

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

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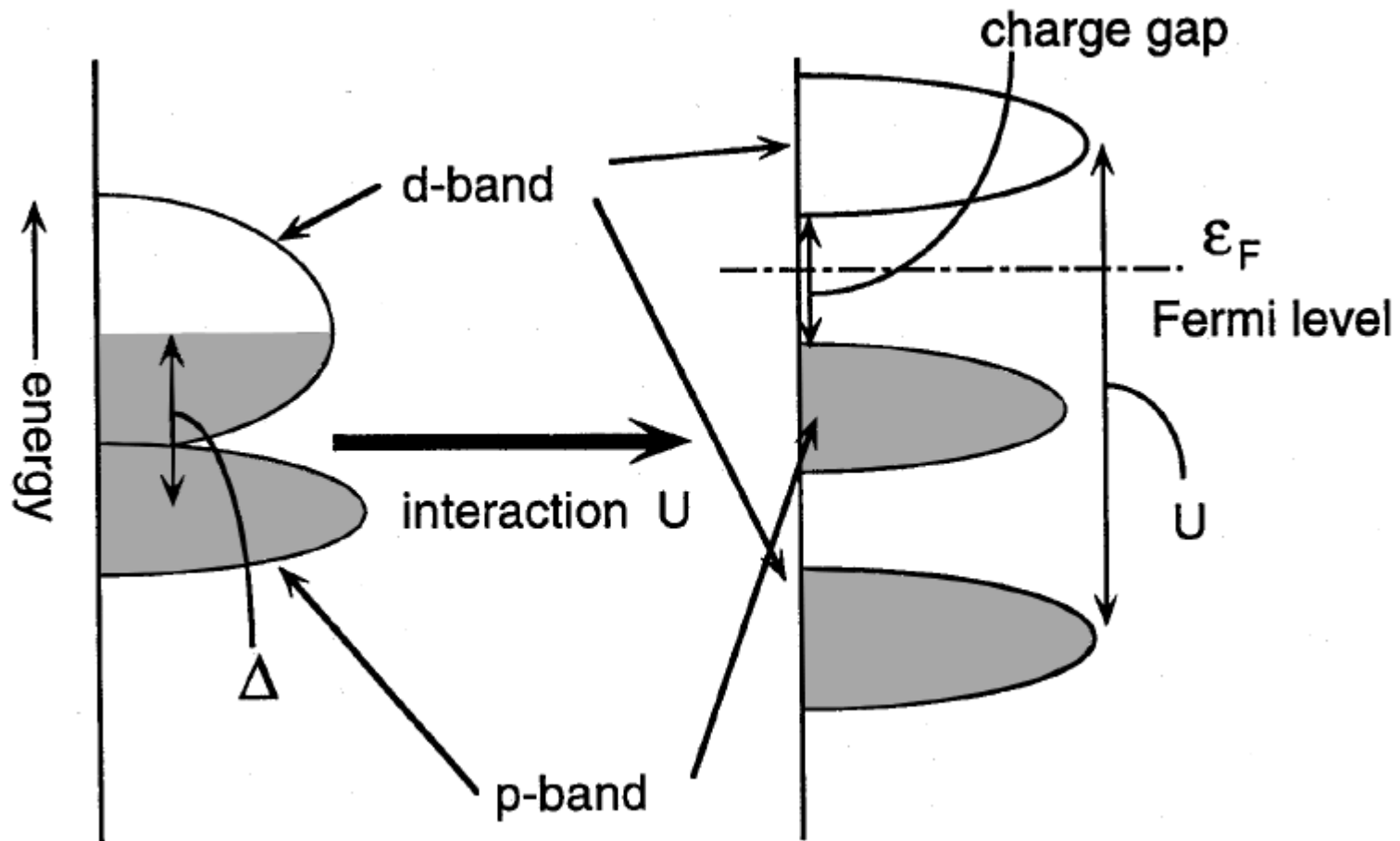
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Abstract. Cubic rocksalt copper monoxide, in contrast to its lighter transition metal neighbours, does not exist in nature nor has it yet been successfully synthesized. Nonetheless, its numerical study as a structurally simpler proxy for the layered cuprate perovskites may prove useful in probing the source of high temperature superconductivity in the latter family of compounds. We report plane-wave pseudopotential DFT (LDA+U) results for both cubic and tetragonal CuO and find rather surprisingly a metallic band structure persists for $0 < U < 6$ eV, and $c/a = 1$ with a Mott-Hubbard gap opening only for finite U under a tetragonal distortion, e.g., above $c/a = 1.1$ for $U = 6$. The metallic states display a Fermi surface with clear nesting tendencies suggesting that high temperature superconductivity in copper oxide compounds may be at least initially mediated by Jahn-Teller electron-phonon coupling as originally proposed by Bednorz and Mueller.

Transition Metal Oxides

“Should be Metals, But Aren’t”
(Charge Transfer Insulators, Instead)



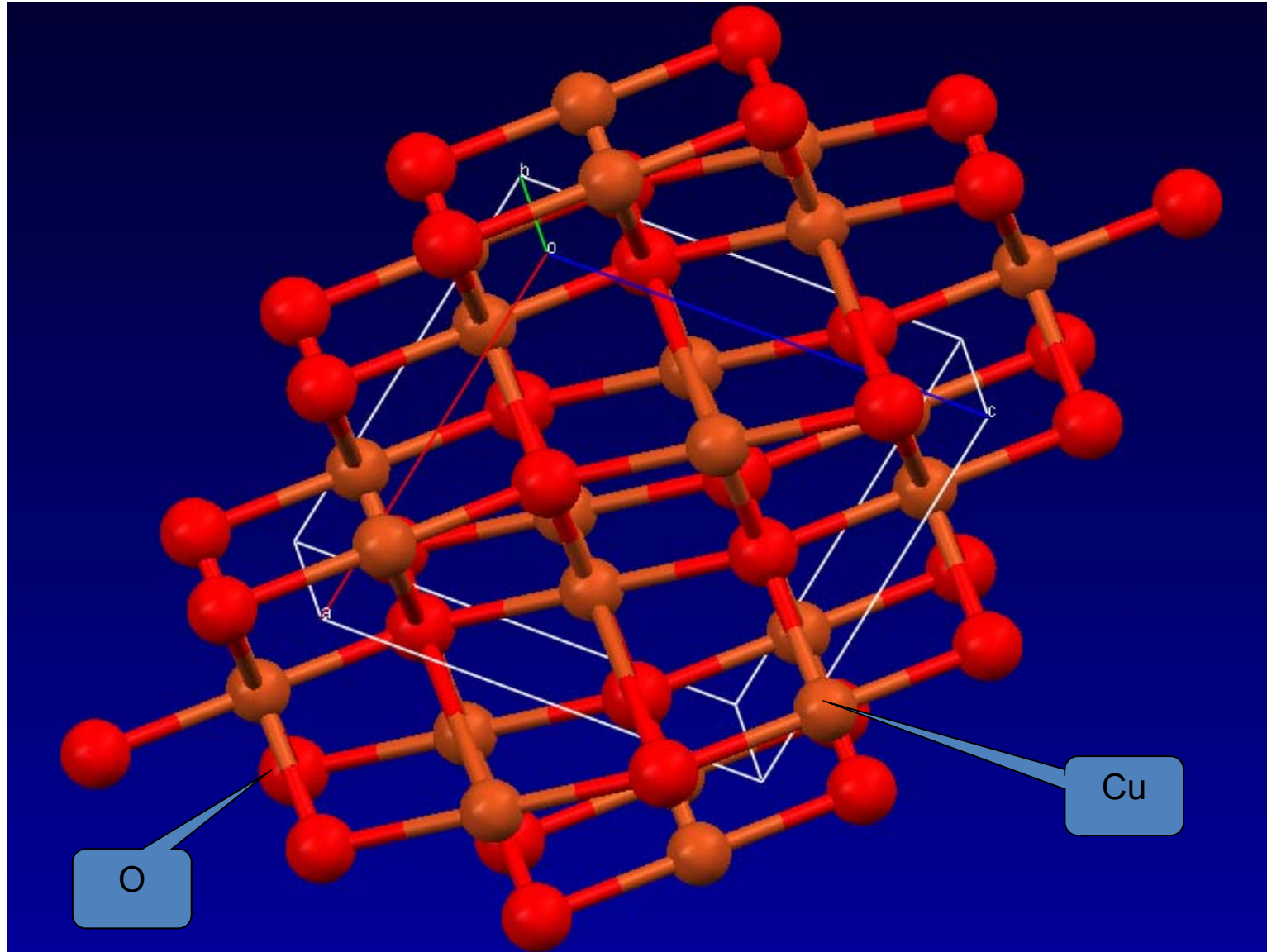
After Imada, et al, RMP 70, 1039 (1998)

Cubic Rocksalt Divalent TMOs

<u>TMO</u>	<u>3d Config</u>	<u>Properties</u>
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	<i>XX Doesn't Exist!</i>

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

Tenorite (Monoclinic CuO)



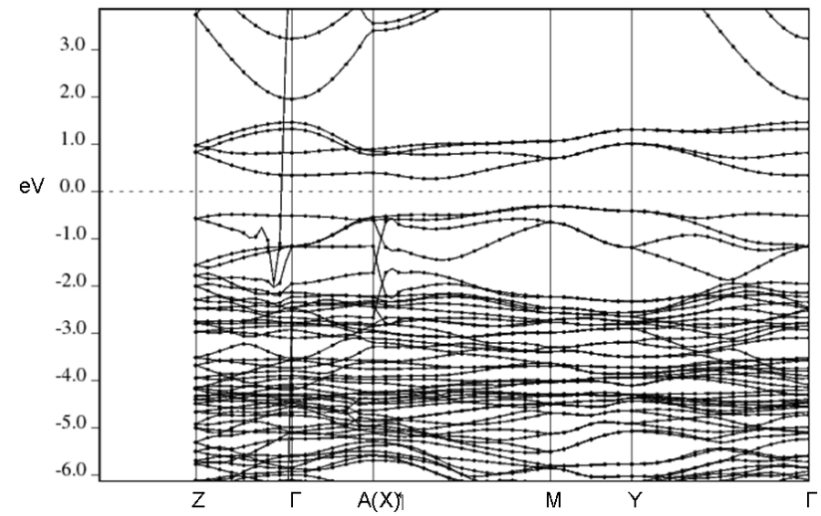
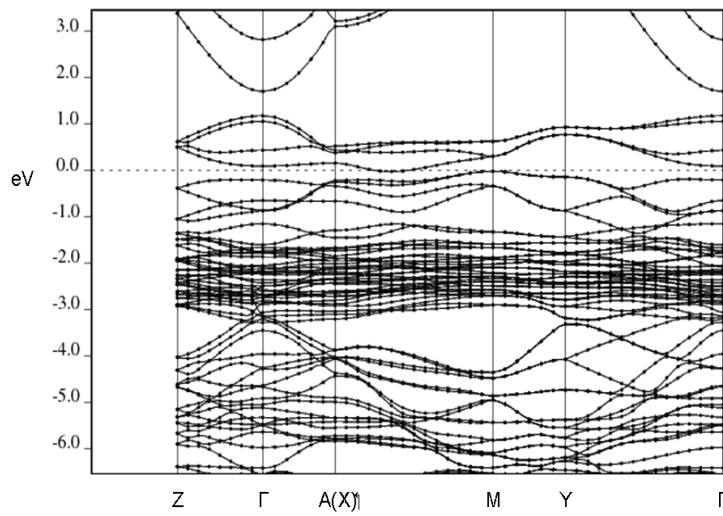
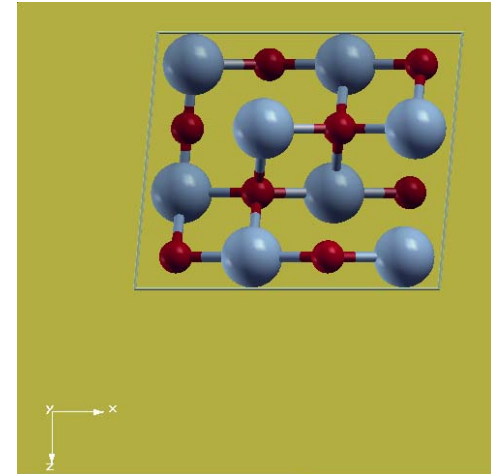
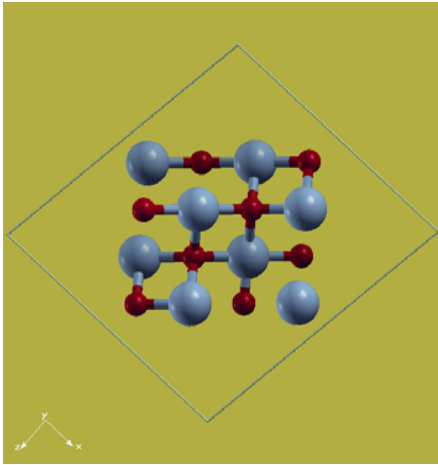
Experimental Equipment (Software)

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

Tenorite “Test”

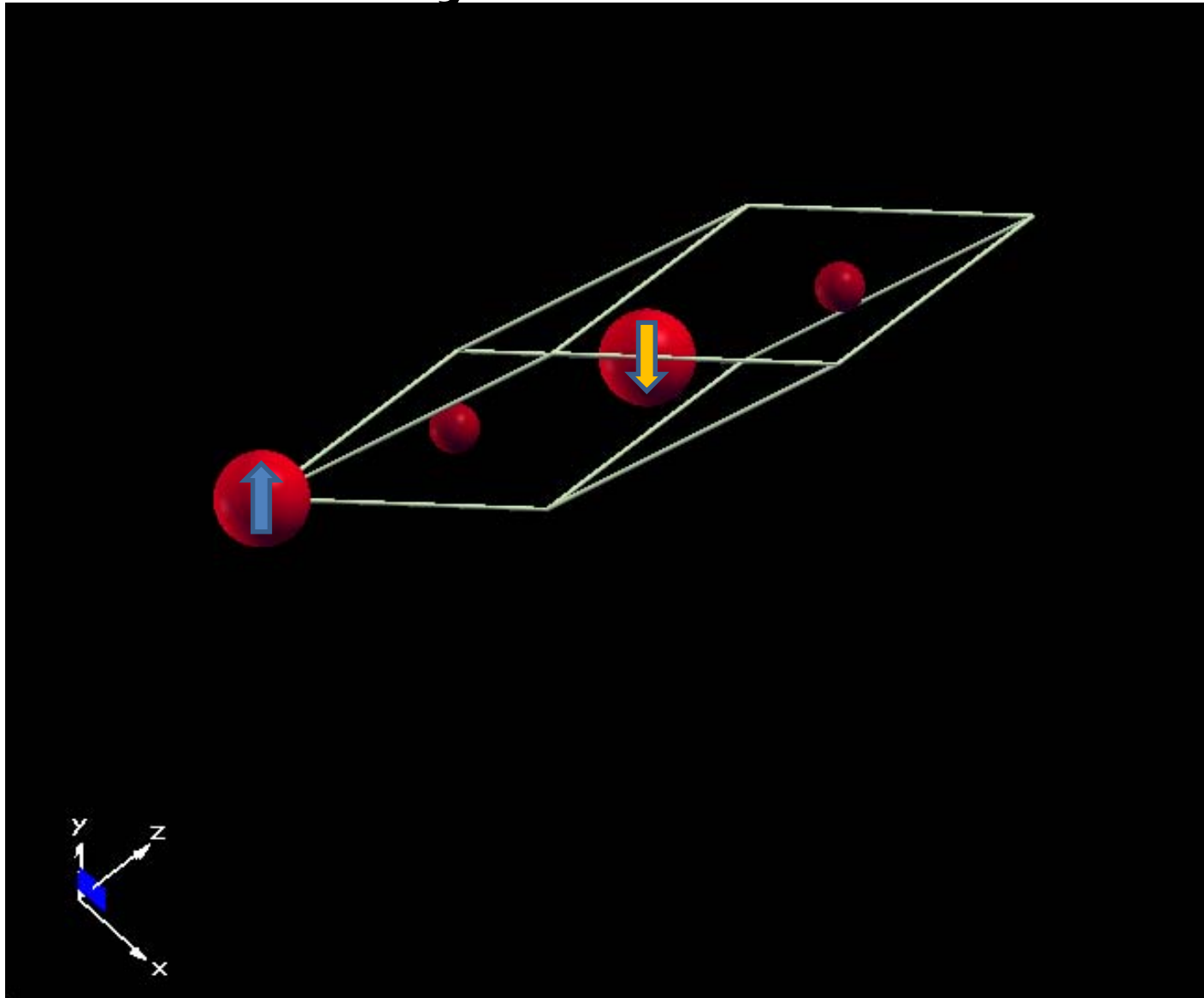
Chemical: $U=0$

AF: $U=6$



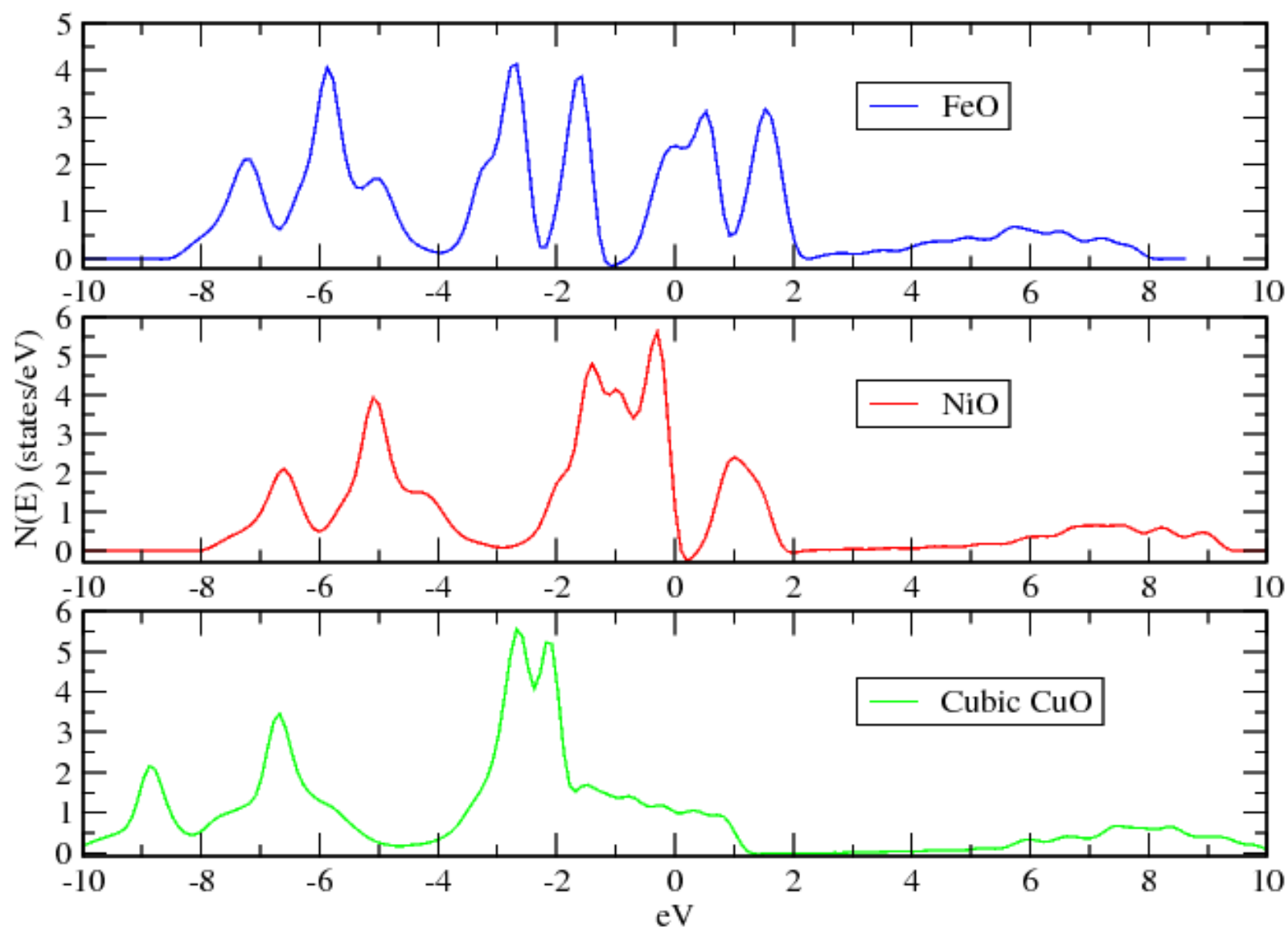
c-rs-CuO

Basic Asymmetric AF Cell



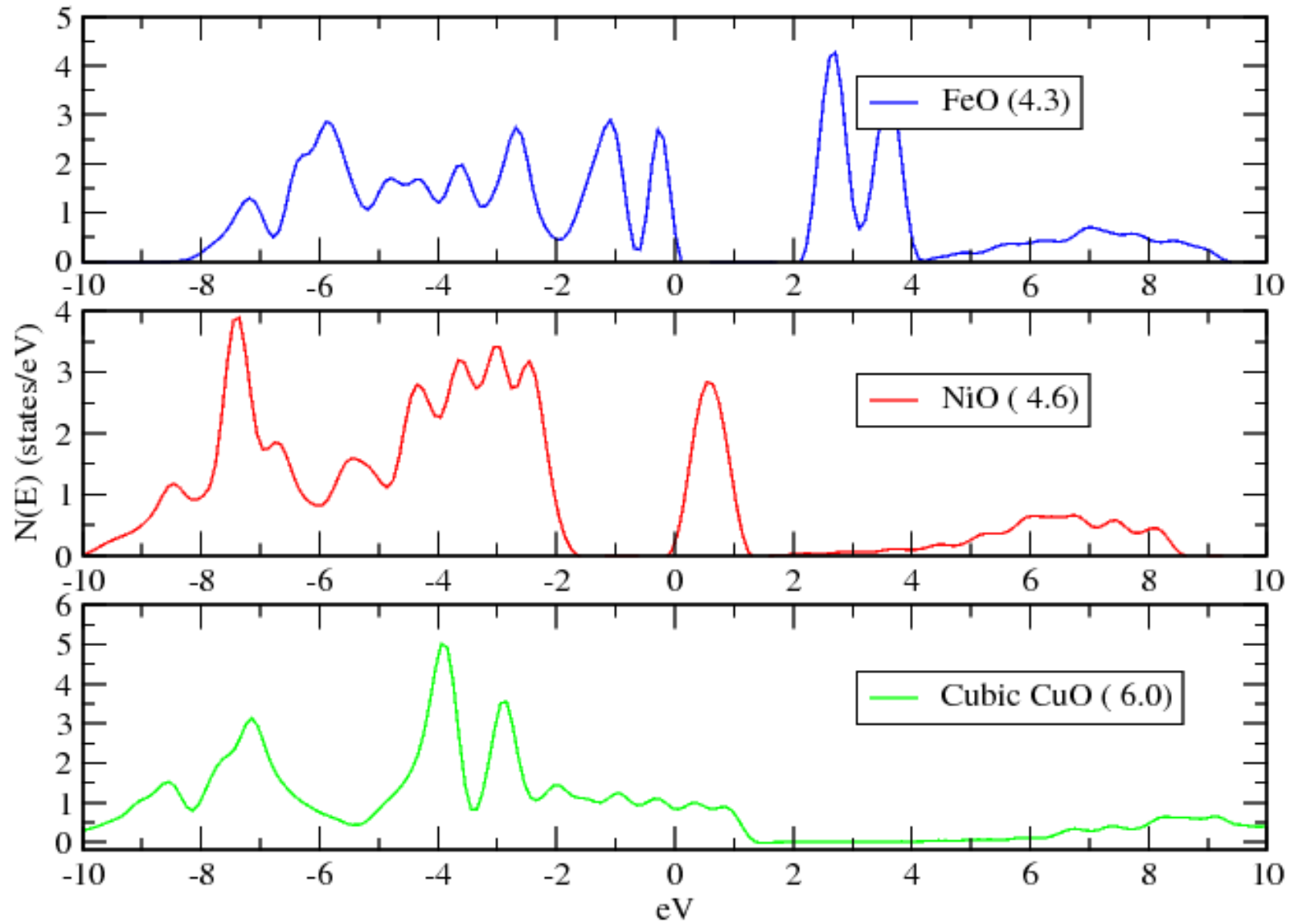
TMO_dos Plot

$U = 0$



TMO_dos Plot

$U > 0$



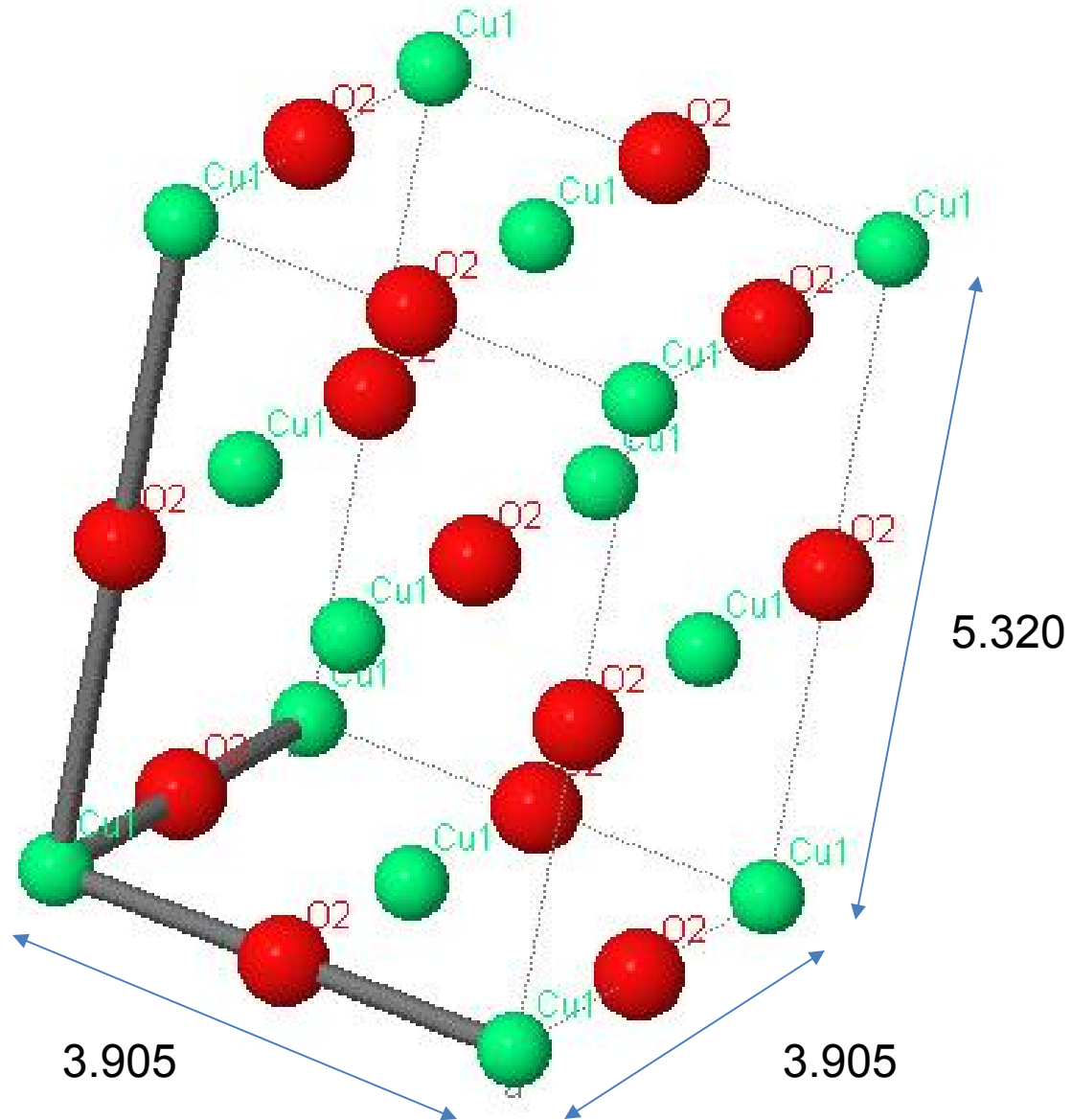
Tetragonal rs-CuO

Fm-3m
a=3.905Å
b=3.905Å
c=5.320Å
 $\alpha=90.0^\circ$
 $\beta=90.0^\circ$
 $\gamma=90.0^\circ$

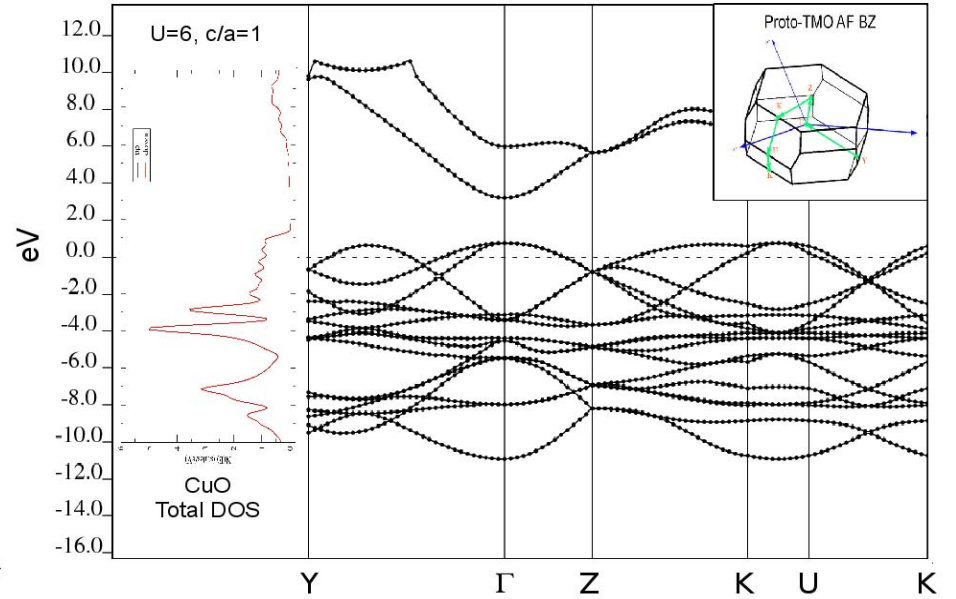
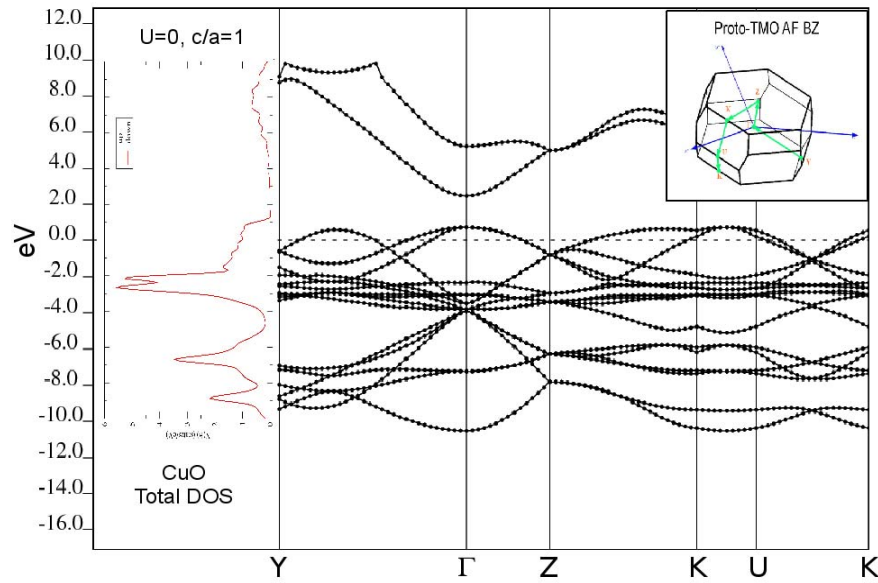
$$c/a = 1.36$$

Measurements (Wolter Siemons)

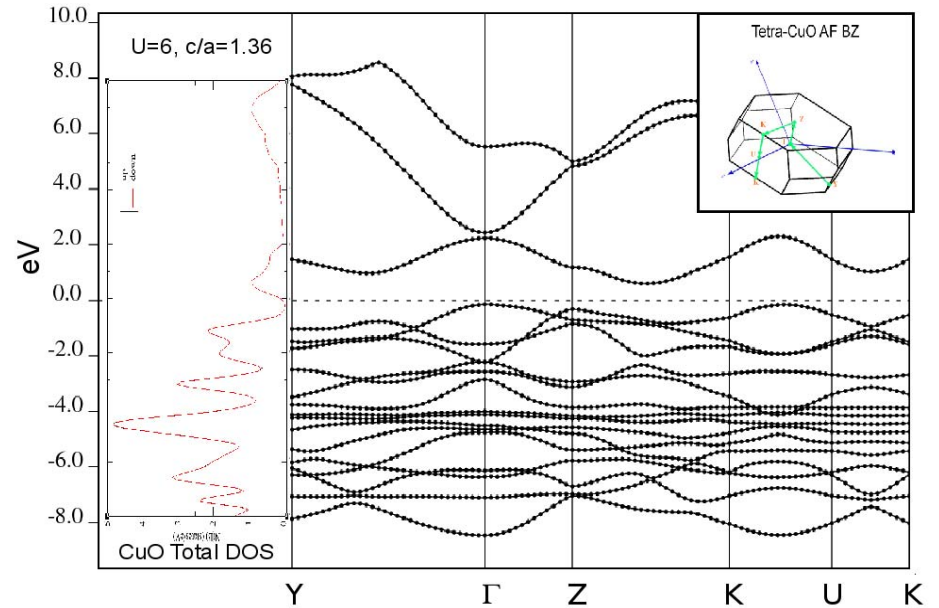
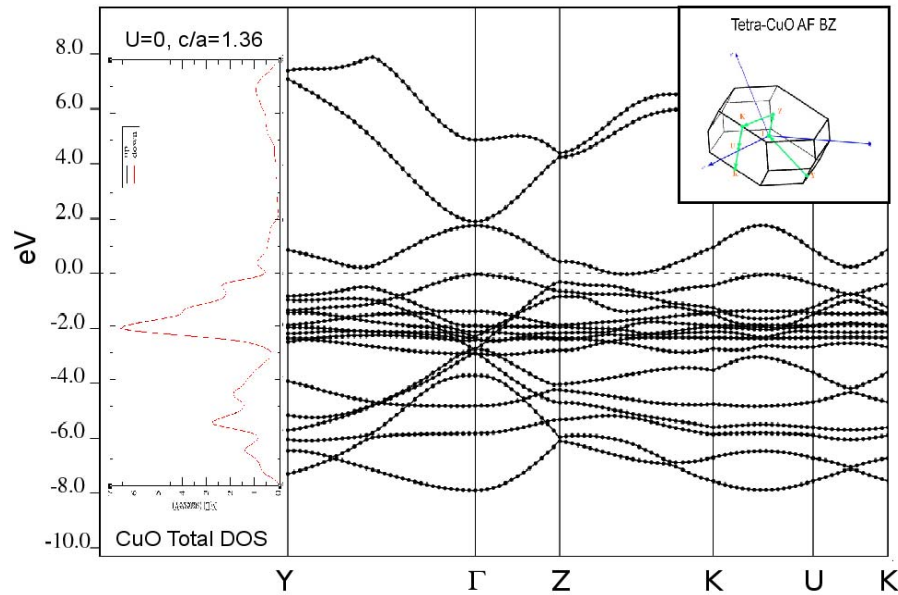
- 2-4 ML epi on STO
- No Fermi Edge
- No Exchange Bias on ferro-SRO (Tc ~ 100-150 K)



Cubic

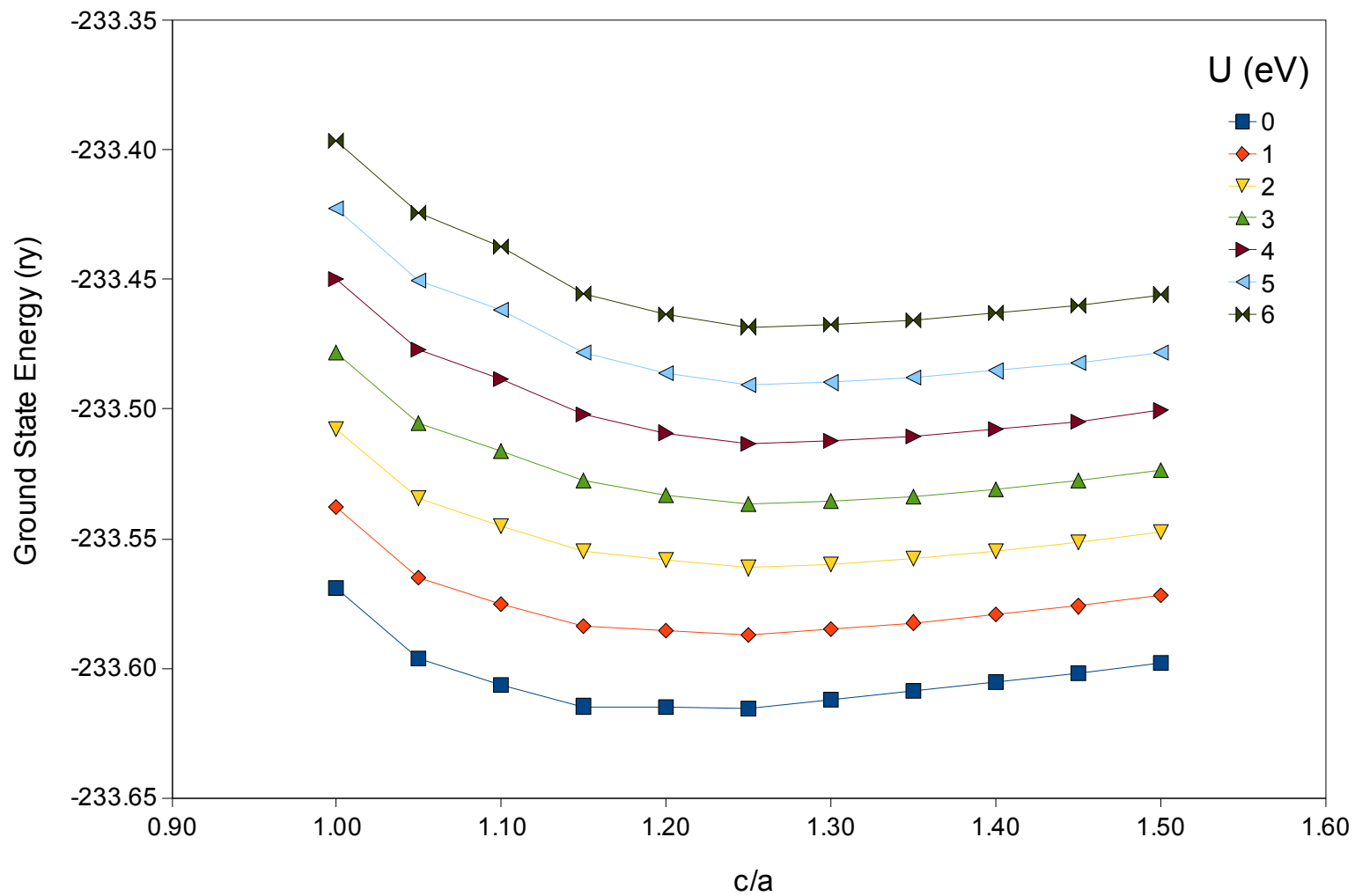


Tetragonal



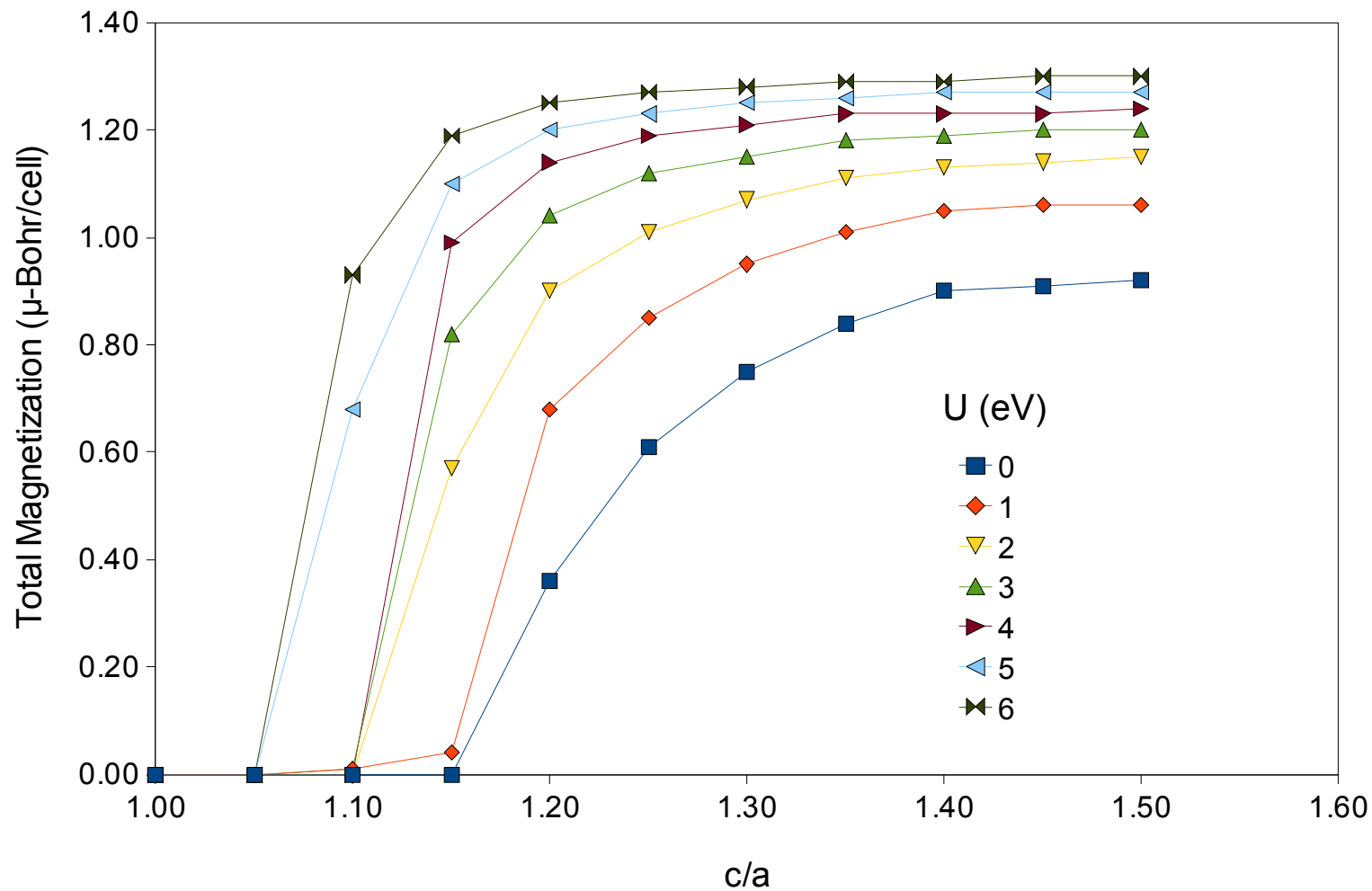
Rocksalt CuO - $a = 3.905$ Angstroms, PP = Cu.pz-3d9_4s2-rrkjus.UPF

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

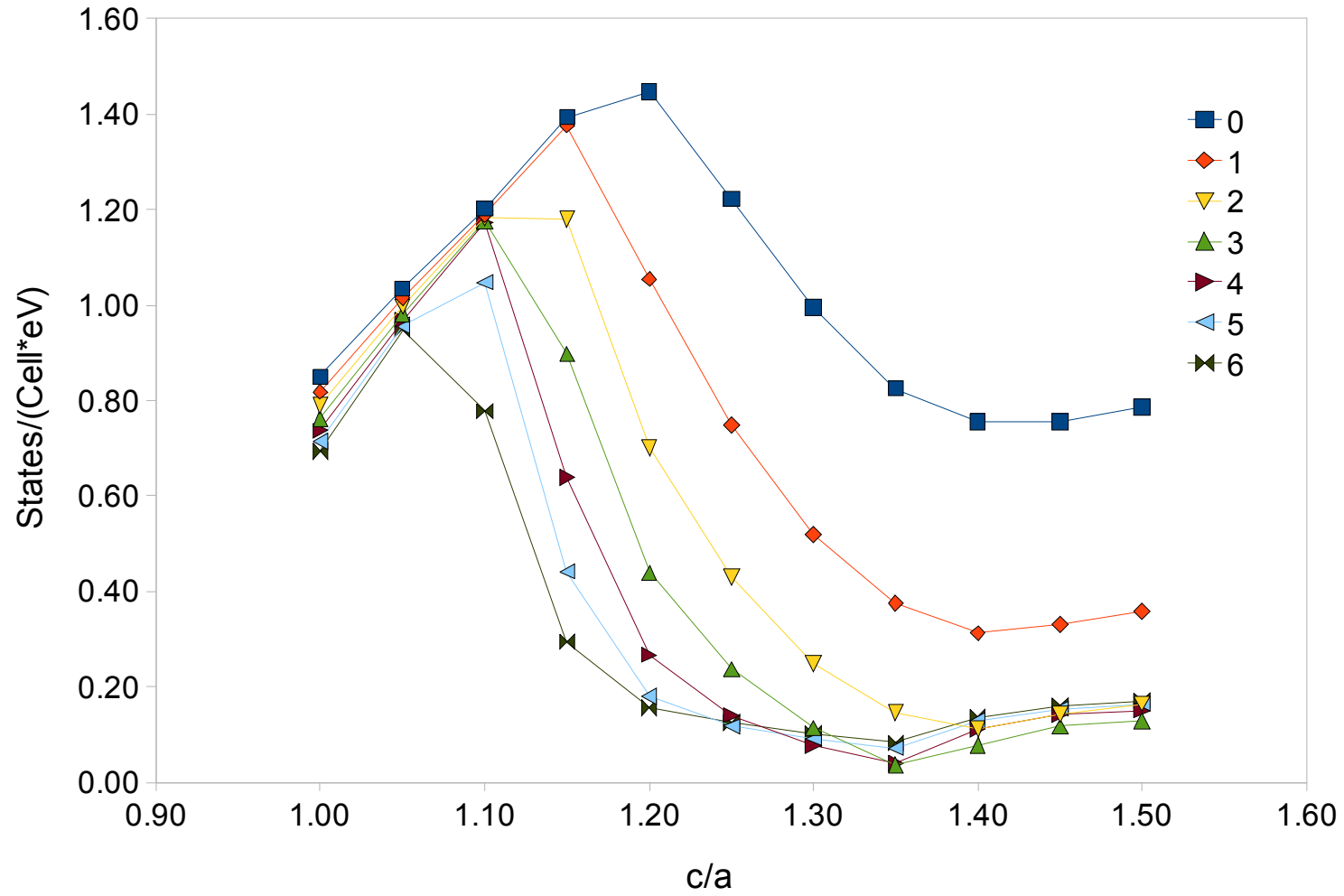


Rocksalt CuO - $a = 3.905 \text{ \AA}$, PP = Cu.pz-3d9_4s2-rrkjus.UPF

Total Magnetization vs c/a & $U(\text{eV})$

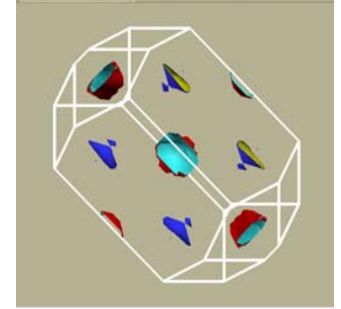
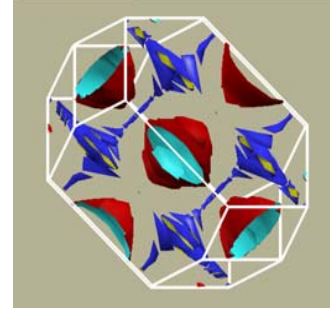
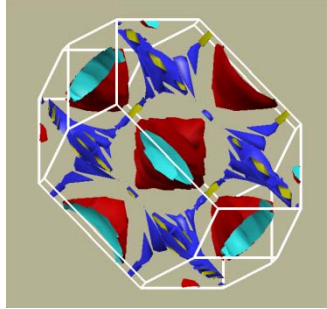
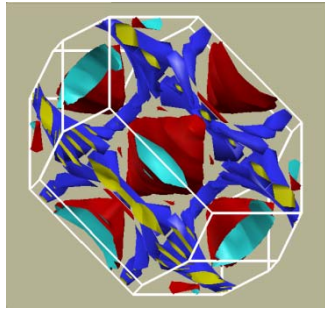
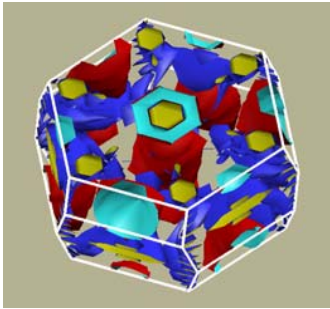


Rocksalt - a = 3.905 Å, PP = Cu.pz-3d9_4s2-rrkjus.UPF
N(E_f) vs c/a & U(eV)



AF-rs-CuO: FS Spin Up

U = 0



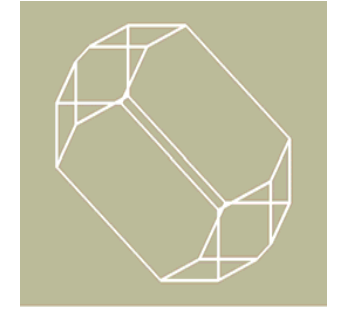
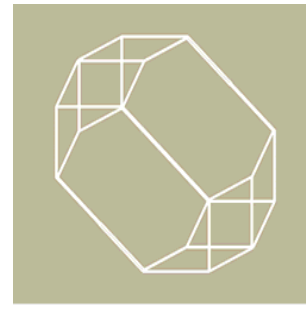
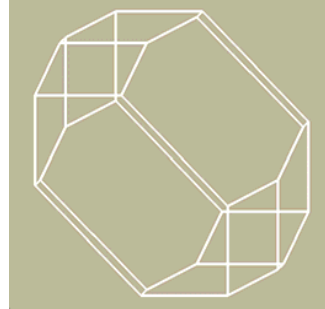
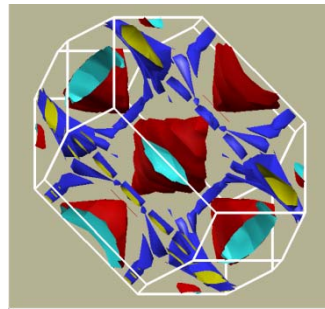
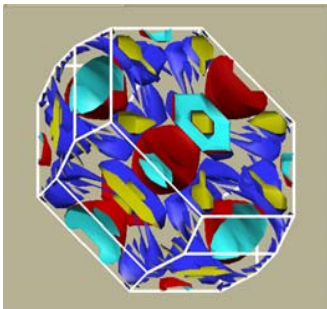
1.0

1.1

c/a
1.115

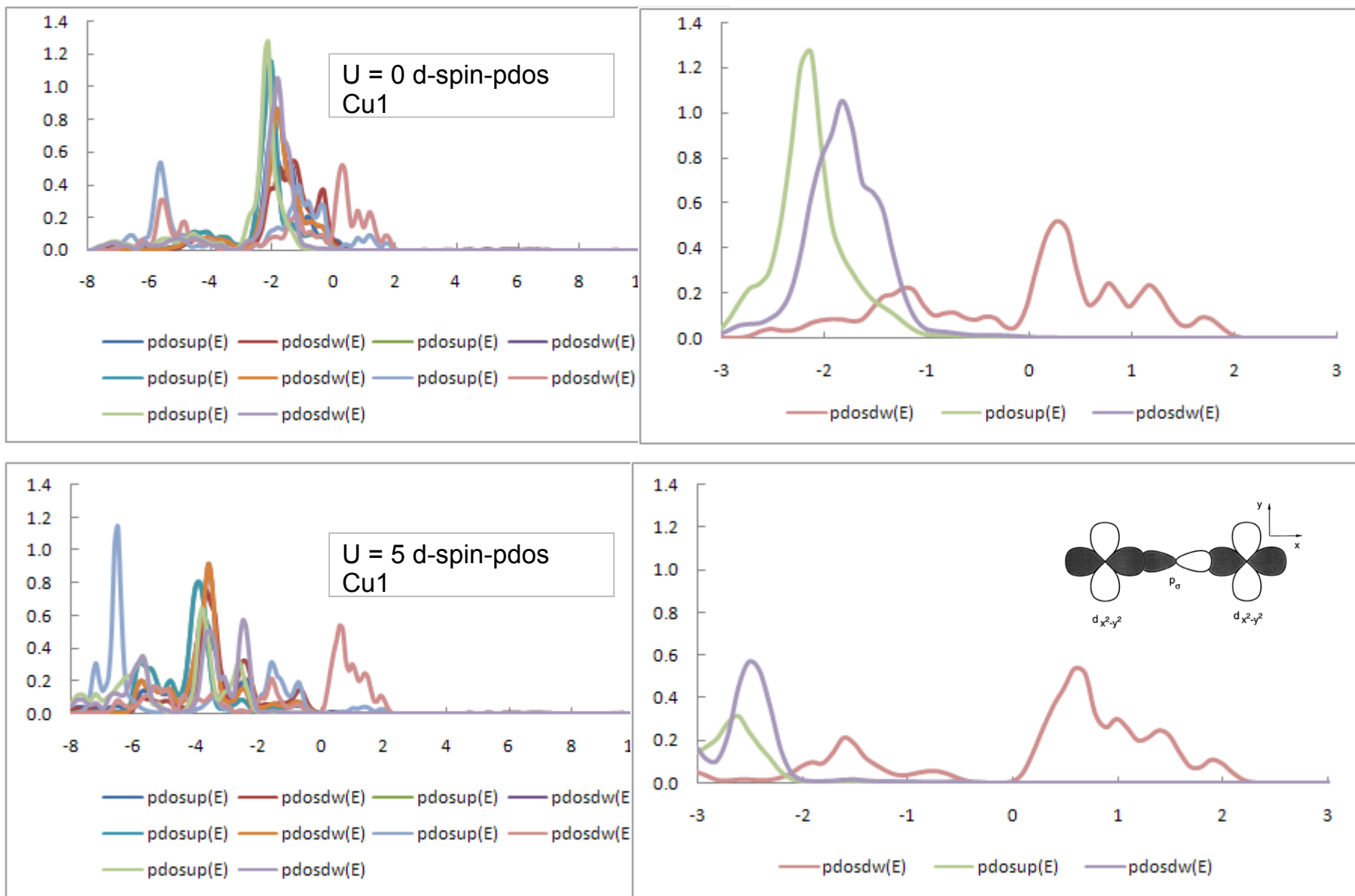
1.2

1.36

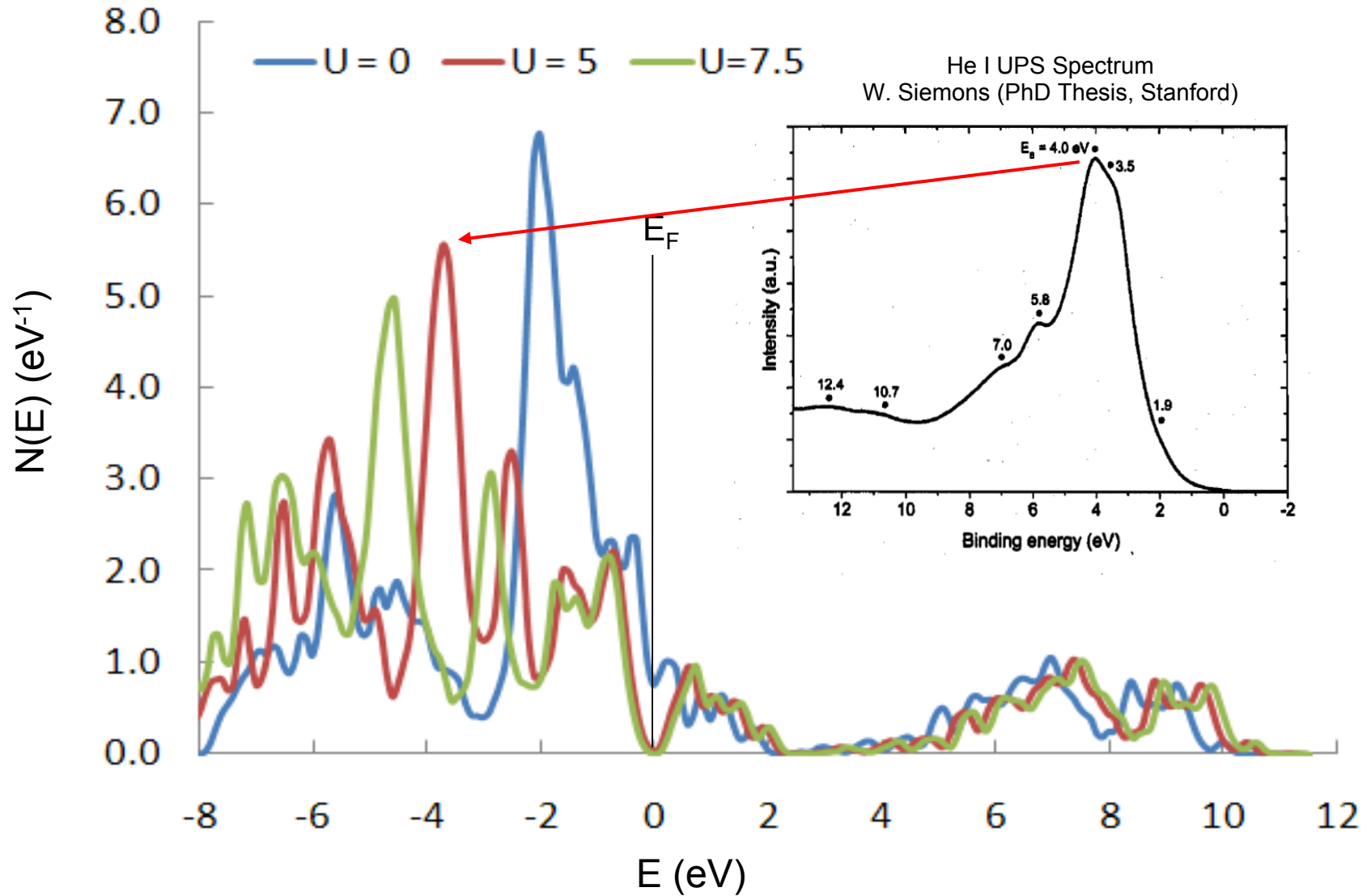


U = 6

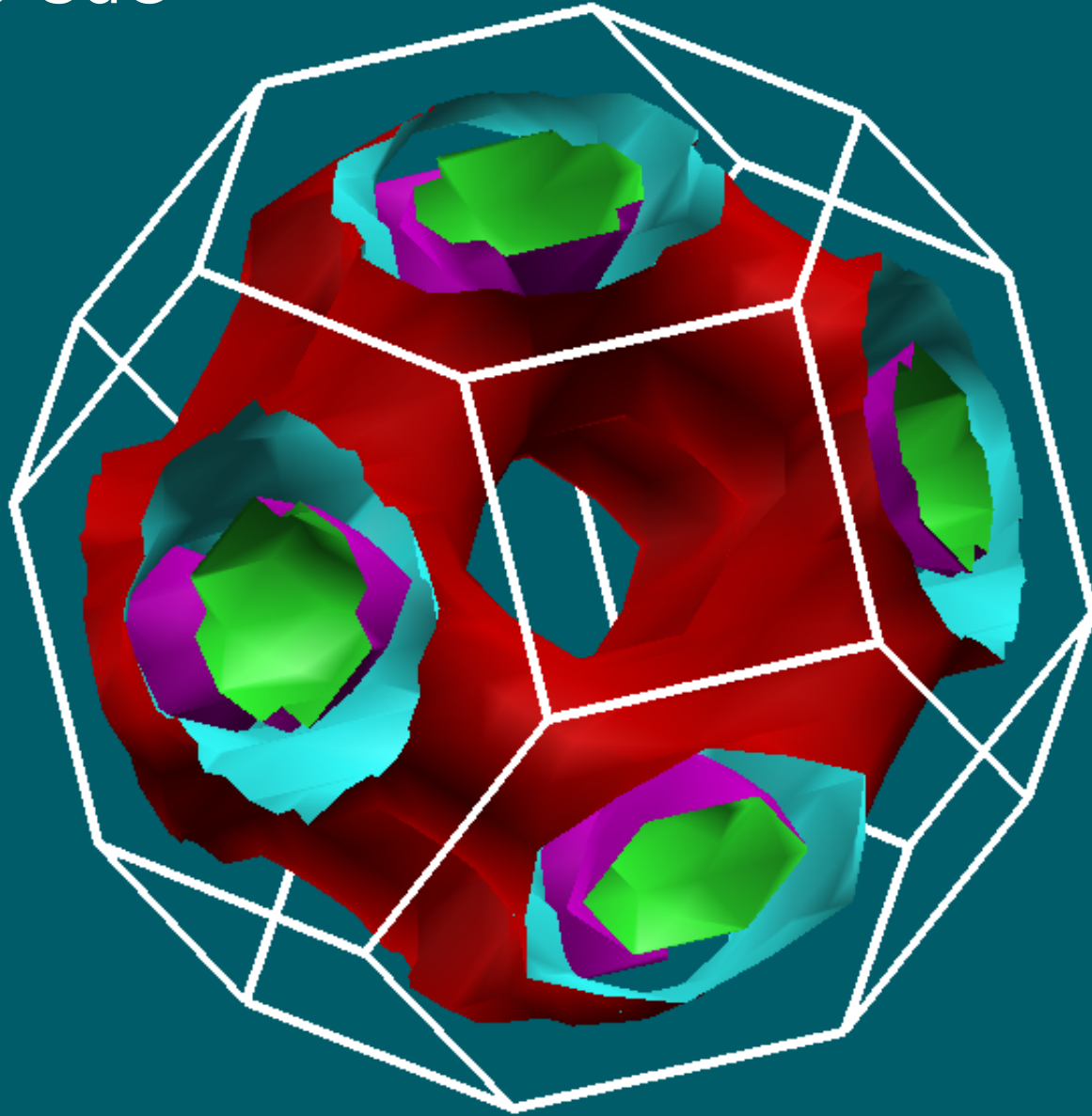
Spin Composition of Cu 3d pDOS as fn(Hubbard): $c/a = 1.36$



t-CuO Density-of-States

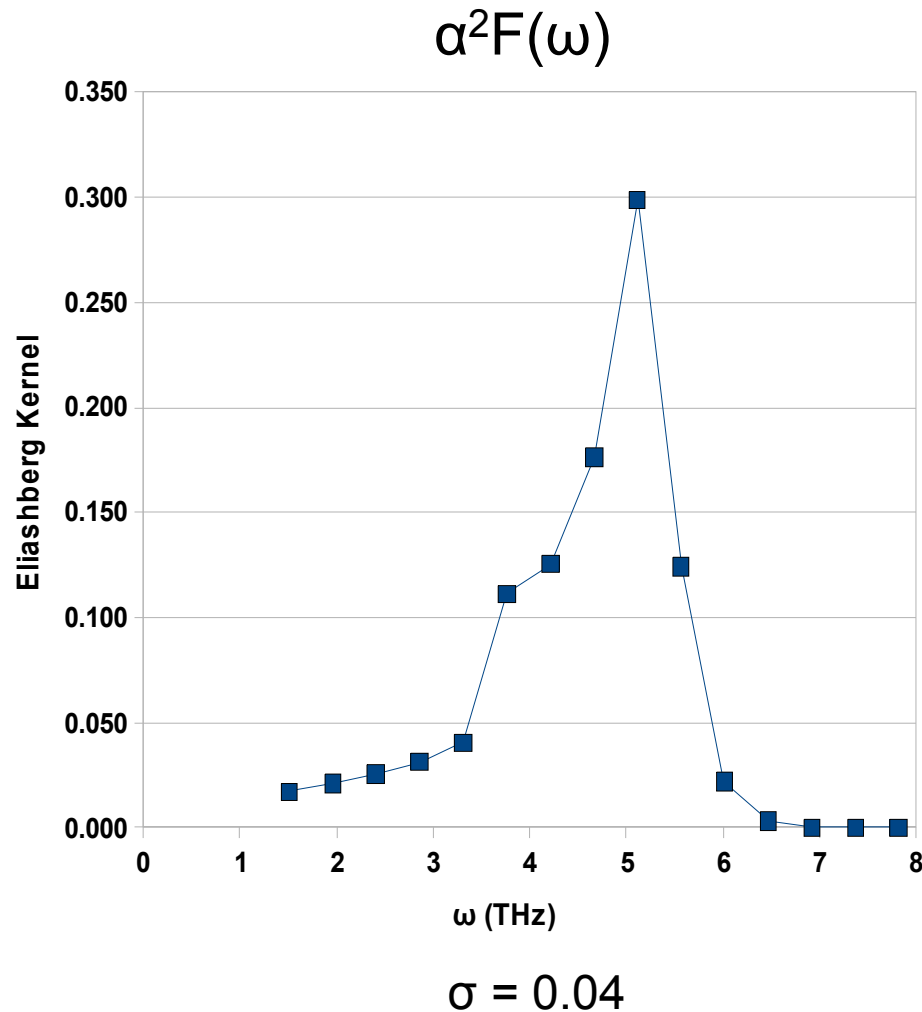


c-rs-CuO



Non-Magnetic Cubic Rocksalt CuO

-- Electron-Phonon Properties --



- $\lambda \sim 0.6 - 0.7$
- Other sc's...

$$T_C = a\Theta e^{-\frac{1}{\lambda - \mu^*}} \quad \lambda k\Theta \ll E_F$$

	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 $c/a > \sim 1.1$, $U > 3$ eV.
- $c/a < 1.1$, 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