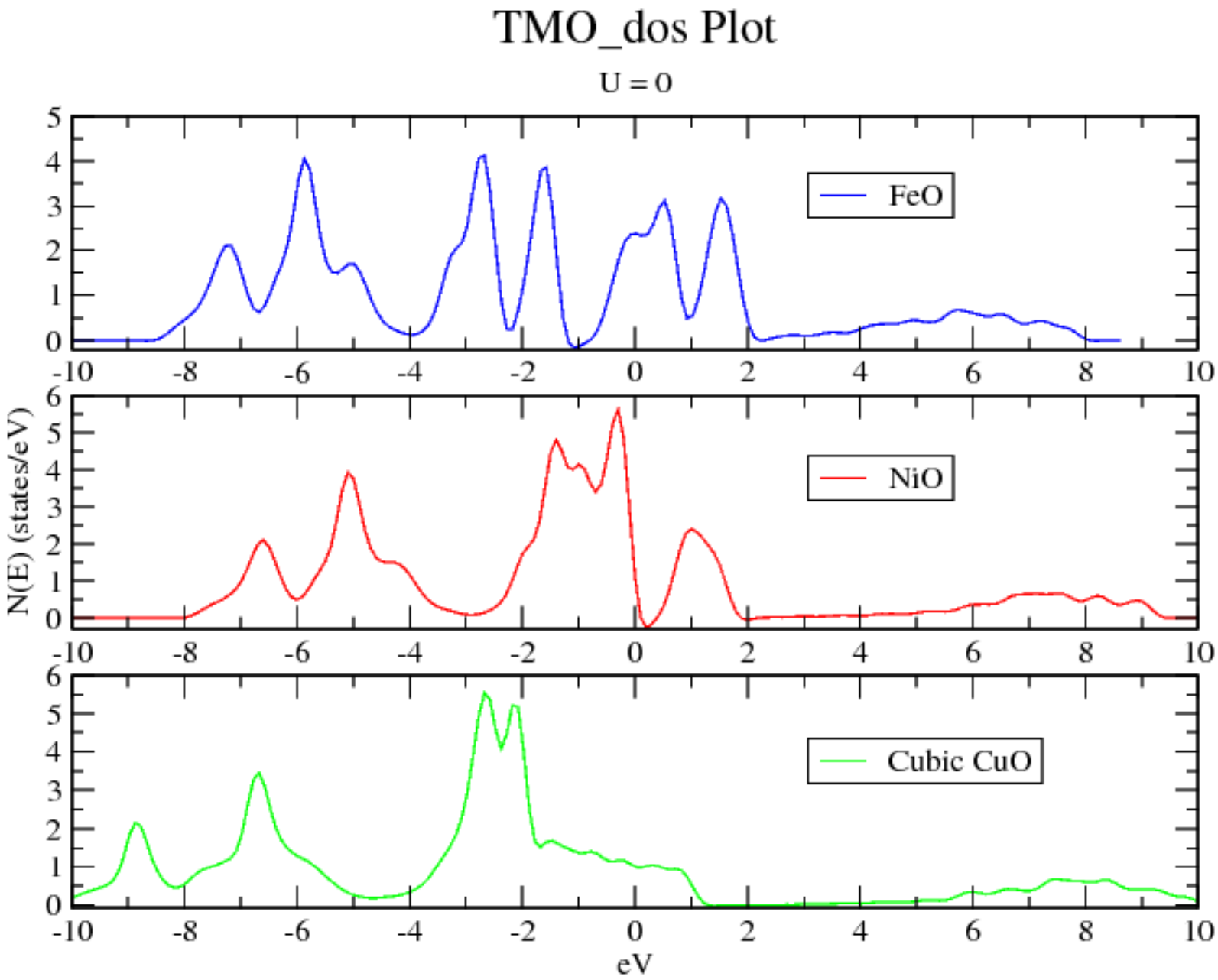


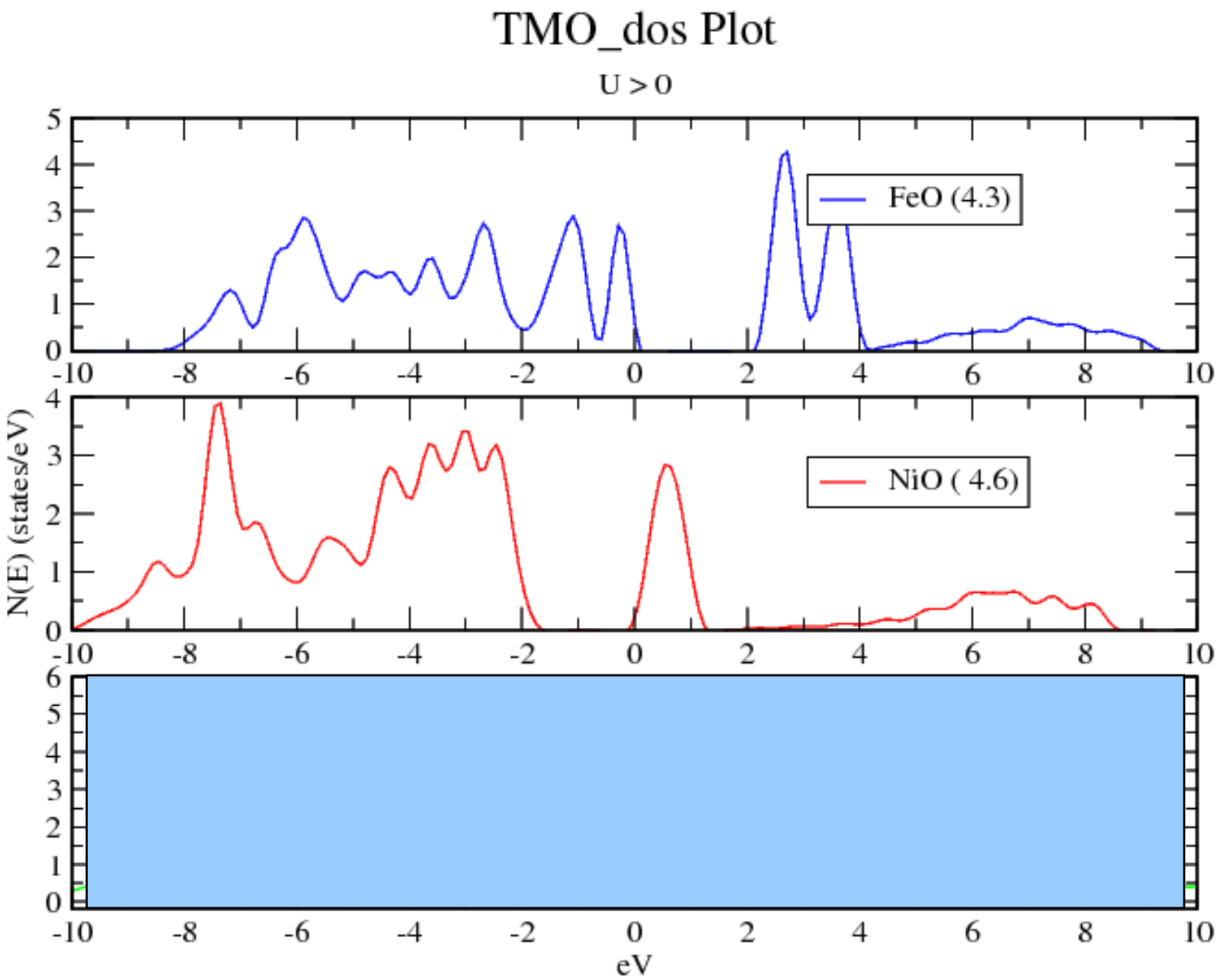
Proto-TMO AF Rock Salt



Basic Asymmetric AF Cell



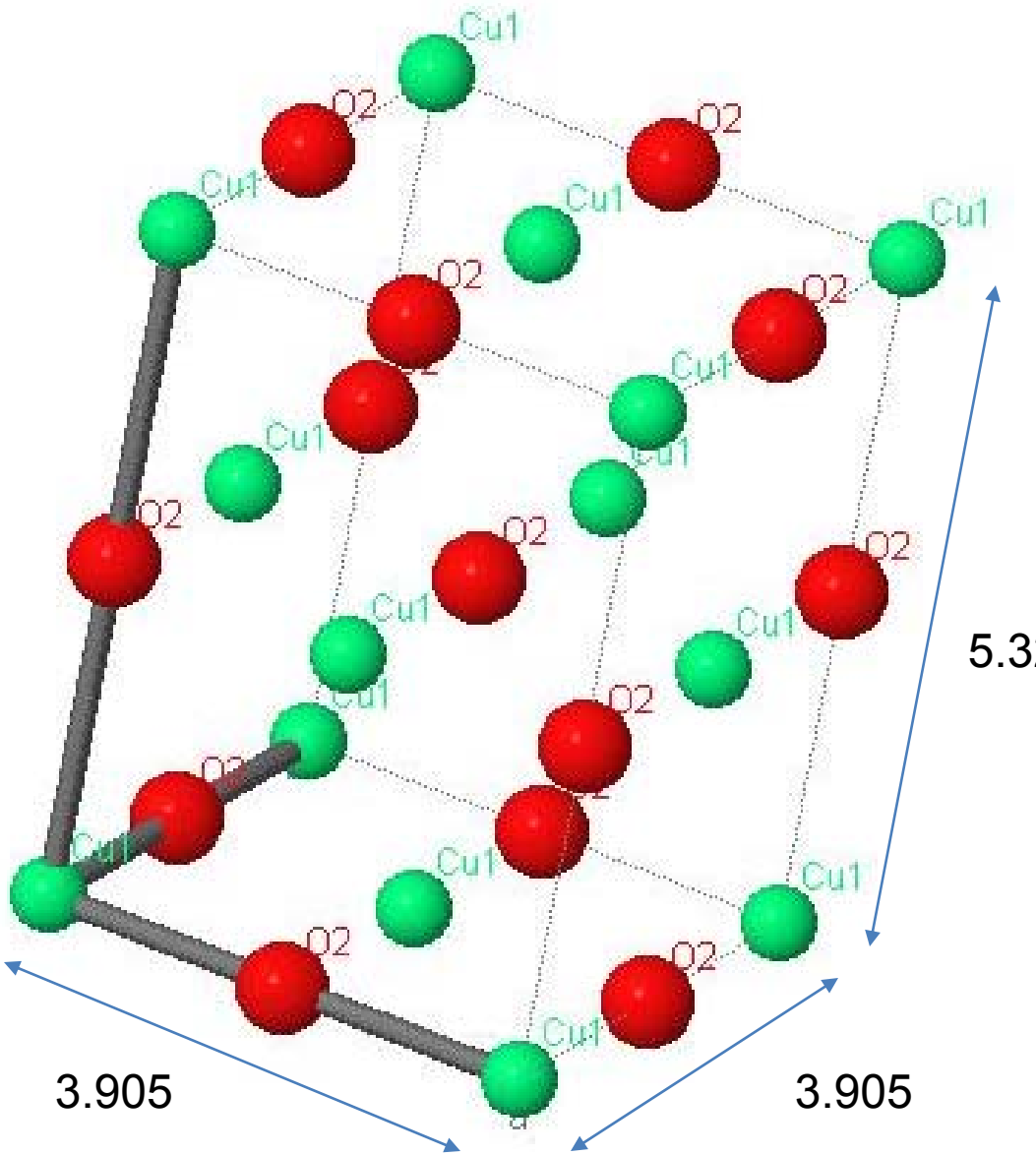

TMO_dos Plot
U = 0
FeO
NiO
Cubic CuO
N(E) (states/eV)
eV
-10
-8
-6
-4
-2
0
2
4
6
8
10


TMO_dos Plot
U > 0
FeO (4.3)
NiO (4.6)
N(E) (states/eV)
eV

Tetragonal CuO

Fm-3m
a=3.905Å
b=3.905Å
c=5.320Å
α=90.0°
β=90.0°
γ=90.0°

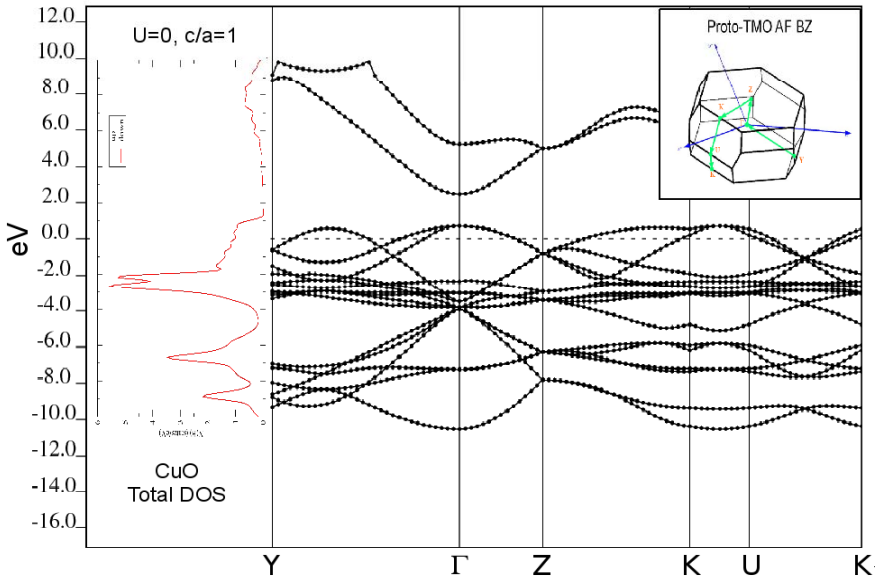
c/a = 1.36

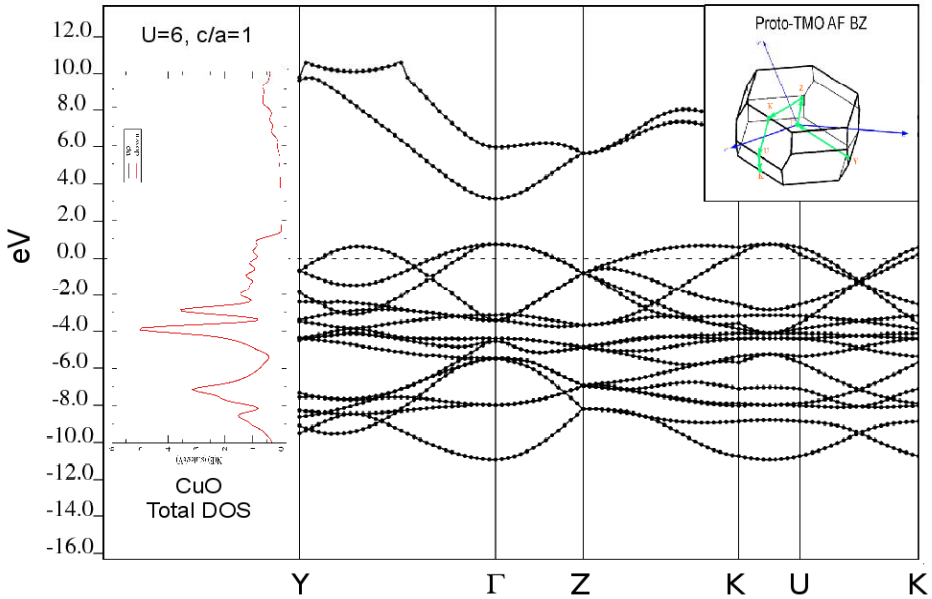


Measurements
(Wolter Siemons)

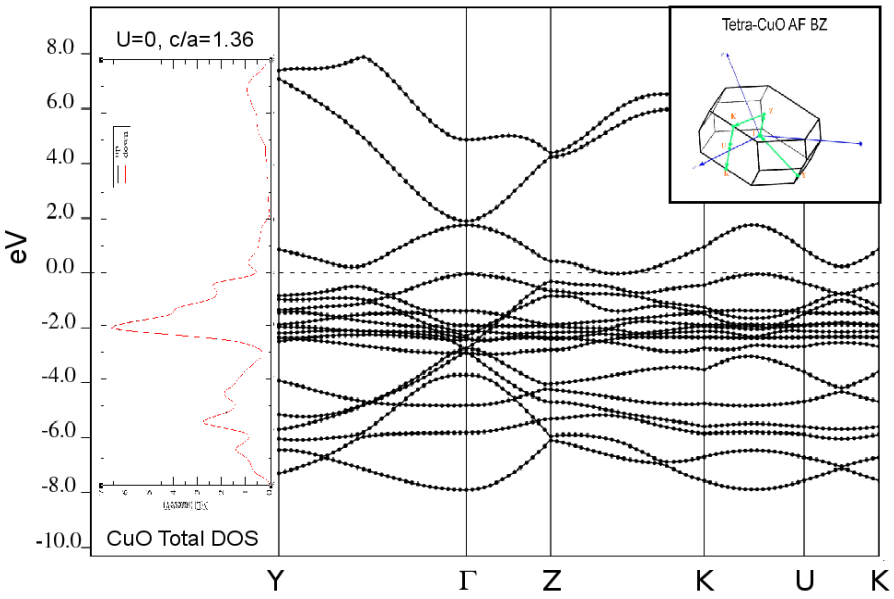
- 2-4 ML epi on STO
- No Fermi Edge
- No Exchange Bias on ferro-SRO (Tc ~ 100-150 K)

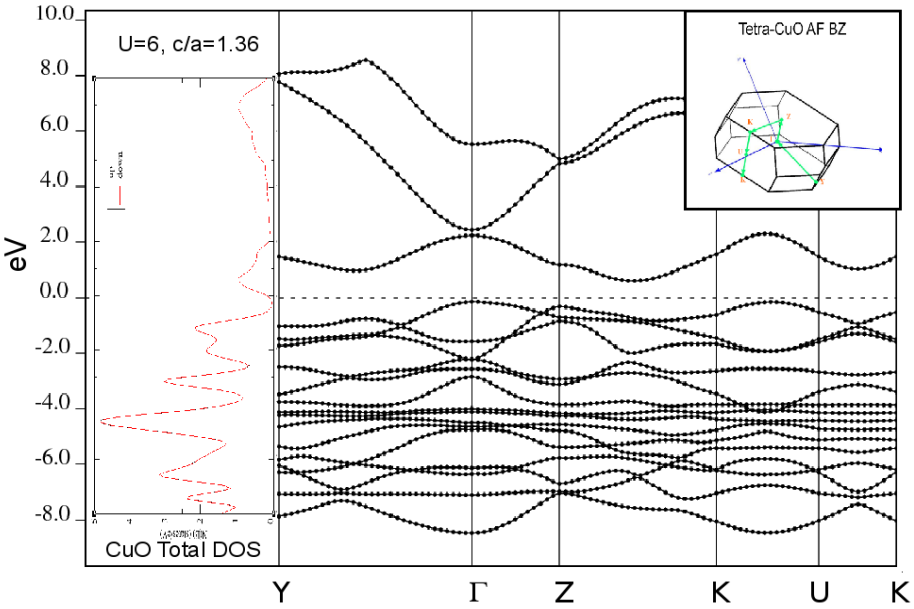
Cubic





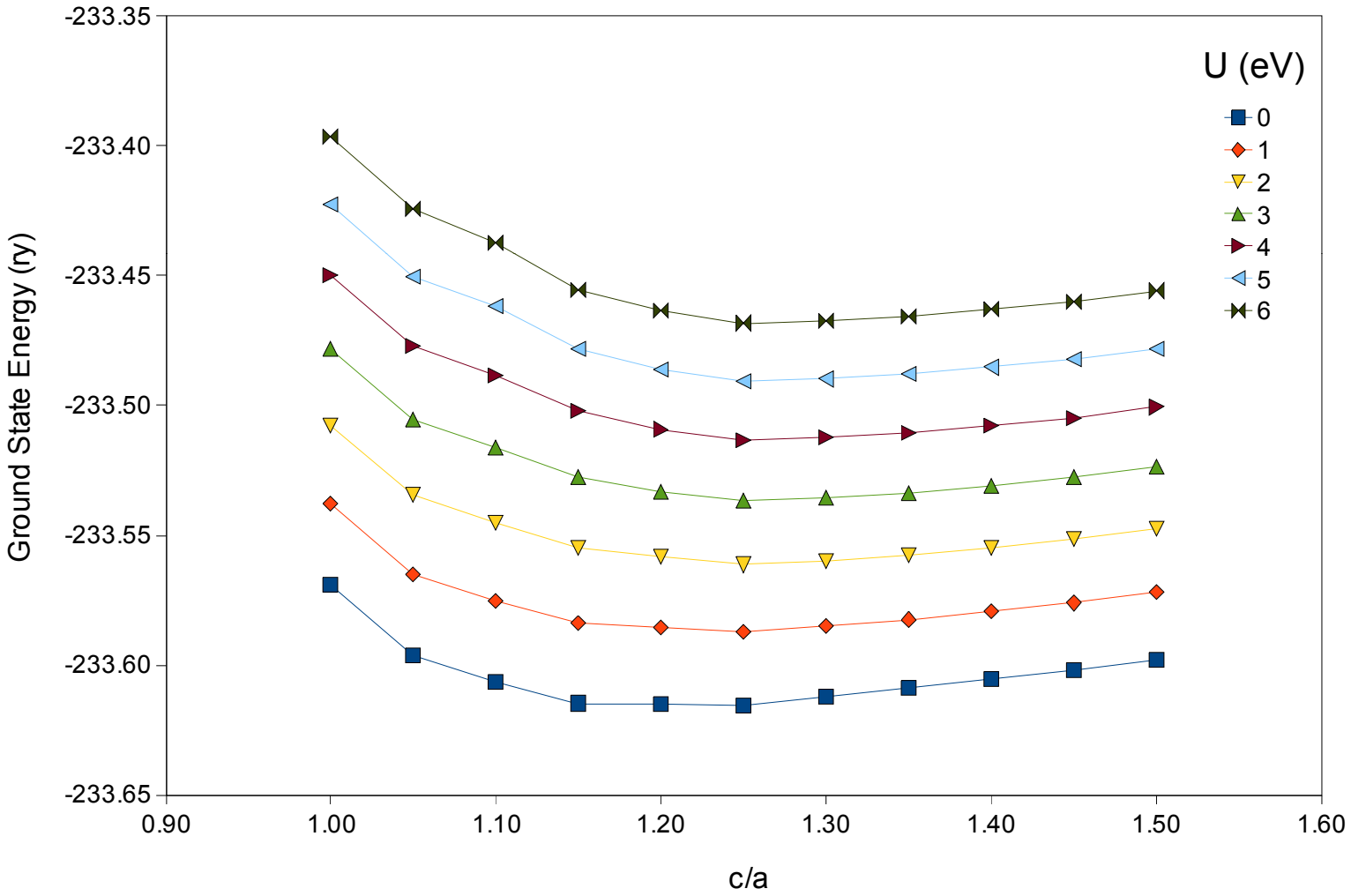
Tetragonal

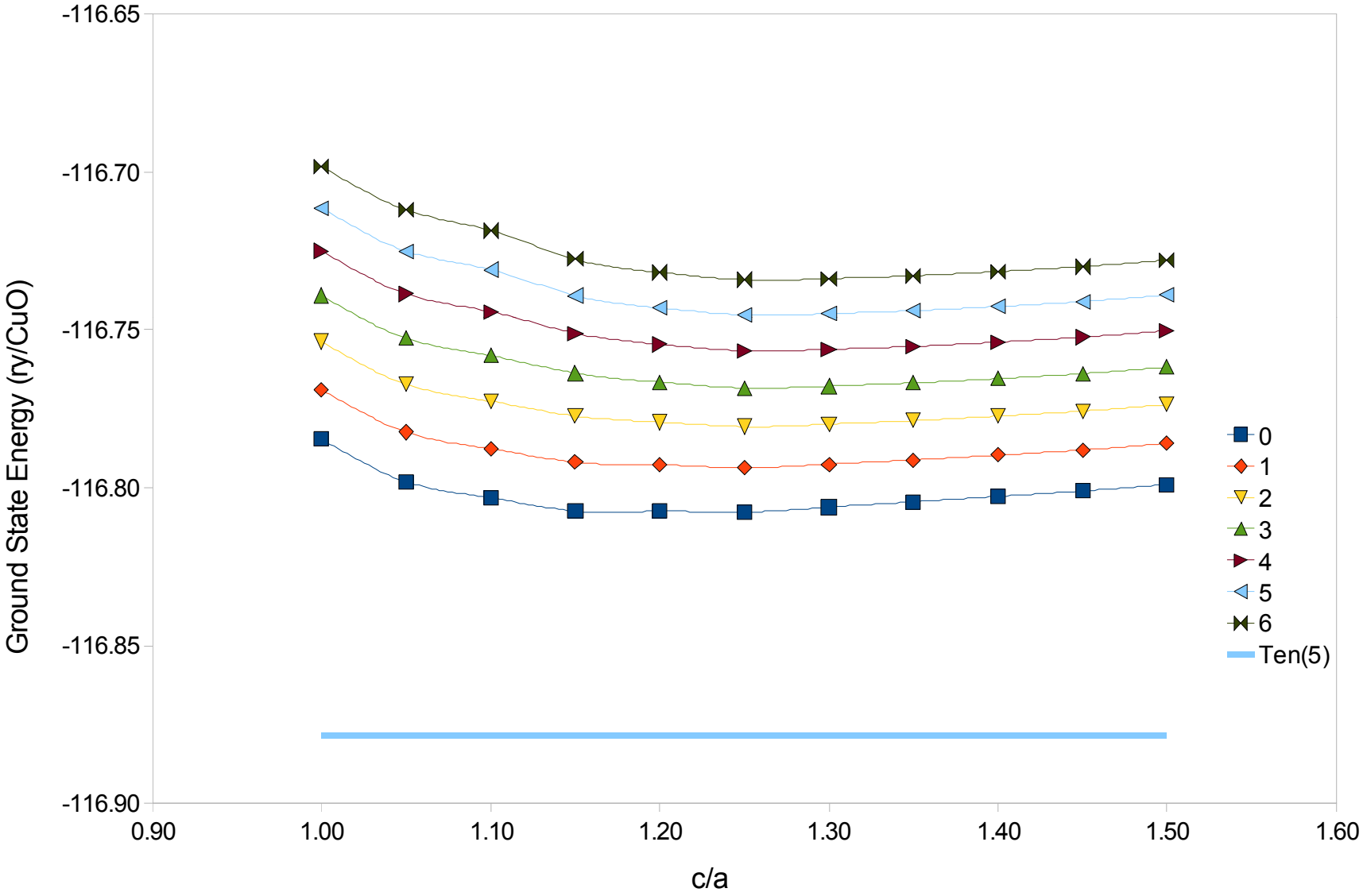




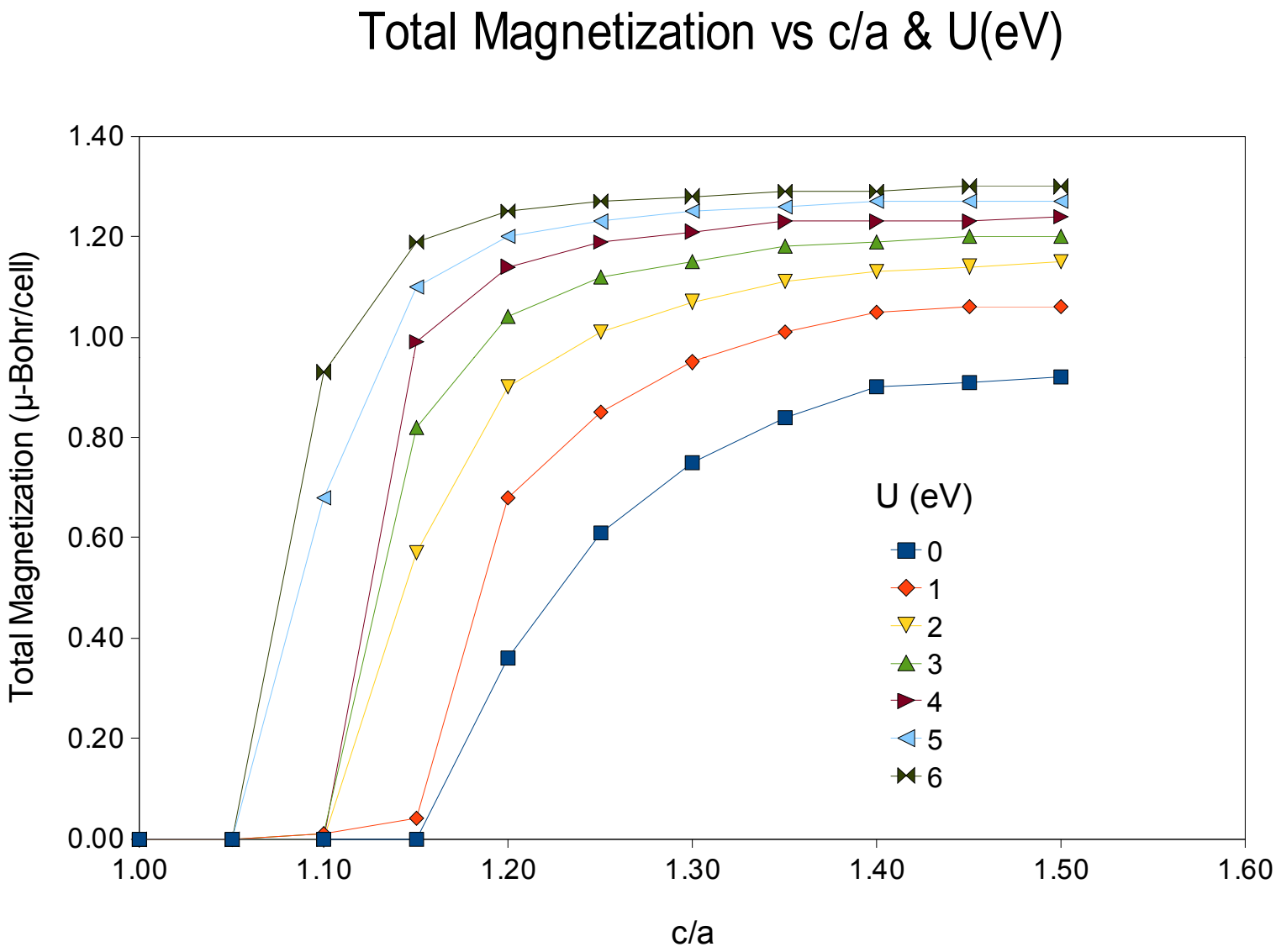
Rocksalt CuO - a = 3.905 Angstroms, PP = Cu.pz-3d9_4s2-rrkjus.UPF

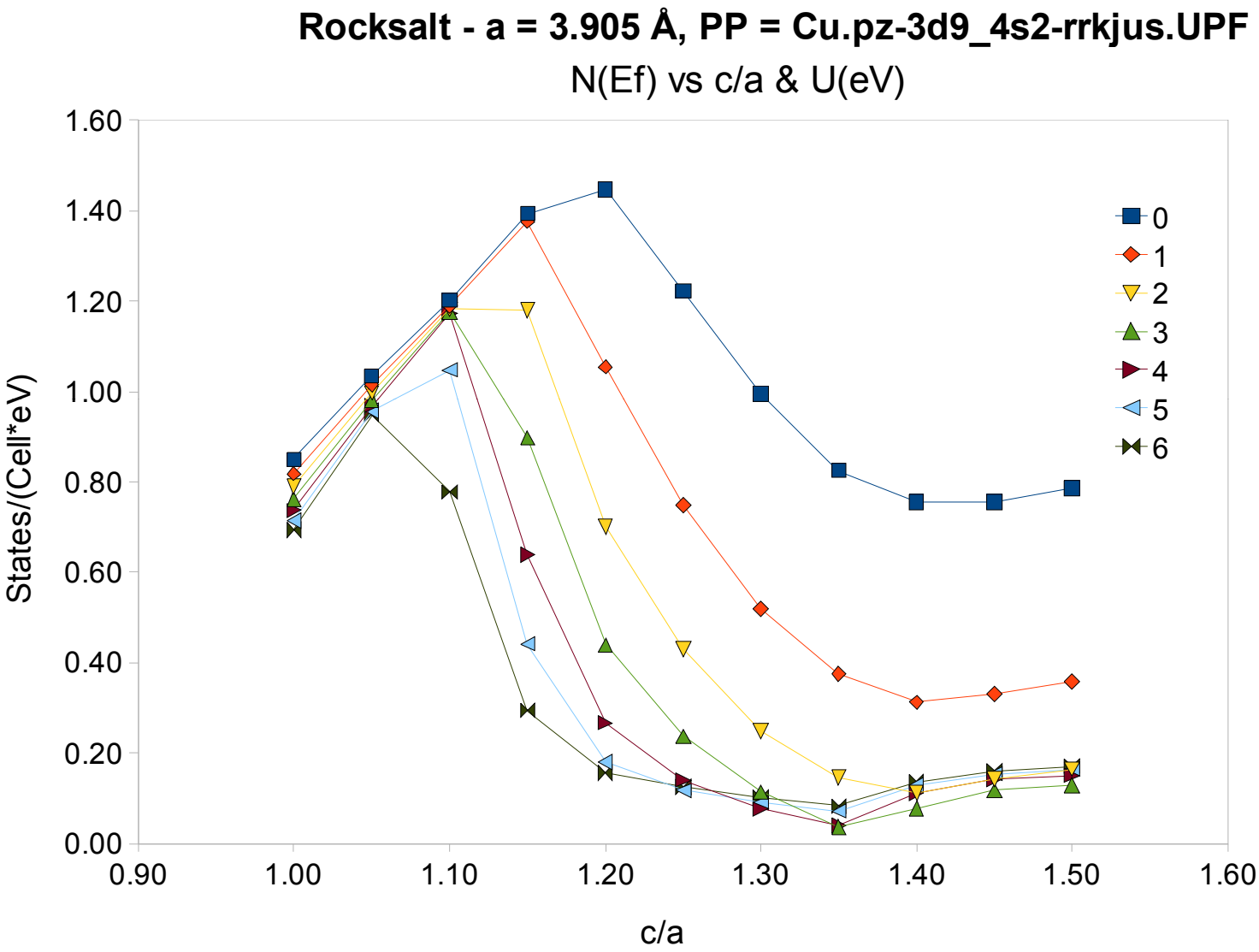
Ground State Energy vs c/a & U(ev)




-116.65
-116.70
-116.75
-116.80
-116.85
-116.90
Ground State Energy (ry/CuO)
0.90
1.00
1.10
1.20
1.30
1.40
1.50
1.60
c/a
0
1
2
3
4
5
6
Ten(5)

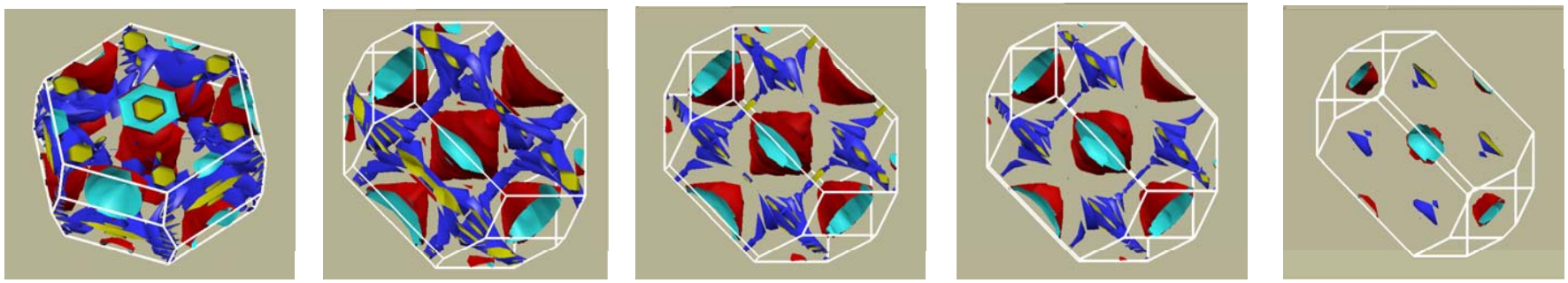
Rocksalt CuO - a = 3.905 Å, PP = Cu.pz-3d9_4s2-rrkjus.UPF




Rocksalt - a = 3.905 Å, PP = Cu.pz-3d9_4s2-rrkjus.UPF
N(Ef) vs c/a & U(eV)
States/(Cell*eV)
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
0.90
1.00
1.10
1.20
1.30
1.40
1.50
1.60
c/a
0
1
2
3
4
5
6

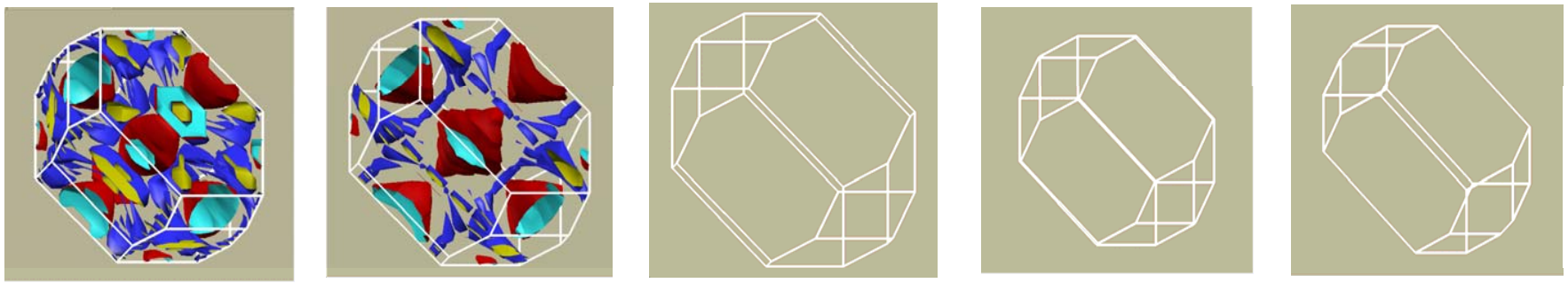
Af-CuO: FS Spin Up

U = 0



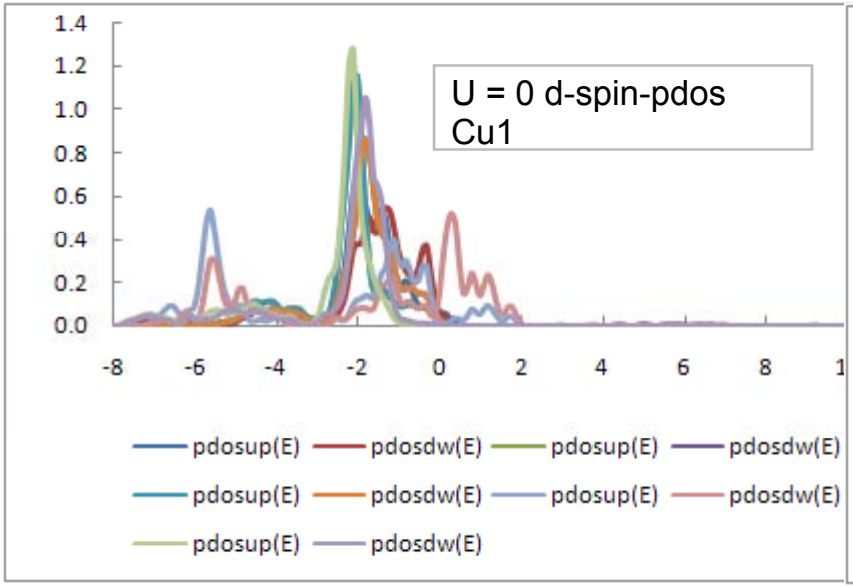
c/a

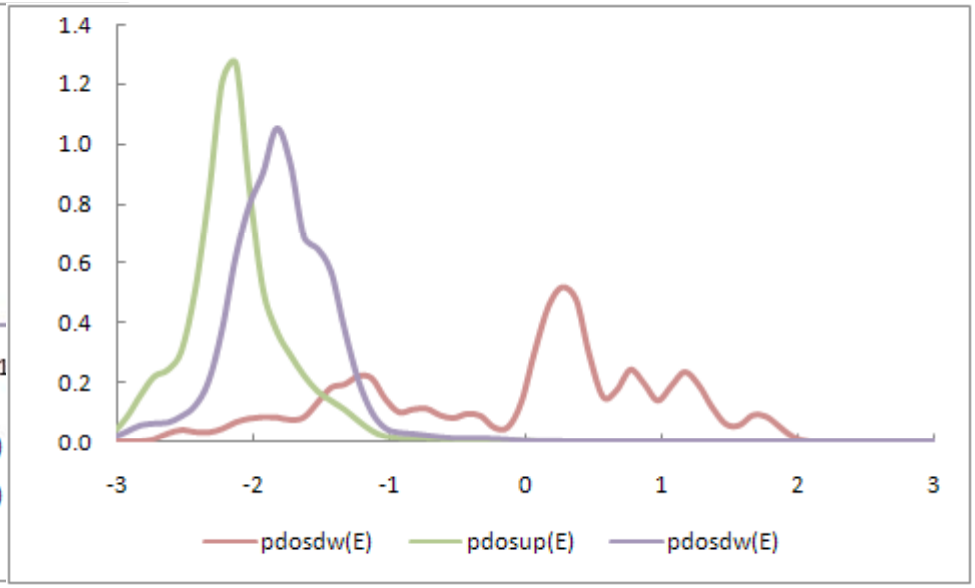
1.0 1.1 1.115 1.2 1.36

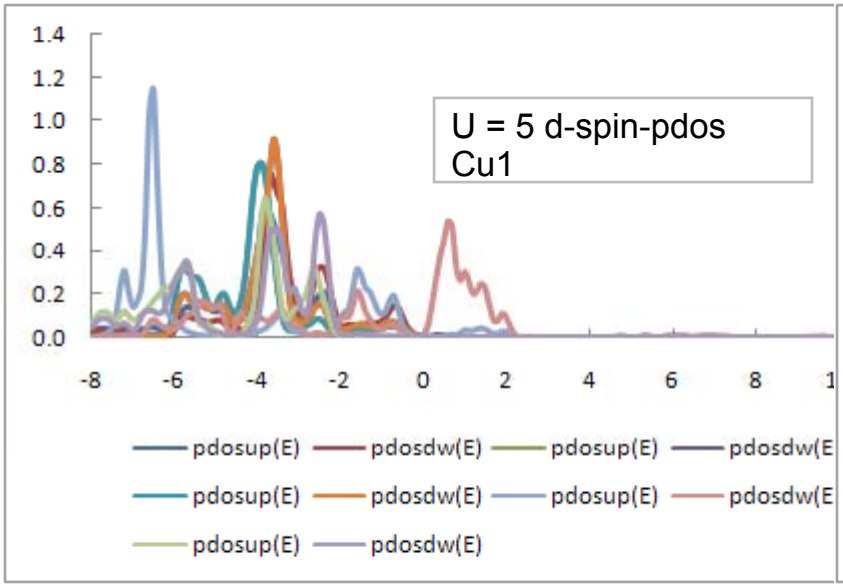


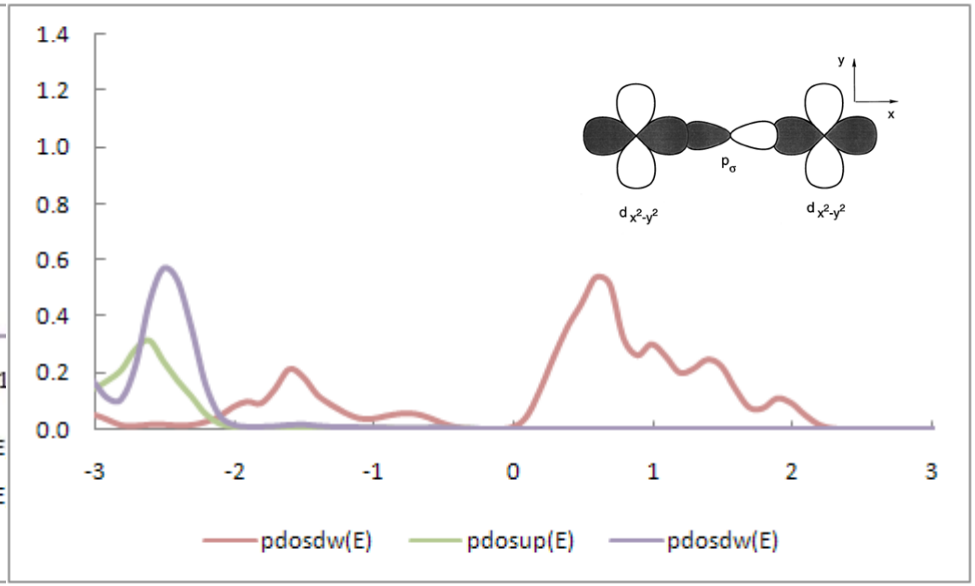
U = 6

Spin Composition of Cu 3d pDOS as fn(Hubbard): c/a = 1.36

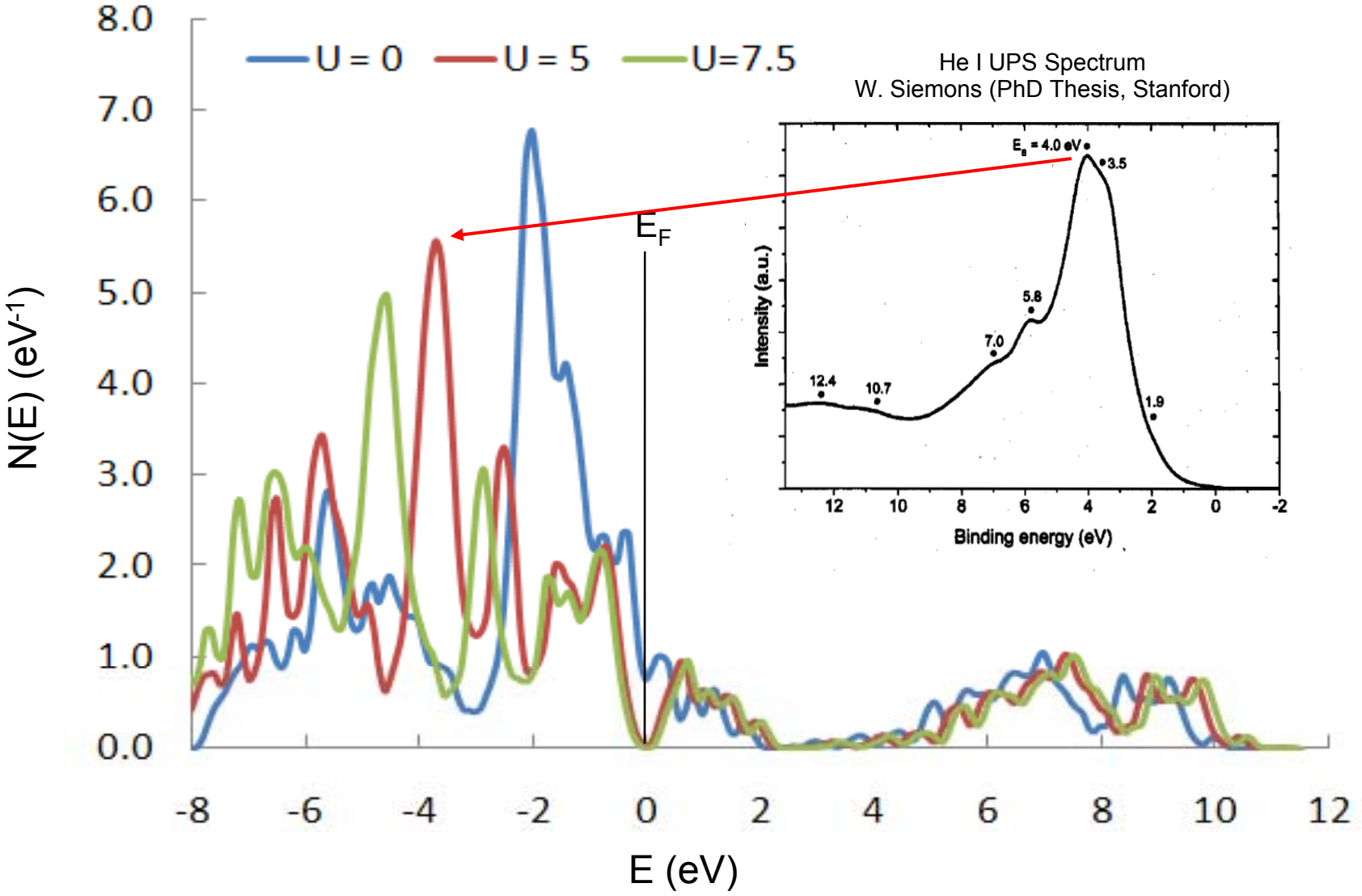


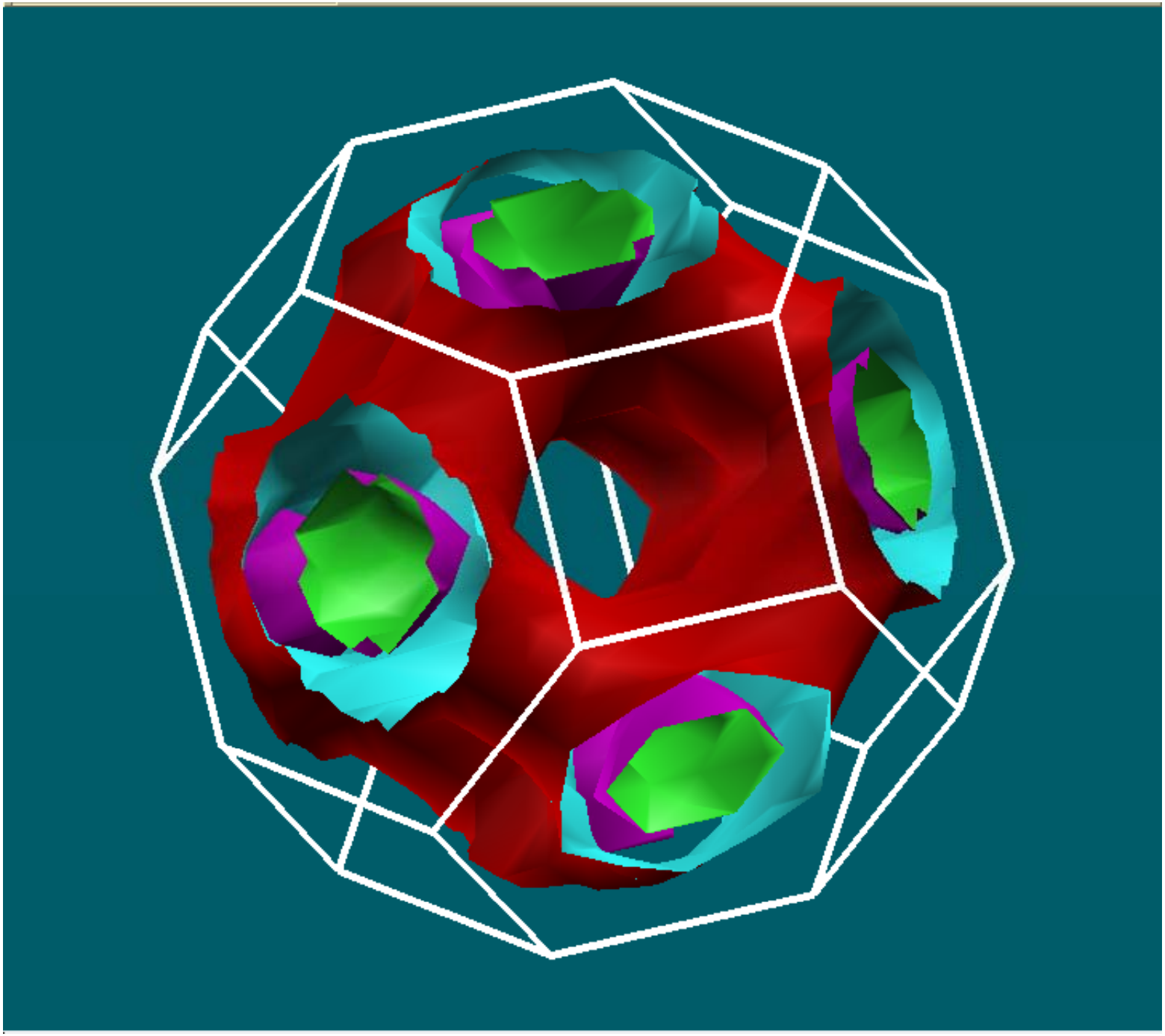




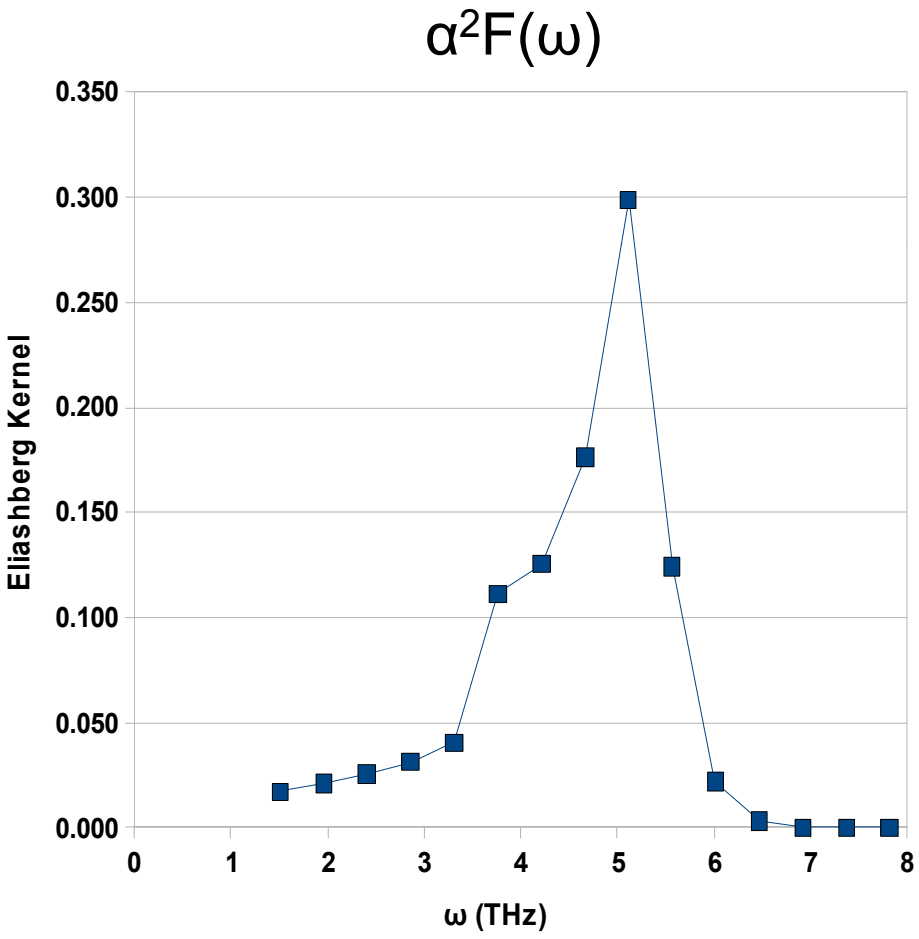


t-CuO Density-of-States





Non-Magnetic Cubic Rocksalt CuO
-- Electron-Phonon Properties --



σ = 0.04

- λ ~ 0.6 – 0.7
- Other sc's…

$$T_C = a\Theta e^{-\frac{1}{\lambda-\mu^*}} \qquad \lambda k\Theta \square \; E_F$$

	T_C (K)	λ	μ*
K_3C_{60}	16.3	0.51	-
Rb_3C_{60}	30.5	0.61	-
Cs_3C_{60}	47.4	0.72	-

Conclusions & Homework

Conclusions

- c-rs-CuO is metallic and thus a proxy for HTSC cuprates.
- e-p $\lambda \sim 0.6 – 0.7$ consistent with $T_C \sim 20 – 50$ K.
- t-rs-CuO becomes a MH-CTI for c/a >~ 1.3.
- c/a < 1.3, t-rs-CuO is “self-doped” metal.
- DFT (LDA+U) + proxy structures a useful exploratory tool for nano-material discovery.

Homework

- Compute e-p coupling λ as f(c/a,U) for t-rs-CuO.
- Compute T_N, μ^*, BCS prefactor, then T_C .
- Compute isotope shift.
- Calculate optical & transport properties as f(c/a).
- Investigate larger values of a-lattice constant
- PAW instead of USPP

DFT & (LDA + U)

$$E_{\mathrm{LDA+U}}\left[n(\mathbf{r})\right] = E_{\mathrm{LDA}}\left[n(\mathbf{r})\right] + E_{\mathrm{HUB}}\left[\left\{n_m^{l\sigma}\right\}\right] - E_{\mathrm{DC}}\left[\left\{n^{l\sigma}\right\}\right]$$

- Implemented in LMTO by Anisimov, et al, JPCM 2, 3973 (1990)
  - Applied to NiO, MnO, FeO, CoO and La_2CuO_4
- Plane-Wave Pseudopotential Implementation by Cococcioni and de Gironcoli, PRB 71, 035105 (2005)
  - Applied to FeO and NiO
  - Download open-source package from http://www.pwscf.org

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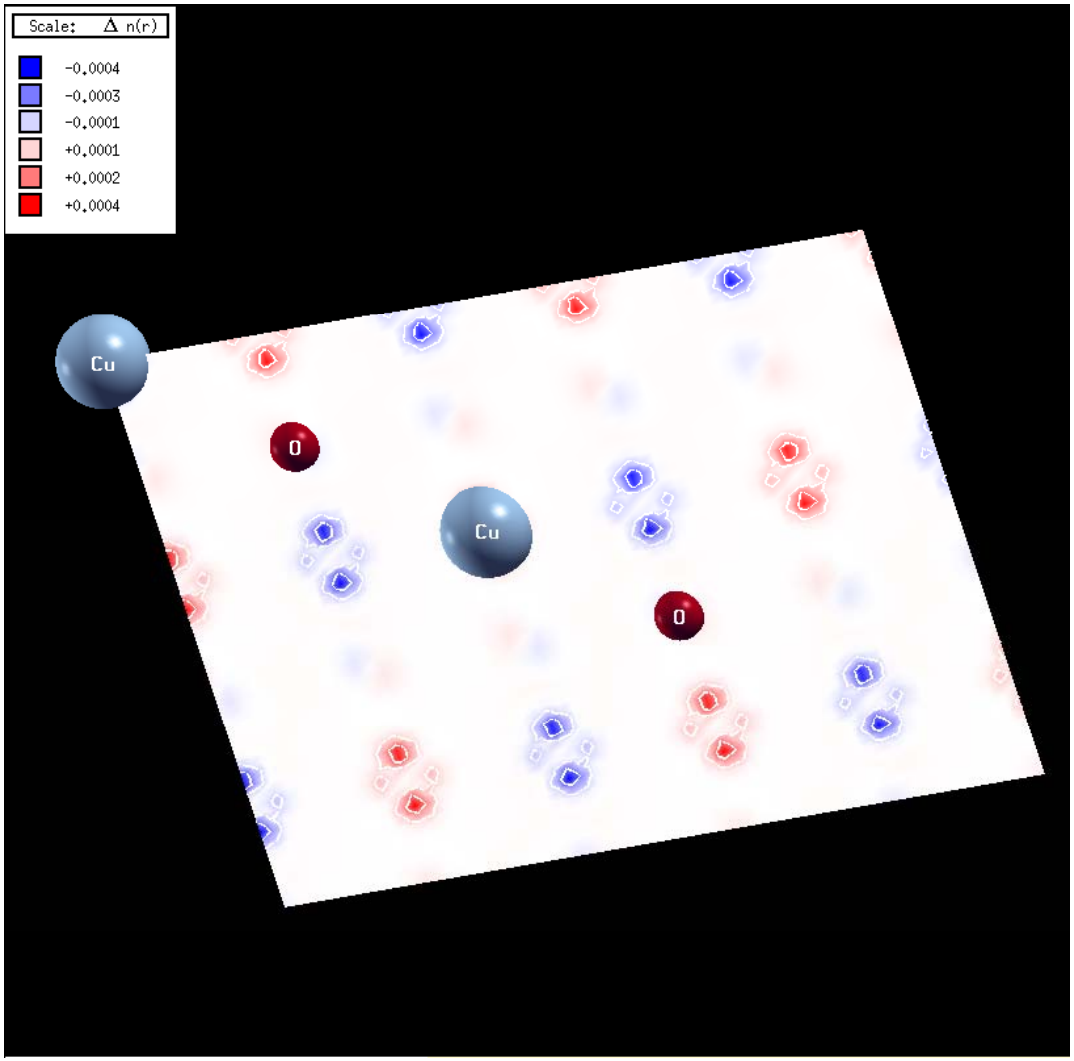

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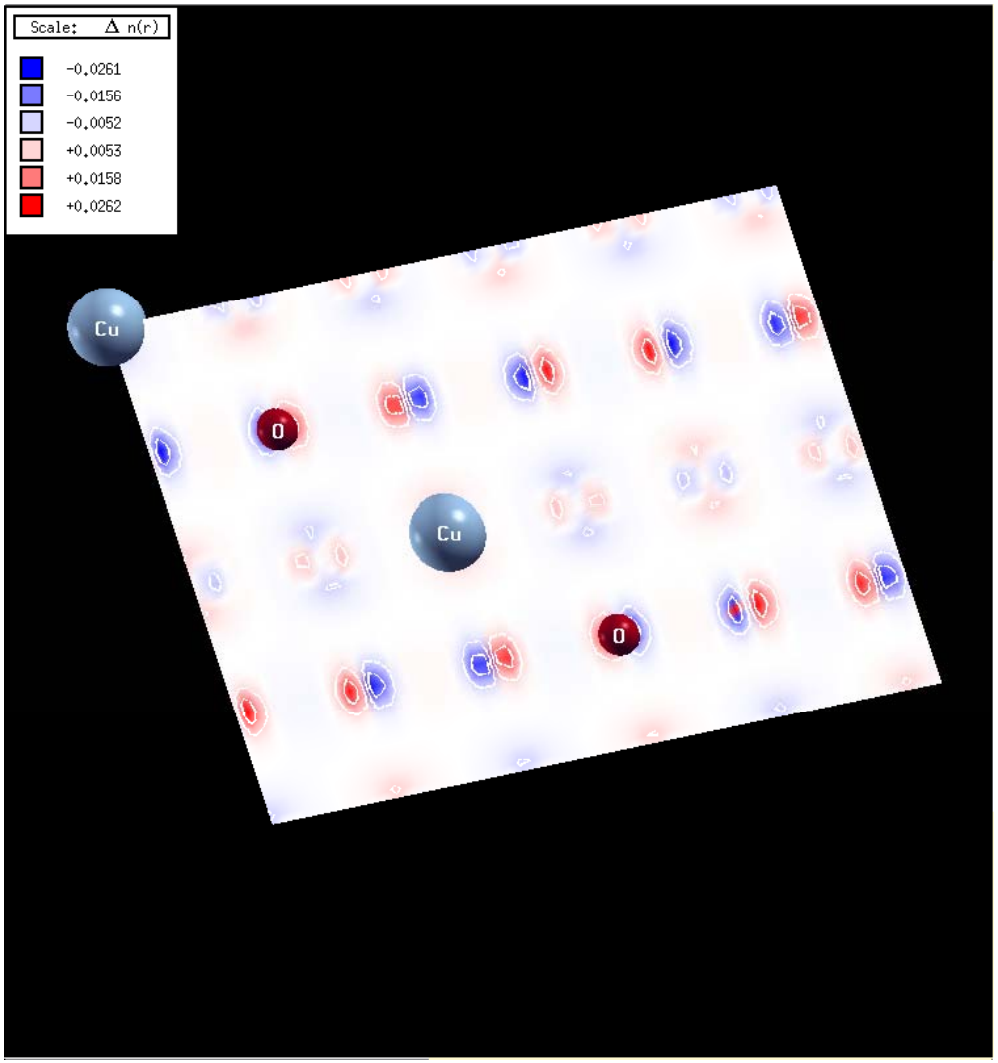

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