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

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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)

### Cubic Rocksalt Divalent TMOs

<table>
<thead>
<tr>
<th>TMO</th>
<th>3d Config</th>
<th>Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>MnO</td>
<td>5</td>
<td>MH-CTI (5.6)</td>
</tr>
<tr>
<td>FeO</td>
<td>6</td>
<td>MH-CTI (5.9)</td>
</tr>
<tr>
<td>CoO</td>
<td>7</td>
<td>MH-CTI (6.3)</td>
</tr>
<tr>
<td>NiO</td>
<td>8</td>
<td>MH-CTI (6.5)</td>
</tr>
<tr>
<td>CuO</td>
<td>9</td>
<td><strong>XX Doesn't Exist!</strong></td>
</tr>
</tbody>
</table>

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 (XCrystDen)
  – www.quantum-espresso.org

• “Dial-in” Parameters
  – $G^2 = 40$ Ry  $\rho = 320$ Ry
  – Convergence $\leq 10^{-6}$ Ry
  – “Smearing” = Methfessel-Paxton
  – Psuedopotentials: Ultrasoft, XC = Perdew-Zunger
  Cu: $3d^94s^2$  O: $2s^22p^4$
Tenorite “Test”

Chemical: U=0

AF: U=6
c-rs-CuO
Basic Asymmetric AF Cell
Tetragonal rs-CuO

$c/a = 1.36$

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 \( c/a \) & \( U(\text{ev}) \)
Rocksalt CuO - $a = 3.905 \, \text{Å}$, PP = Cu.pz-3d9_4s2-rrkjus.UPF

Total Magnetization vs $c/a$ & $U$(eV)
Rocksalt - $a = 3.905 \text{ Å}$, PP = Cu.pz-3d9_4s2-rrkjus.UPF

$N(E_f)$ vs $c/a$ & $U(\text{eV})$
AF-rs-CuO: FS Spin Up

\( U = 0 \)

1.0  
1.1  
\( \frac{c}{a} \) 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

He I UPS Spectrum

$E_F$
c-rs-CuO
Non-Magnetic Cubic Rocksalt CuO
-- Electron-Phonon Properties --

\[ \lambda \sim 0.6 - 0.7 \]

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

<table>
<thead>
<tr>
<th></th>
<th>( T_C ) (K)</th>
<th>( \lambda )</th>
<th>( \mu^* )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( K_3C_{60} )</td>
<td>16.3</td>
<td>0.51</td>
<td>-</td>
</tr>
<tr>
<td>( Rb_3C_{60} )</td>
<td>30.5</td>
<td>0.61</td>
<td>-</td>
</tr>
<tr>
<td>( Cs_3C_{60} )</td>
<td>47.4</td>
<td>0.72</td>
<td>-</td>
</tr>
</tbody>
</table>
Conclusions & Homework

Conclusions
- c-rs-CuO is metallic and thus a proxy for HTSC cuprates.
- $e\cdot p\lambda \sim 0.6 - 0.7$ consistent with $T_c \sim 20 - 50$ K.
- t-rs-CuO becomes a MH-CTI for $c/a > 1.1$, $U > 3$ 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 $e\cdot p$ coupling $\lambda$ as $f(c/a, U)$ for t-rs-CuO.
- Compute $T_N$, $\mu^*$, BCS prefactor, then $T_c$.
- Compute isotope shift.
- Calculate optical & transport properties as $f(c/a)$.
- Investigate larger values of a-lattice constant.