Opening…

A DFT (LDA+U) Study of the Electronic Properties of Layered, Square-Planar Coordinated Copper Monoxide Structures

-- Proxies for High Temperature Superconductivity --

Paul M. Grant
IBM Research Staff Member, Emeritus

Aging IBM Pensioner

Financial Support From:
IBM Retiree Pension Fund Prior to 1990

Prelude

The International Conference on Theoretical Physics 'Dubna-Nano2008' IOP Publishing
Journal of Physics: Conference Series **129** (2008) 012042 doi:10.1088/1742-6596/129/1/012042

Electronic properties of rocksalt copper monoxide: A proxy structure for high temperature superconductivity

Paul M. Grant*
W2AGZ Technologies

"**Electronic Properties of Rocksalt Copper Monoxide**,"
APS MAR09-2008-006217, P. M. Grant, Pittsburgh (2009)

PHYSICAL REVIEW B **79**, 195122 (2009)

Tetragonal CuO: End member of the 3*d* transition metal monoxides

Wolter Siemons,[1,2] Gertjan Koster,[1,2,*] Dave H. A. Blank,[1] Robert H. Hammond,[2]
Theodore H. Geballe,[2] and Malcolm R. Beasley[2]

Tools

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

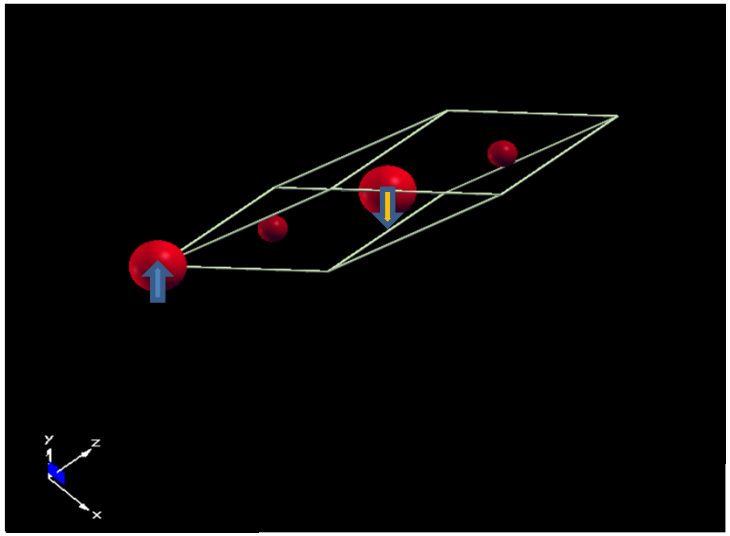
Psuedopotentials: Ultrasoft, XC = Perdew-Zunger

Cu: $3d^9 4s^2$ O: $2s^2 2p^4$

Hardware

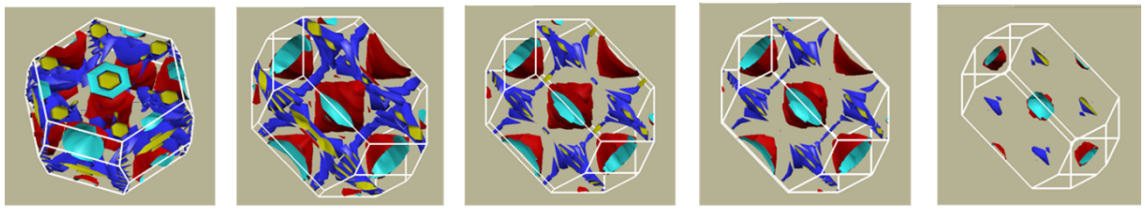
3.33 GHz Intel Core i7 – 12 GB+

Findings



Basic Asymmetric af-CuO Cell

U = 0



Spin Up

c/a

1.0 1.1 1.115 1.2 1.36

U = 6

Are There Phonons w/ High-Tc in YBCO?

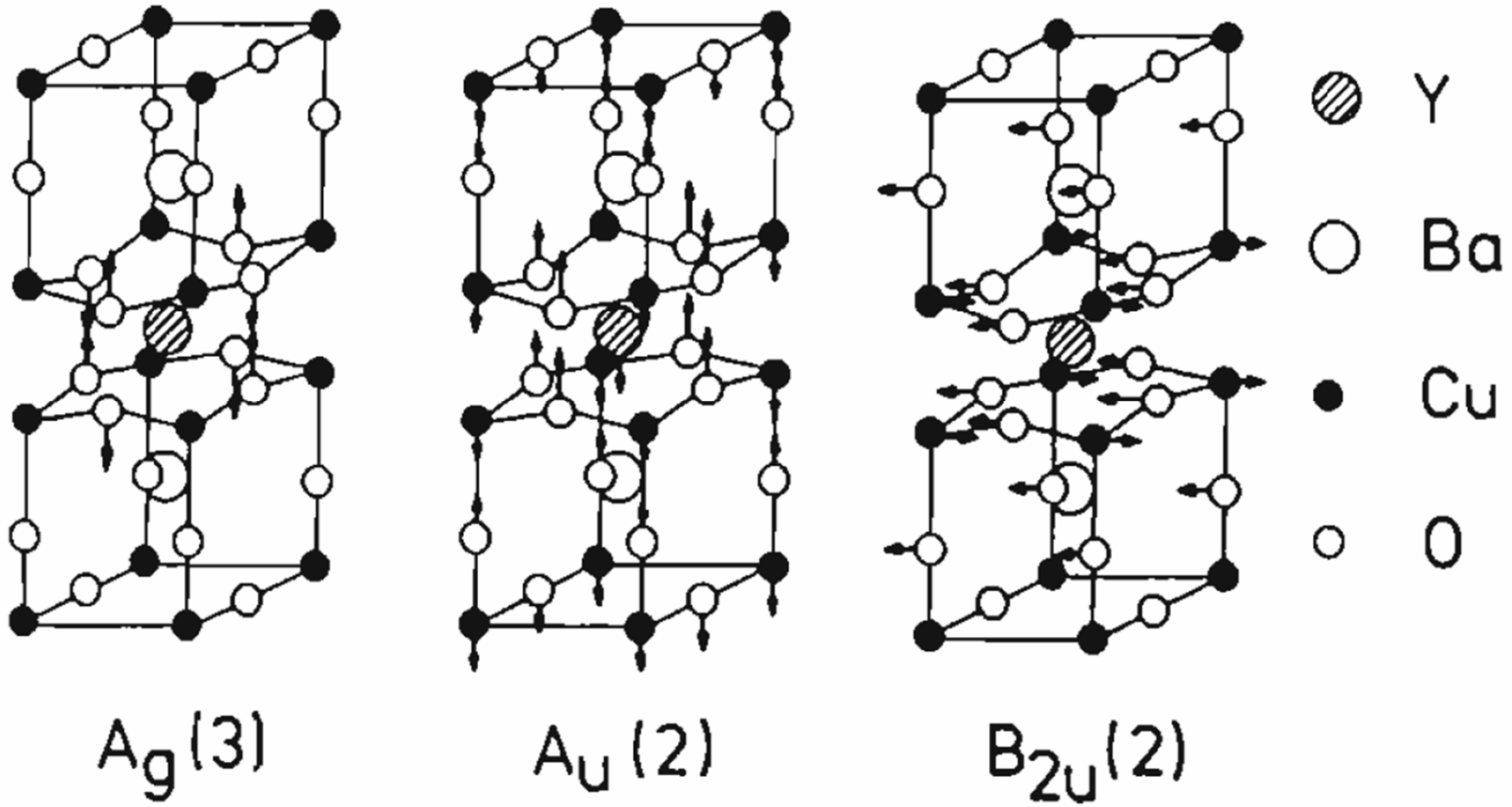
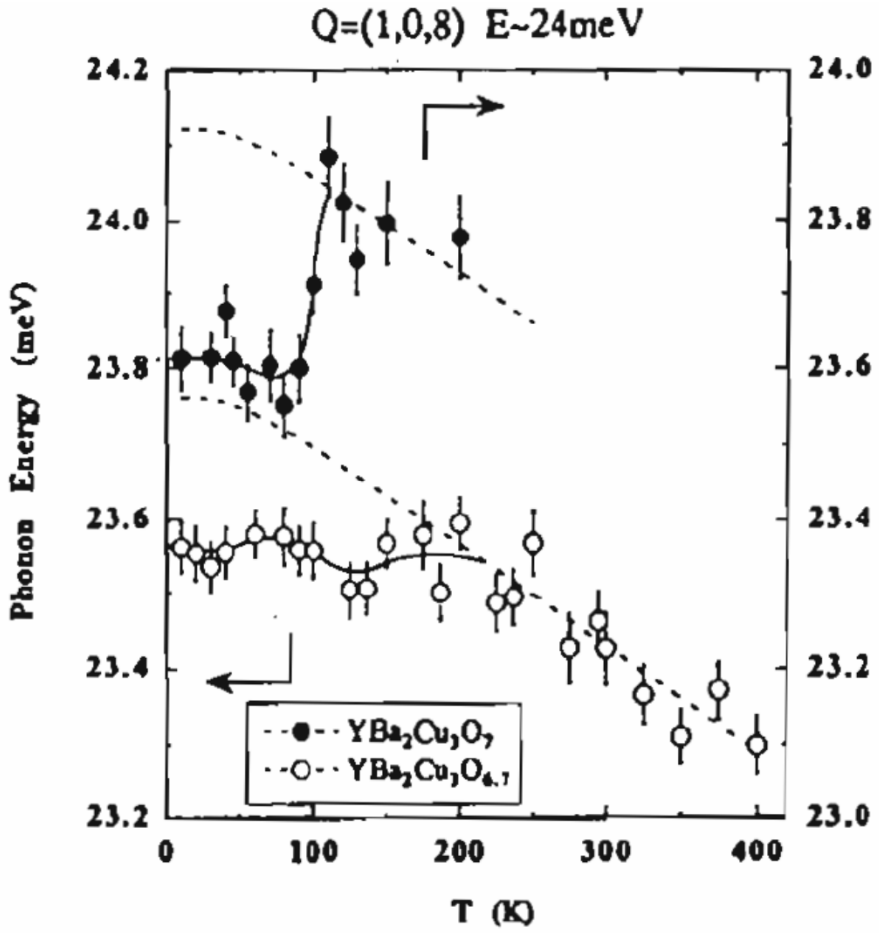
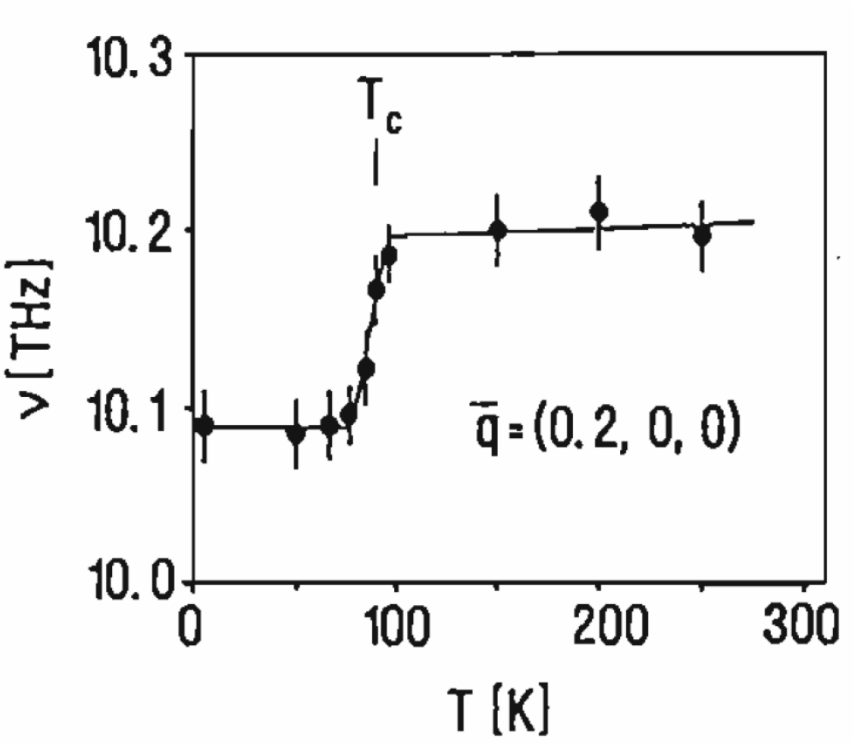


Fig. 38: Pintschovius and Reichardt, in Furrer, ISBN 0-7923-5226-2

Yes -- They're There!



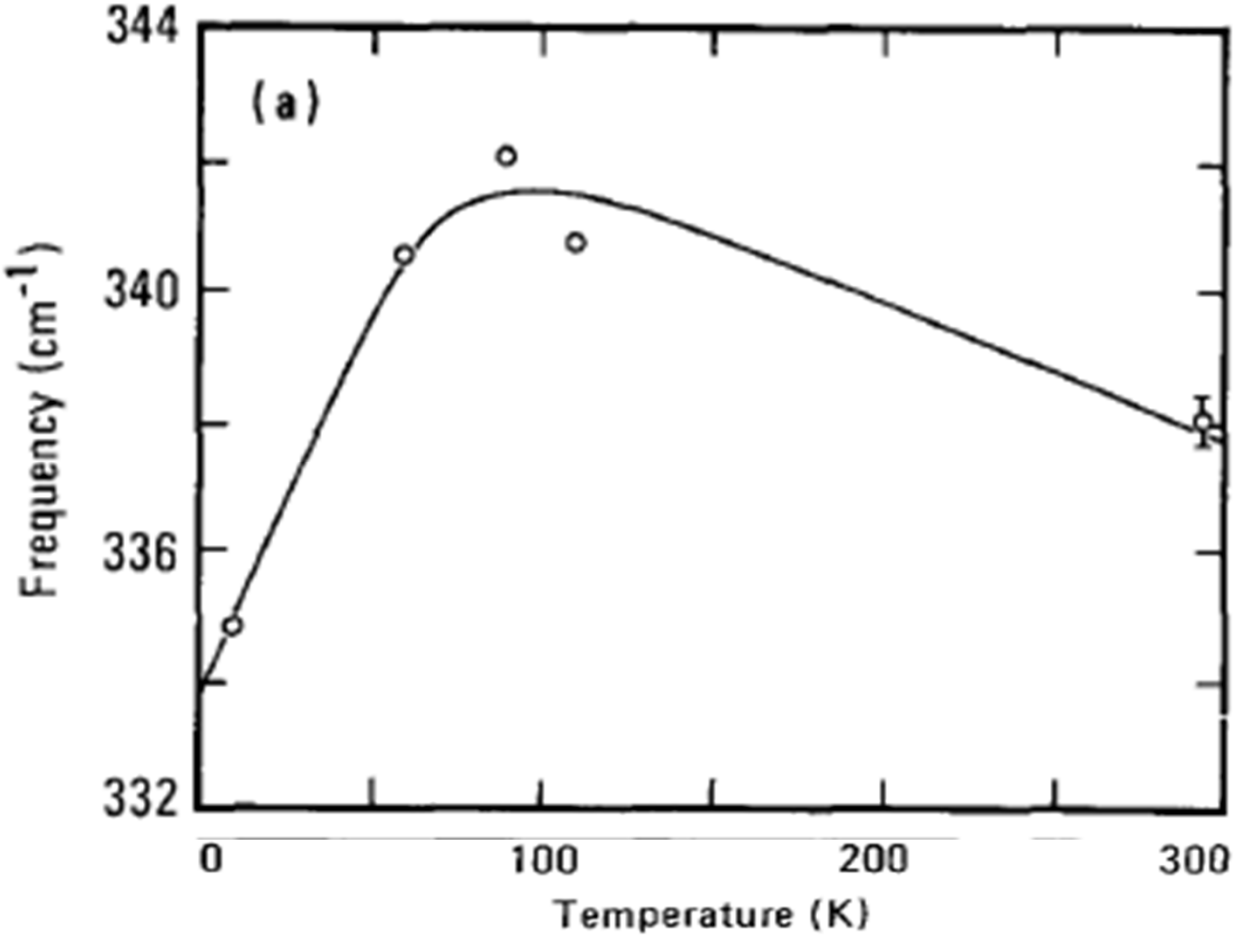
Harashima, et al., Physica C263, 257 (1996)



Pyka, et al., PRL 70, 1457, (1993)

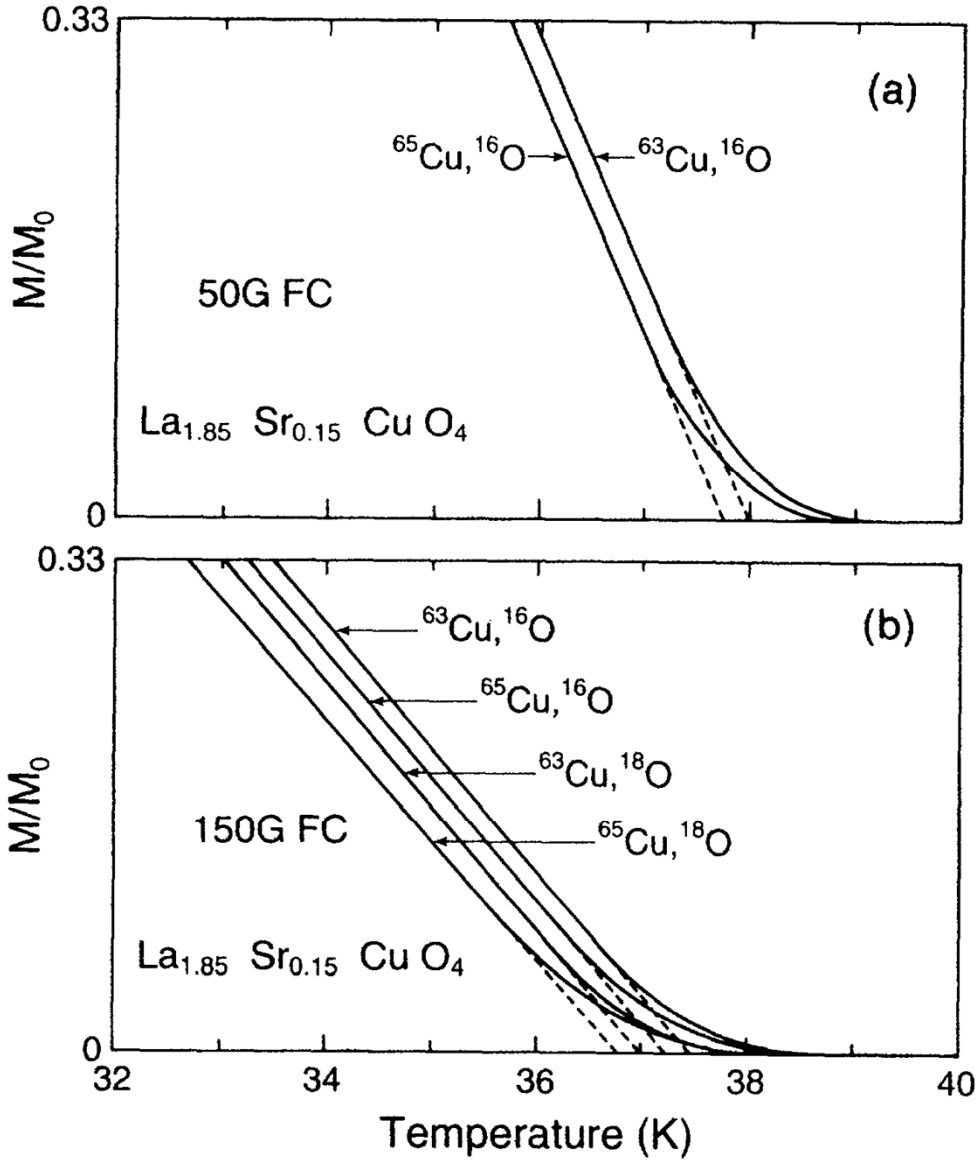
Macfarlane, Rosen, Seki, SSC 63, 831 (1987)

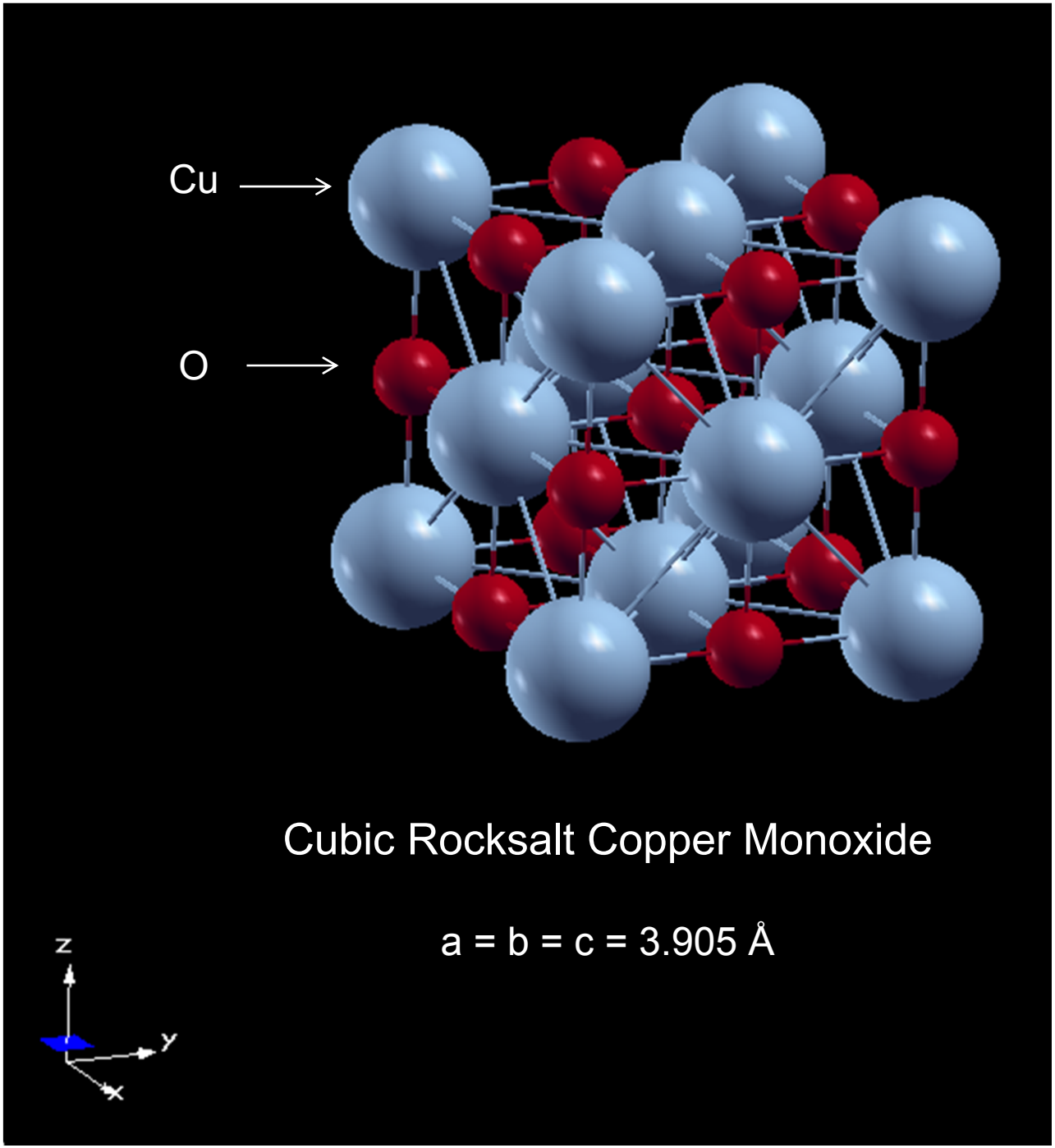
Raman Spectroscopy of YBCO



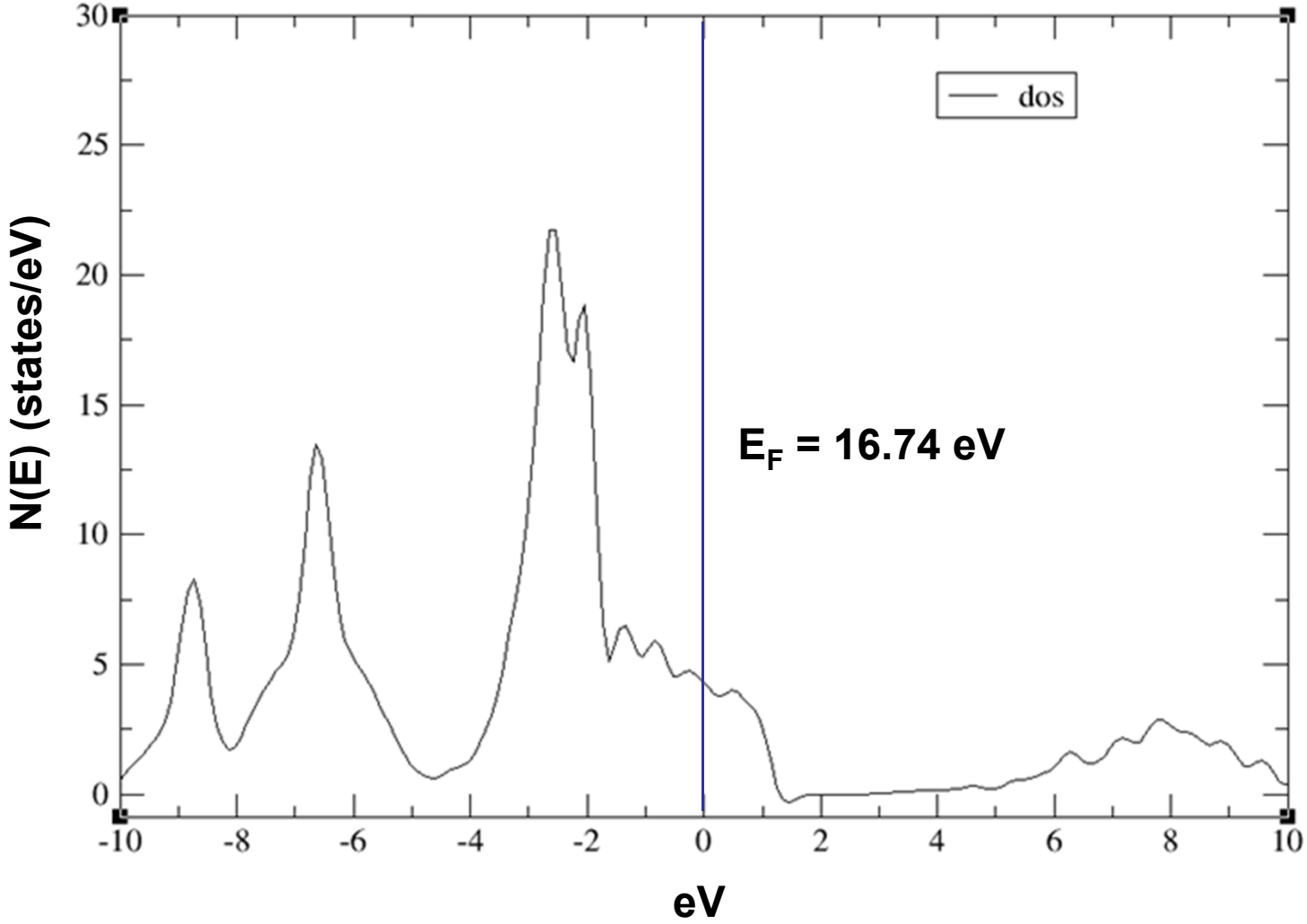
Copper and Oxygen Isotope Effects in $La_{2-x}Sr_xCuO_4$

J. P. Franck,[1] S. Harker,[1] and J. H. Brewer[2]

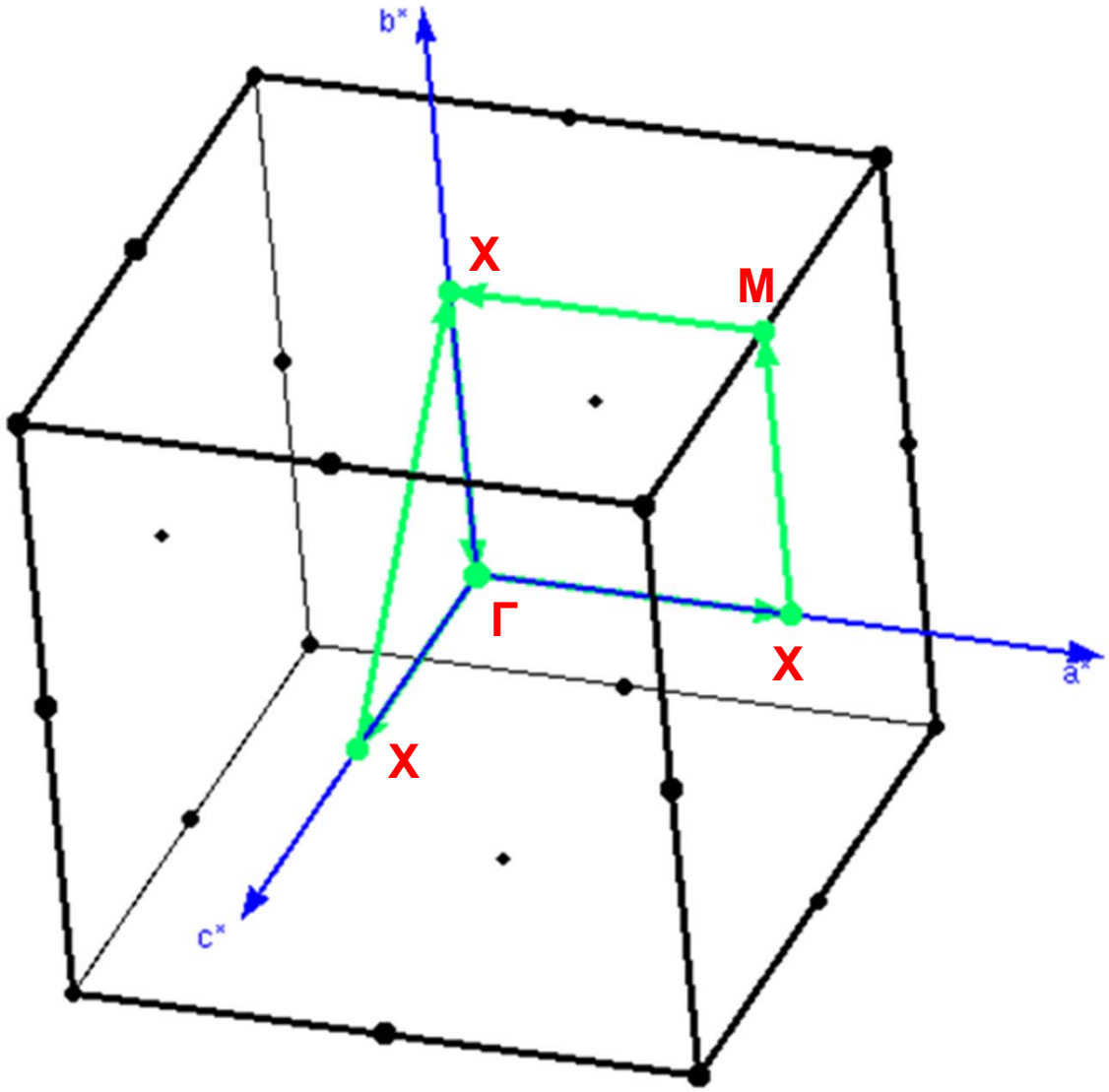



Cu
O
Cubic Rocksalt Copper Monoxide
a = b = c = 3.905 Å
z
y
x

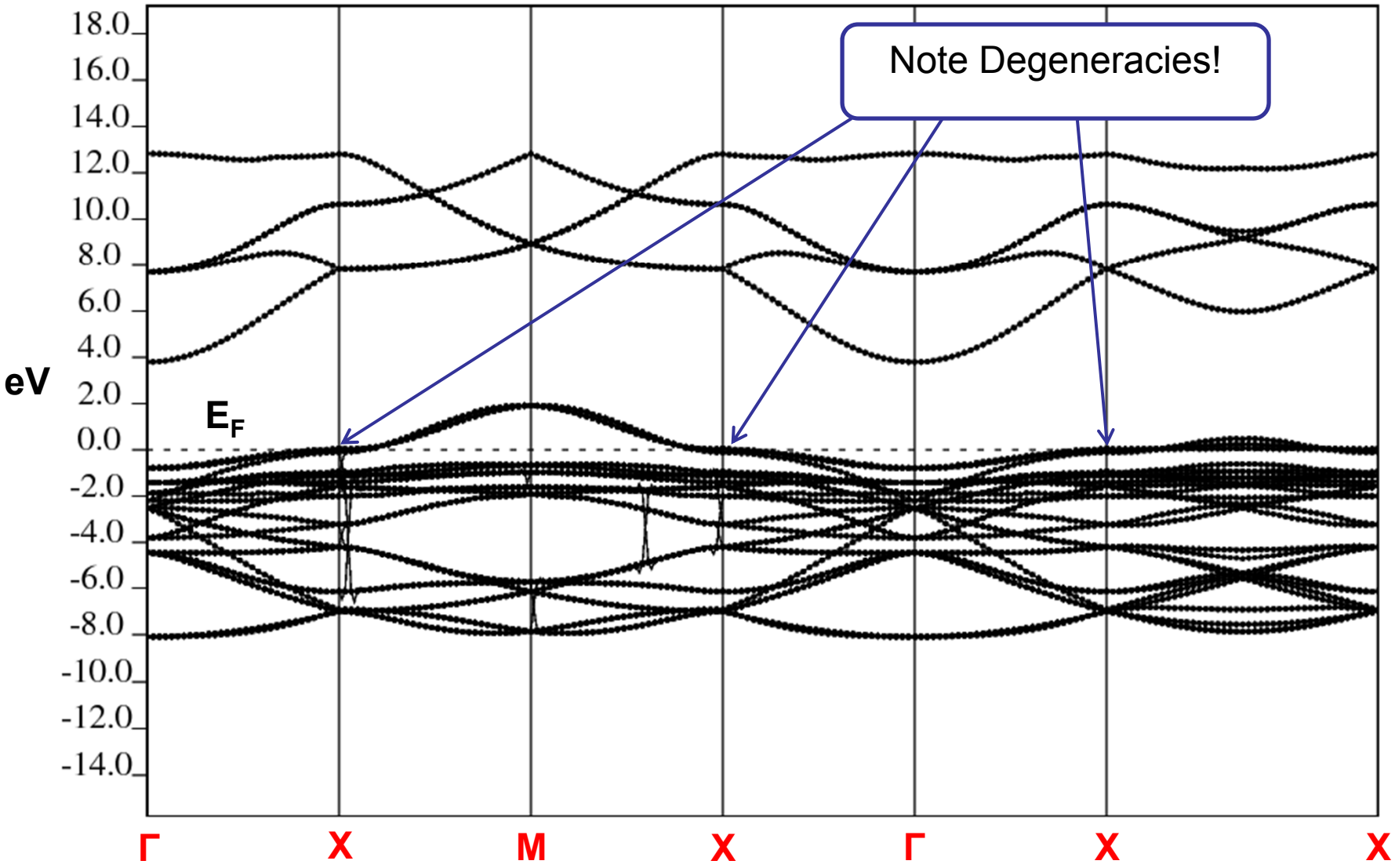
Rocksalt CuO
Combined DOS



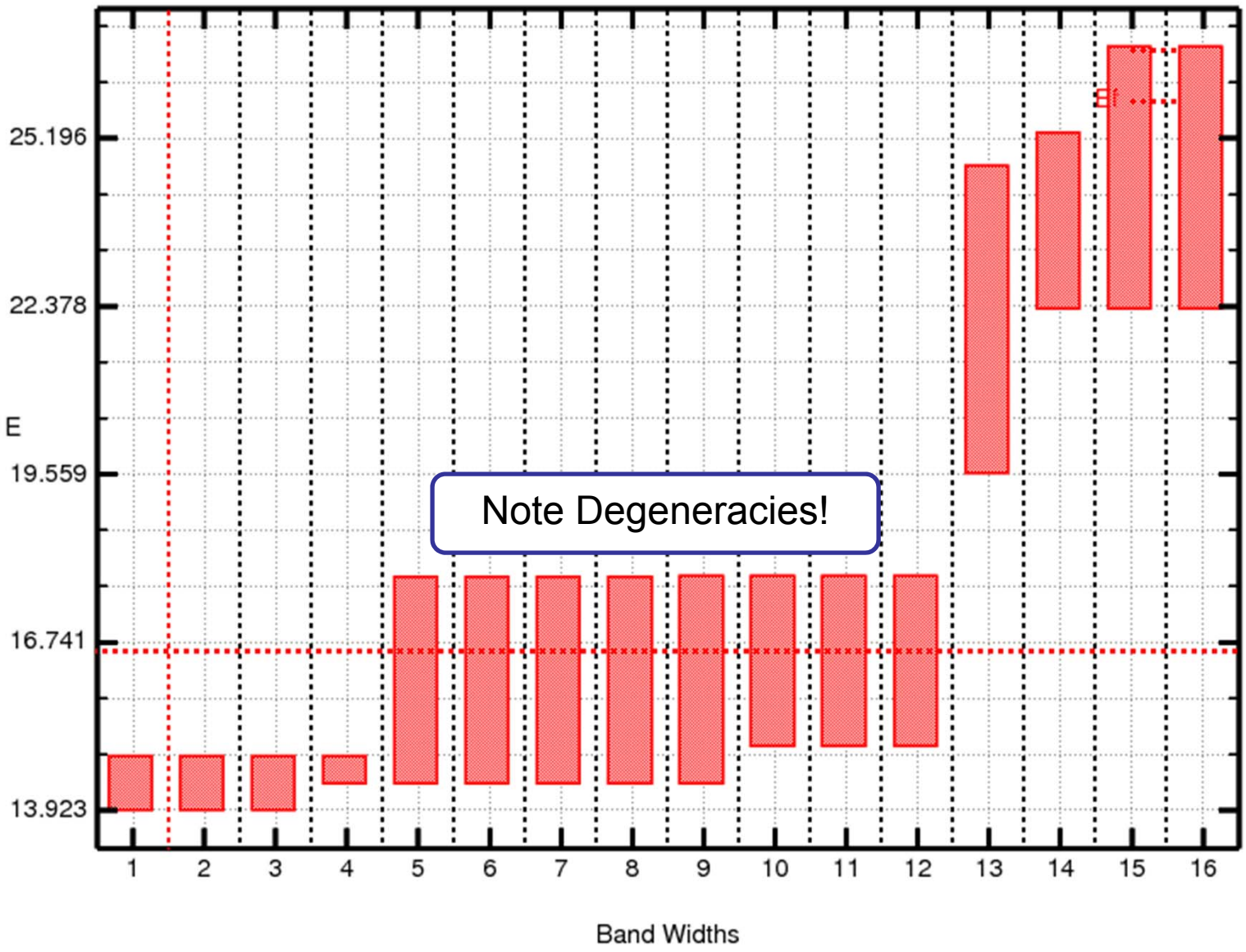
Rocksalt CuO BZ



Rocksalt CuO Bands

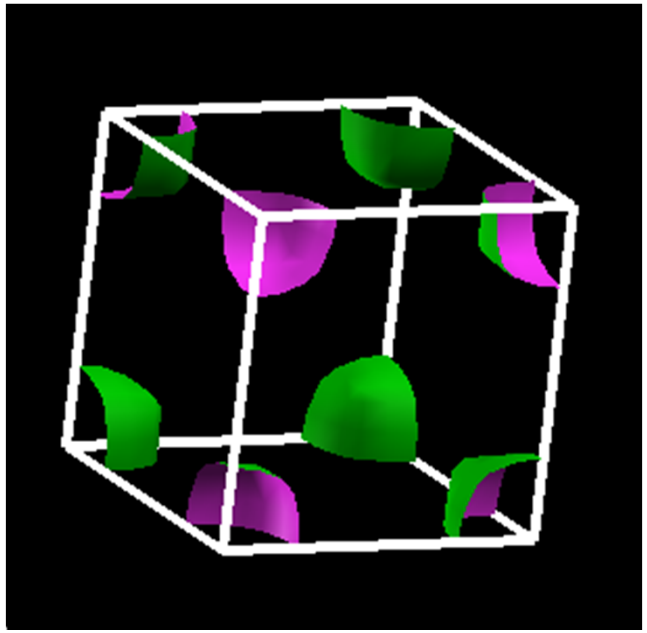


Rocksalt CuO Band Widths

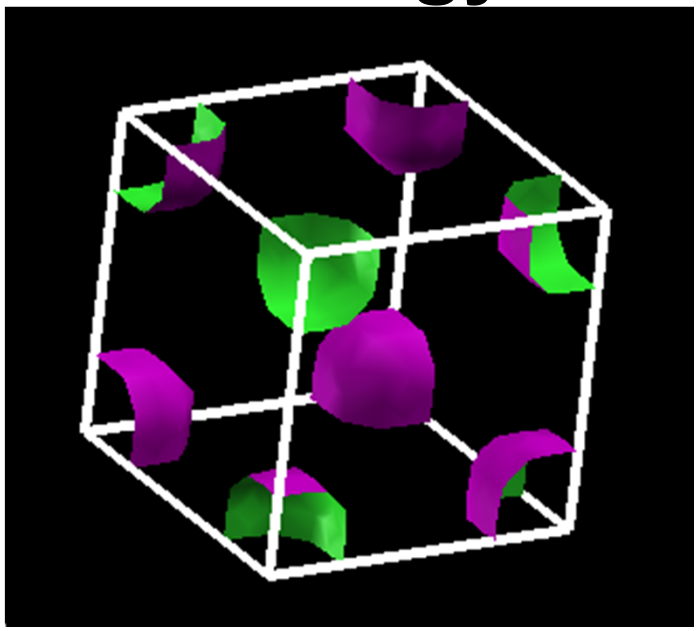


Rocksalt CuO Fermiology

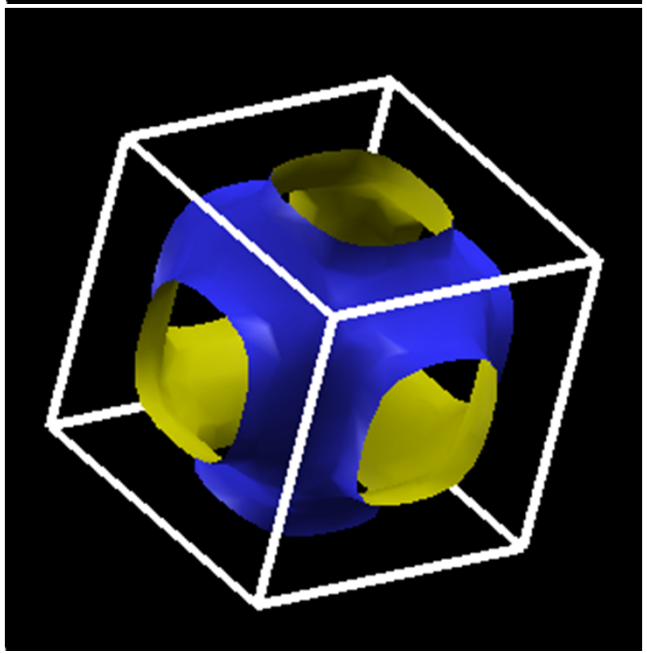
5



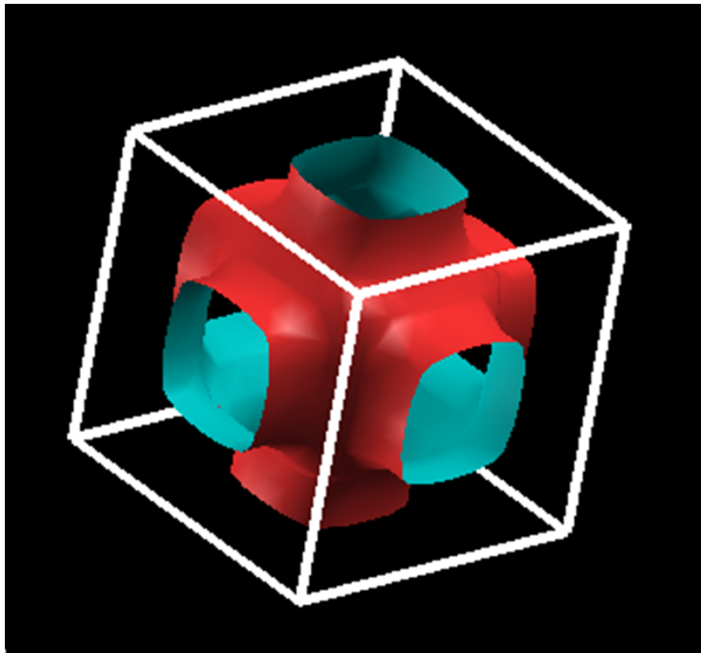
8



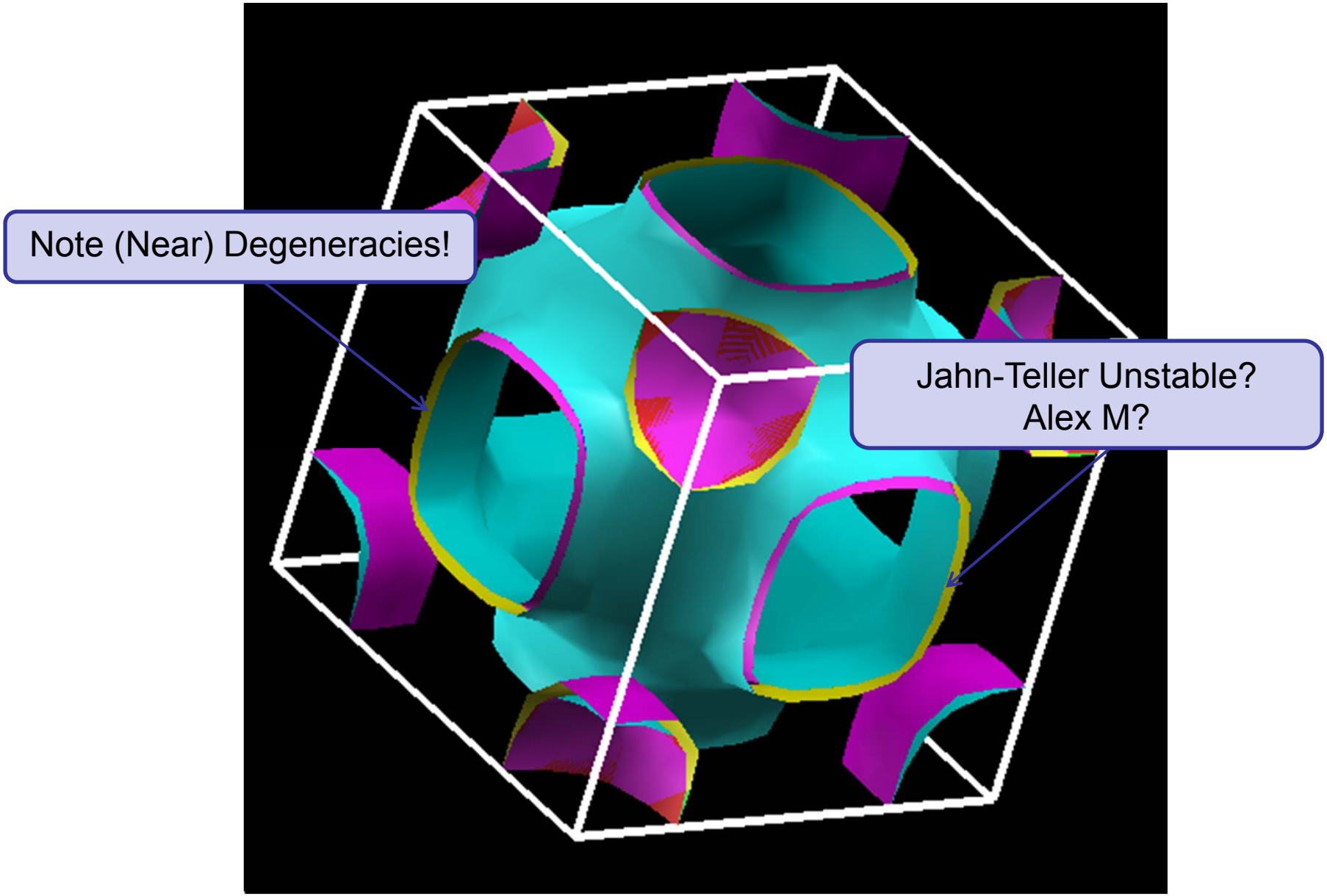
10



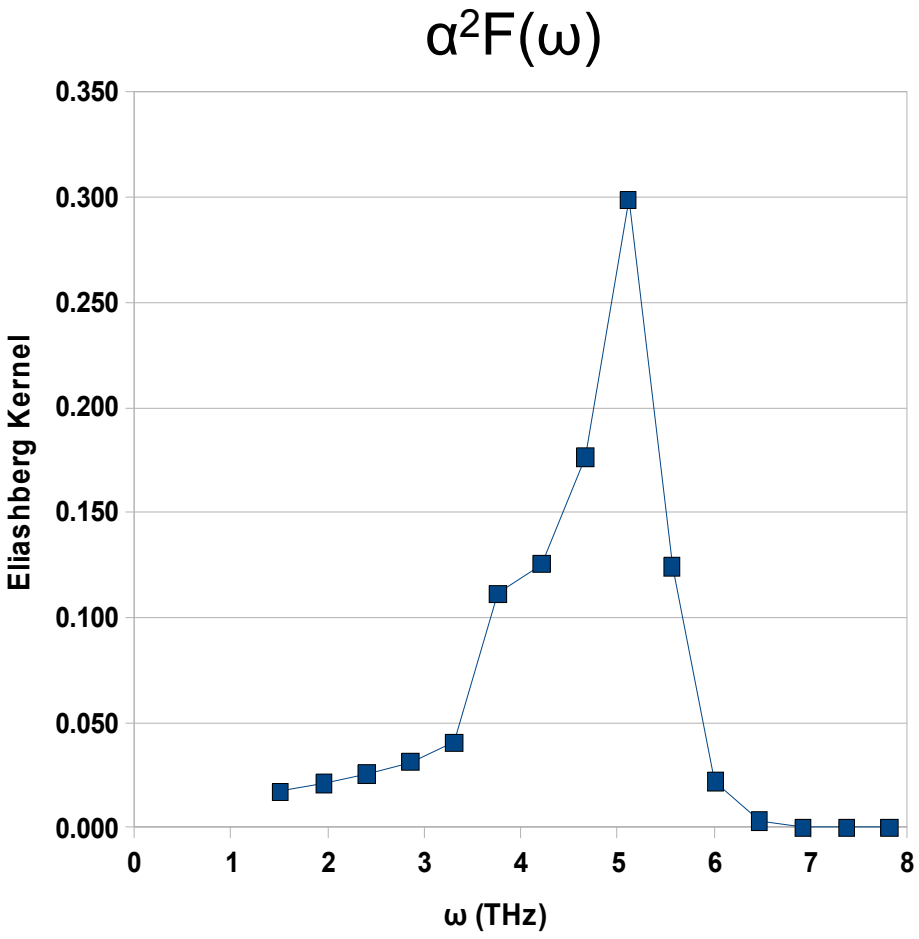
12



Rocksalt CuO Fermiology (Combined)



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



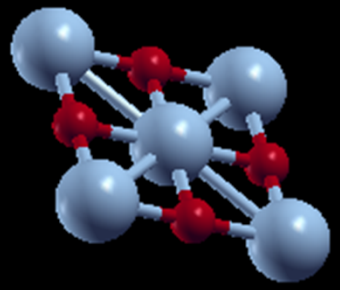
σ = 0.04

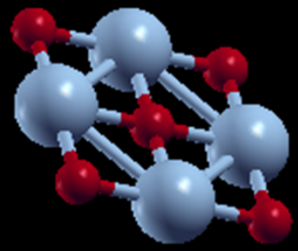
- λ ~ 0.6 – 0.7
- Other sc's…

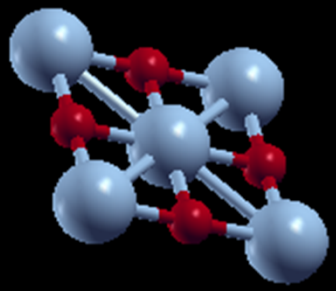
$$T_C = a\Theta e^{-\frac{1}{\lambda-\mu^*}} \qquad \lambda k\Theta \ll E_F$$

	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	-

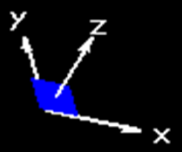
Square-Planar Copper Monoxide
“Film”



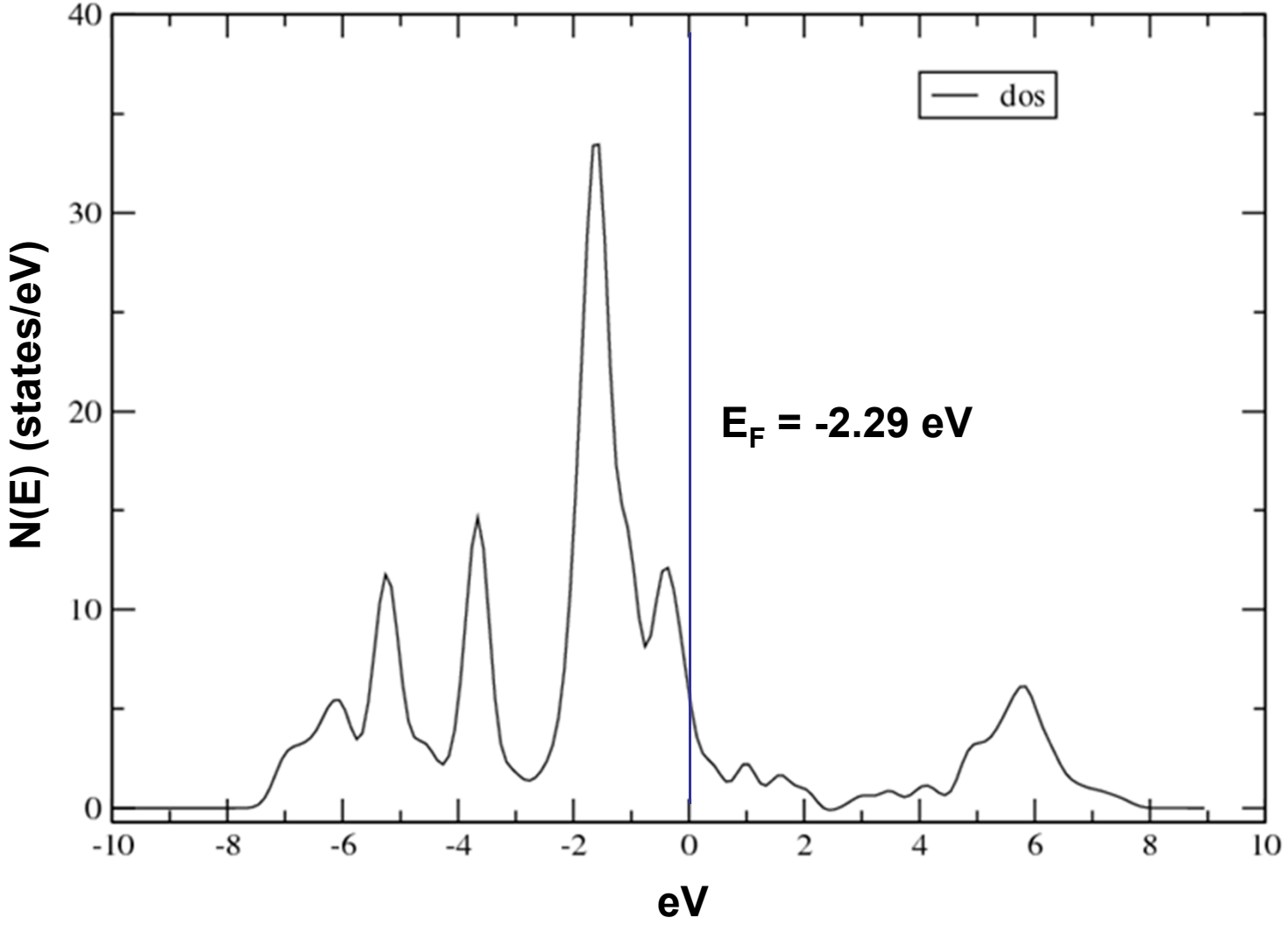




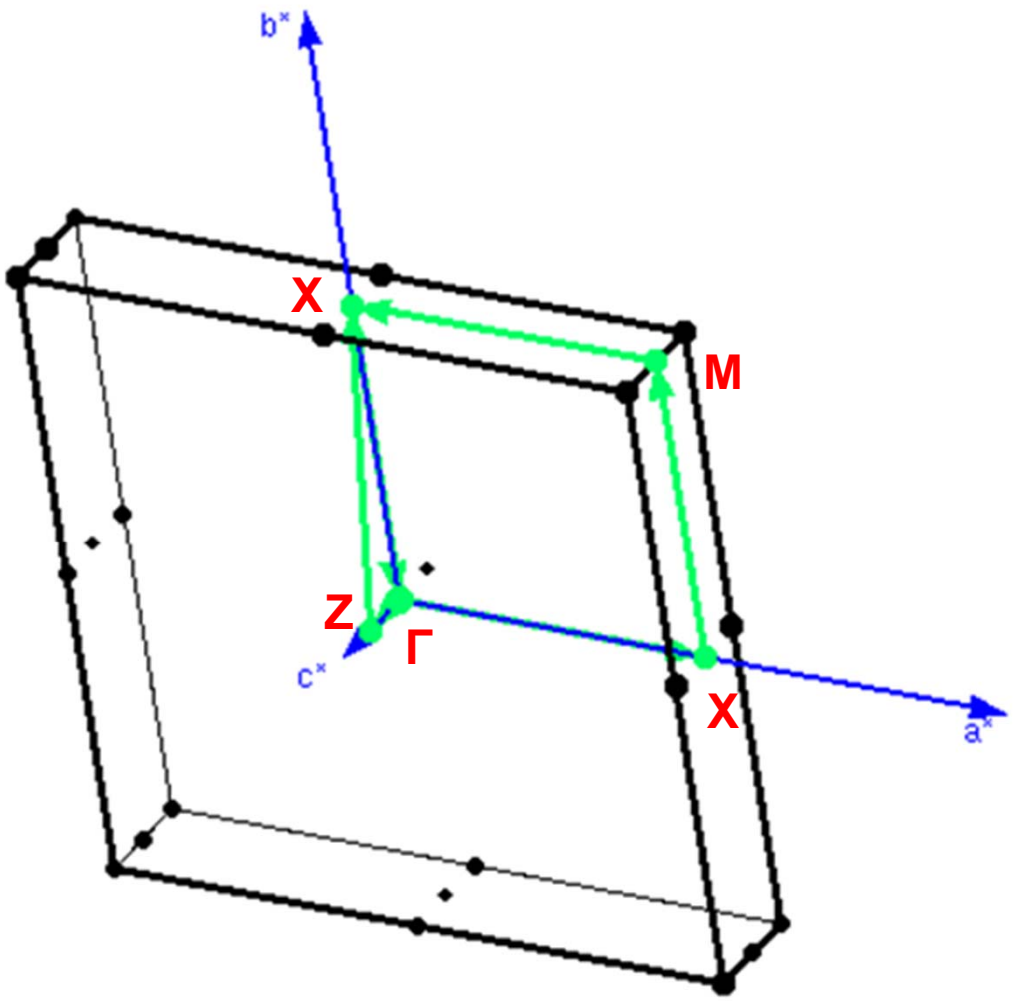
a = b = 3.905 Å
c = 6 x 3.905 = 23.43 Å



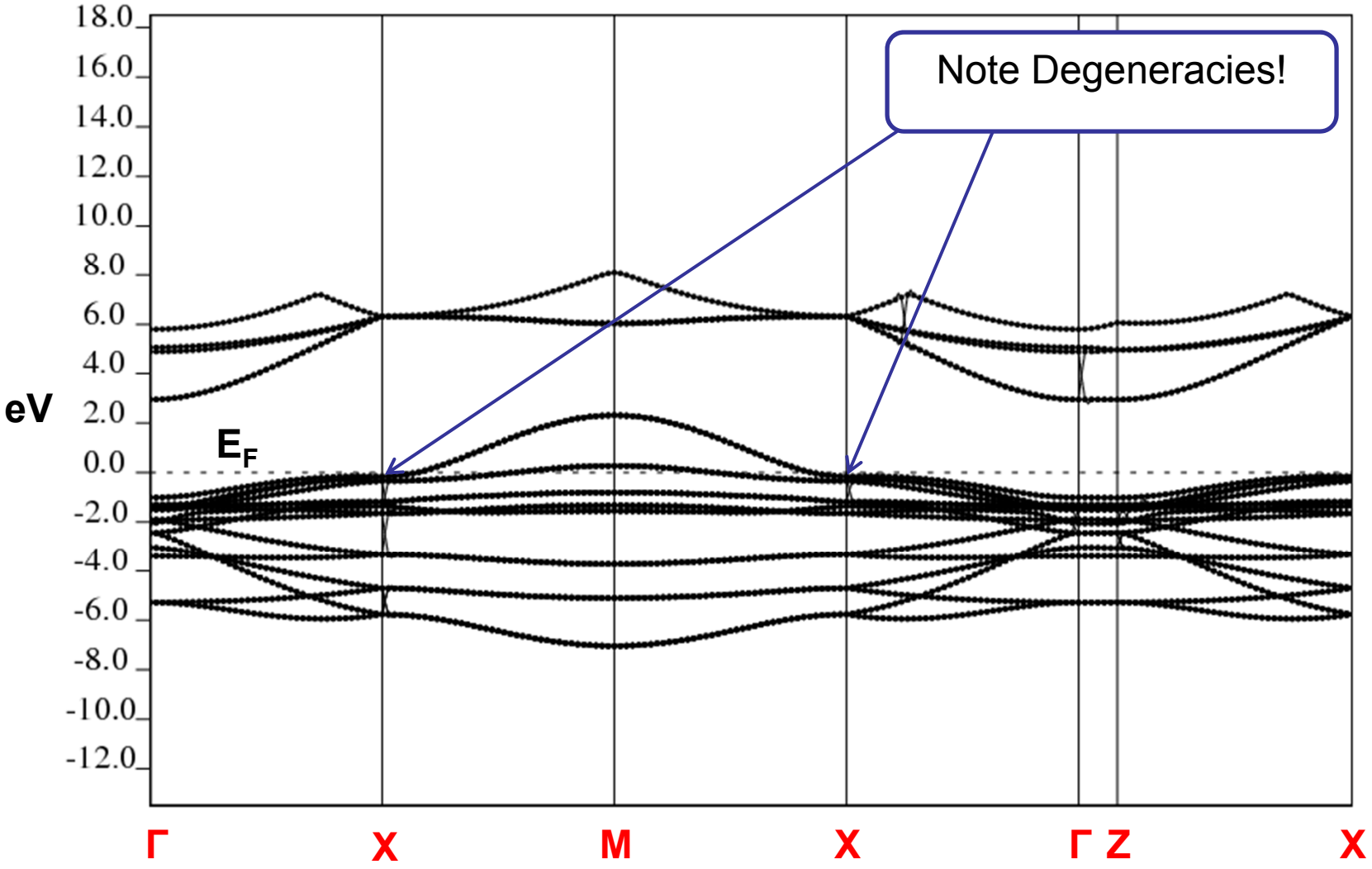
“Thin Film” Rocksalt CuO
Combined DOS



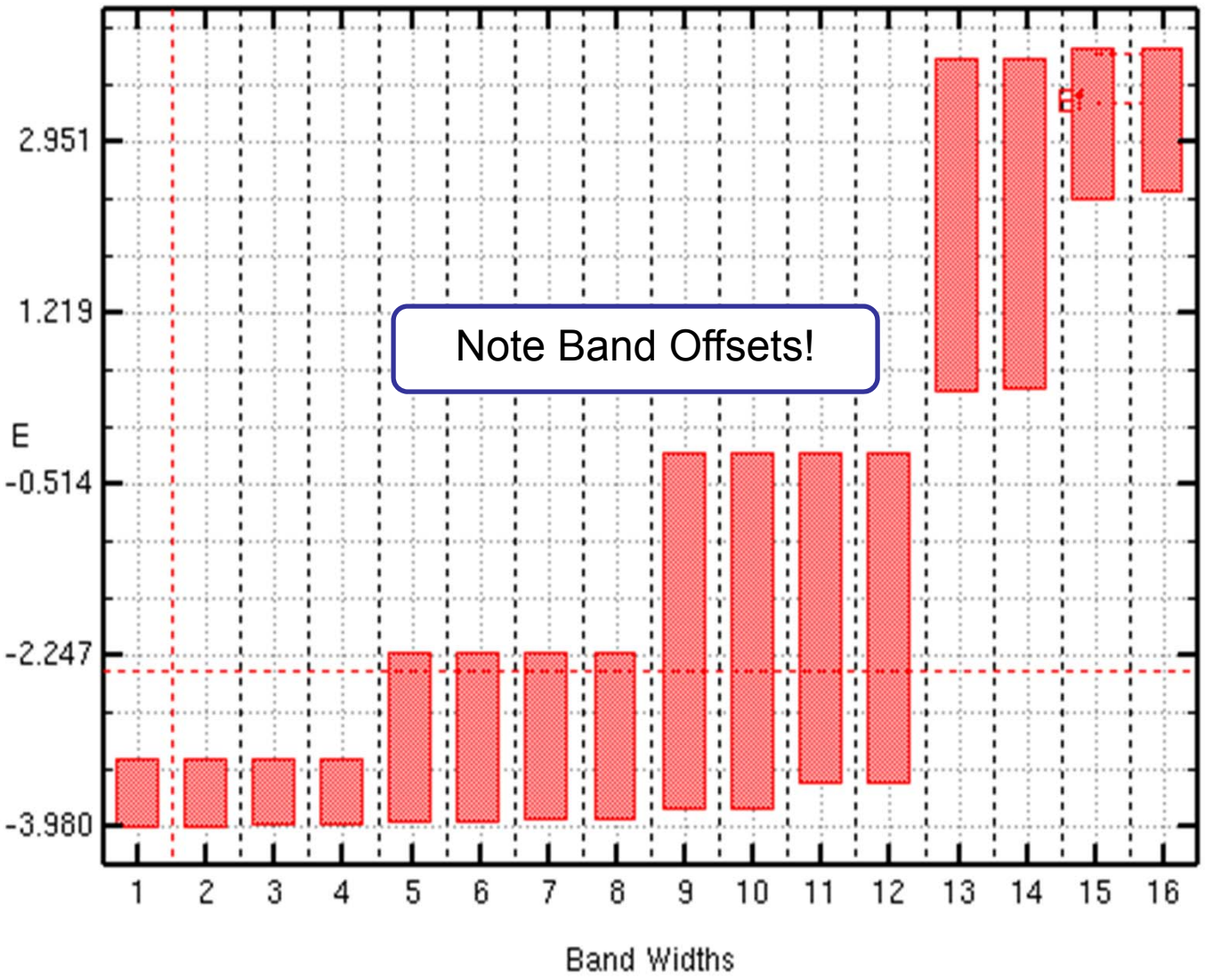
“Thin Film” CuO BZ



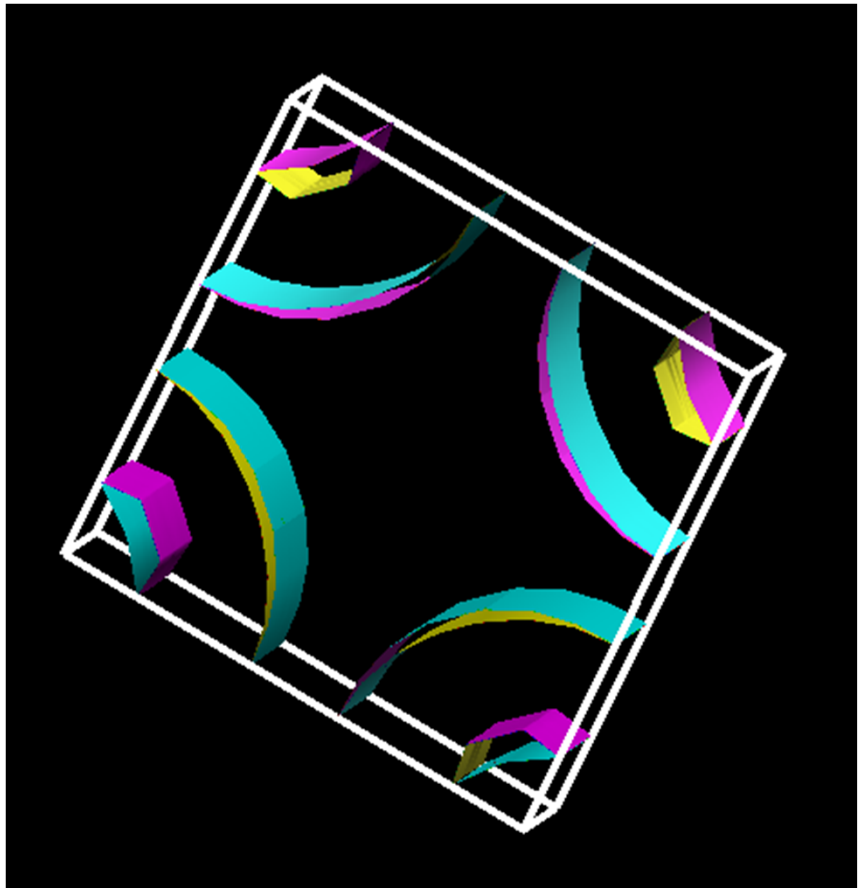
“Thin Film” CuO Bands

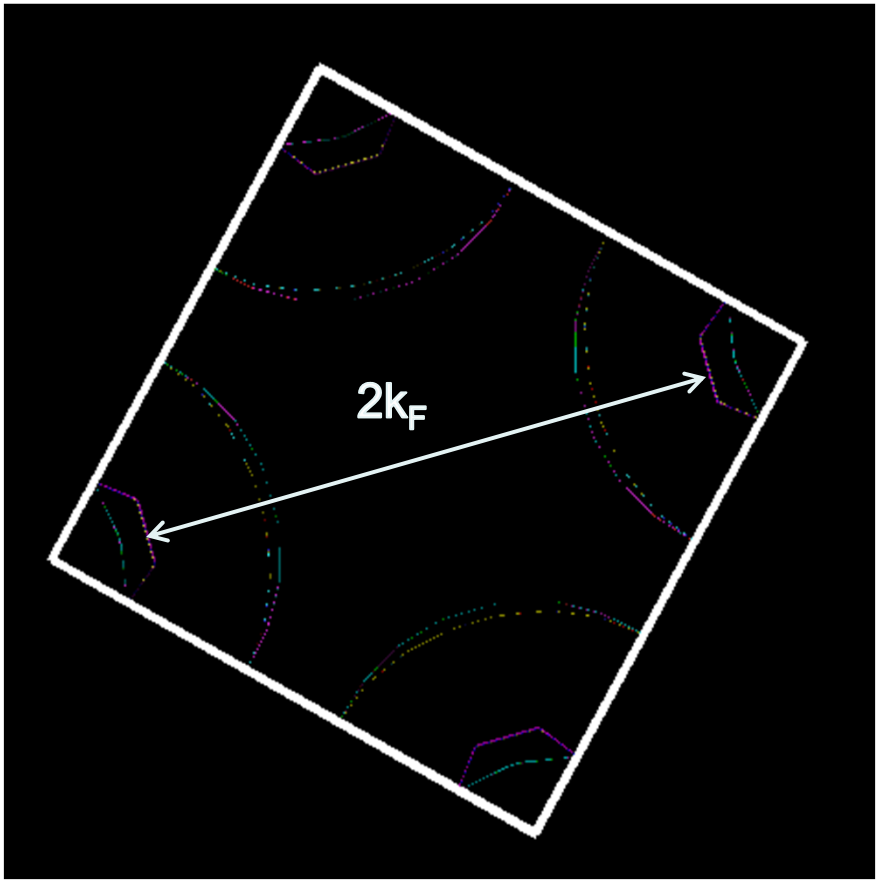


“Thin Film” CuO Band Widths



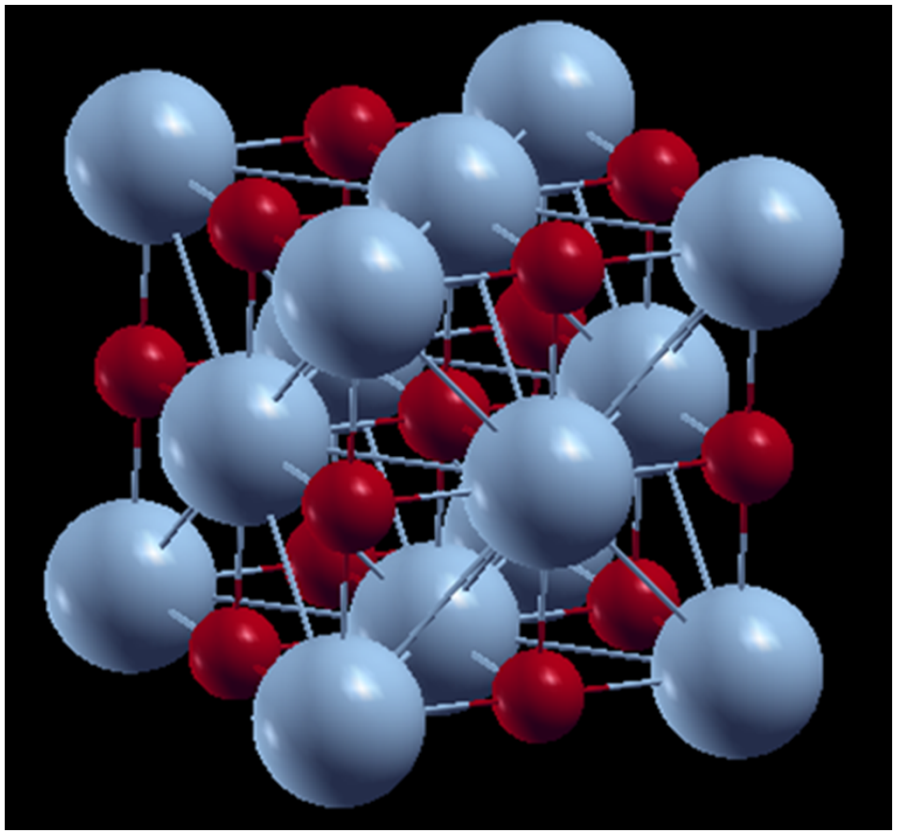
“Thin Film” CuO Fermiology (Combined)



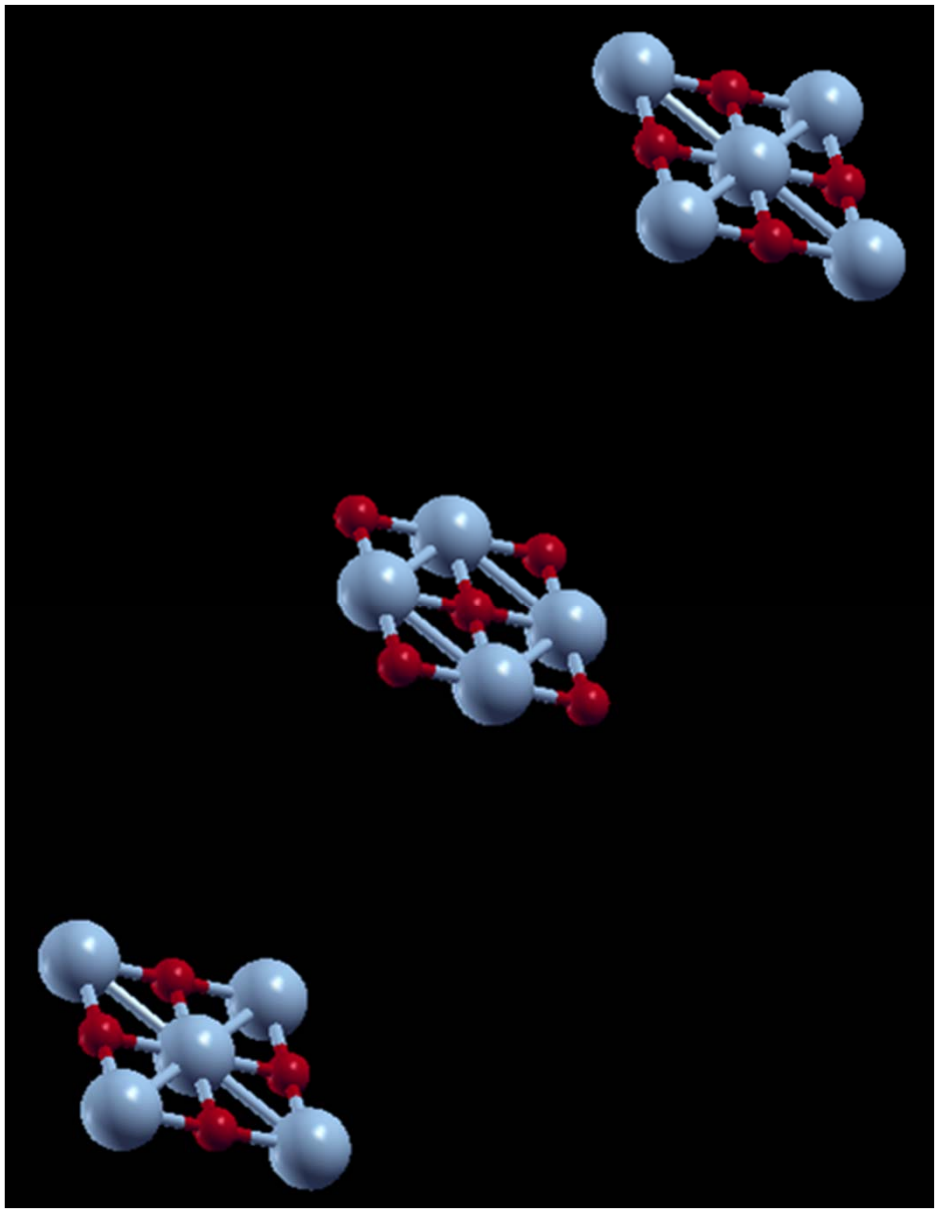


- “Nesting Fermi Lines”
- → CDW? → SDW? → HTSC?
- $\lambda \sim$?

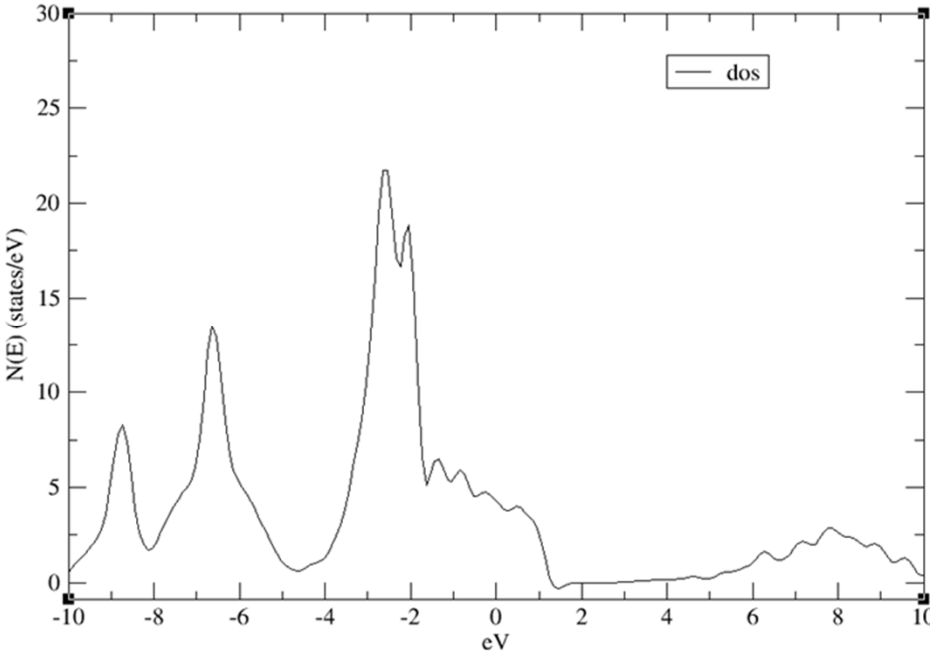
“Rocks”



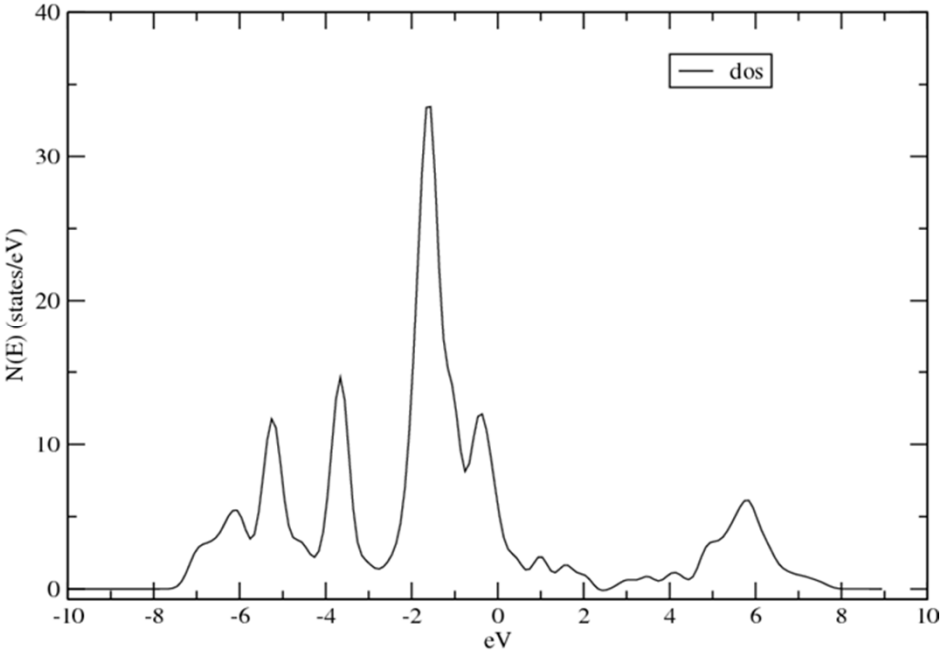
“Films”



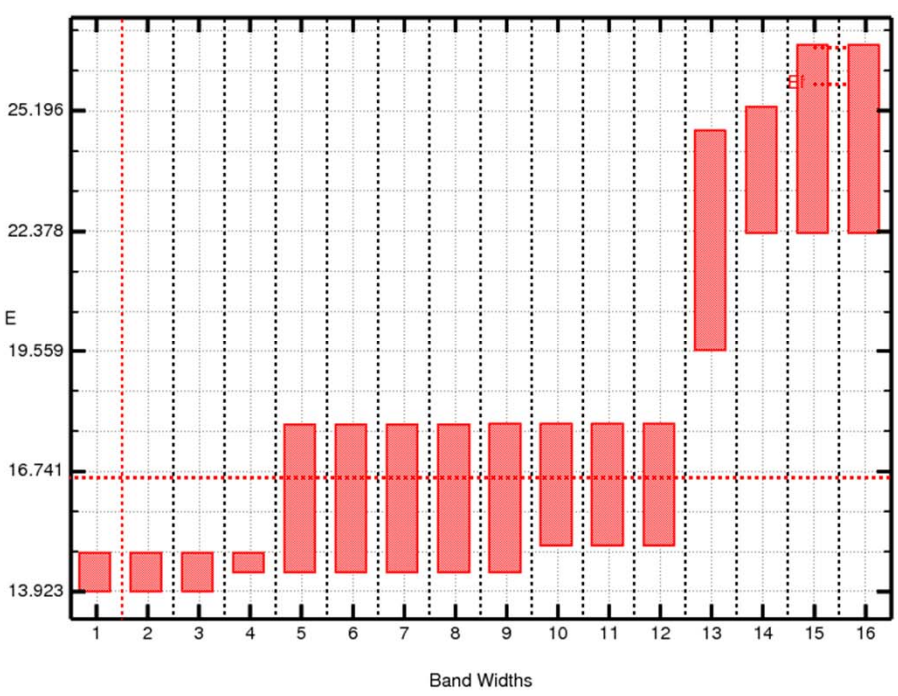
“Rocks”


dos
N(E) (states/eV)
eV
30
25
20
15
10
5
0
-10
-8
-6
-4
-2
0
2
4
6
8

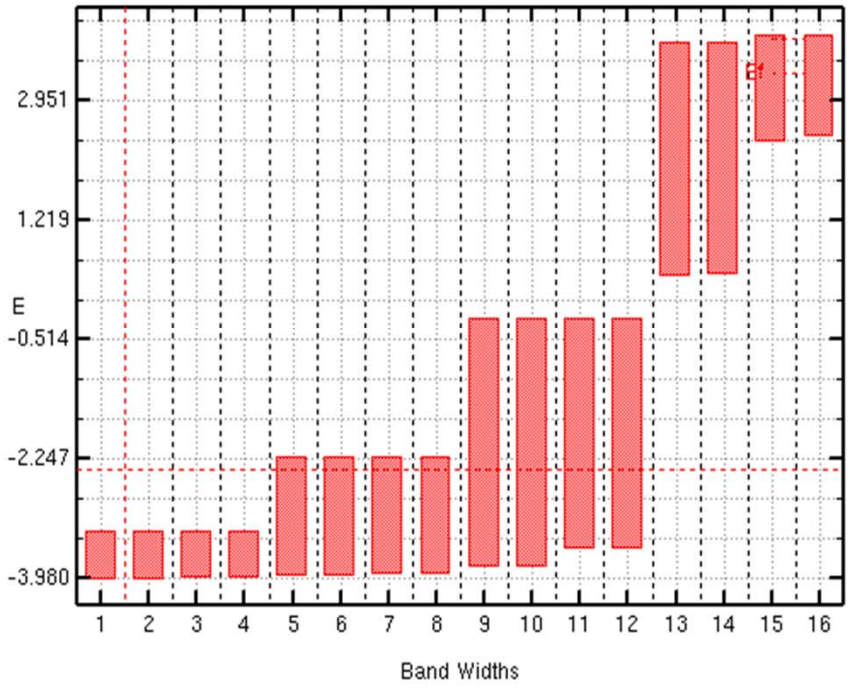
“Films”


dos
N(E) (states/eV)
eV
40
30
20
10
0
-10
-8
-6
-4
-2
0
2
4
6
8
10

“Rocks”

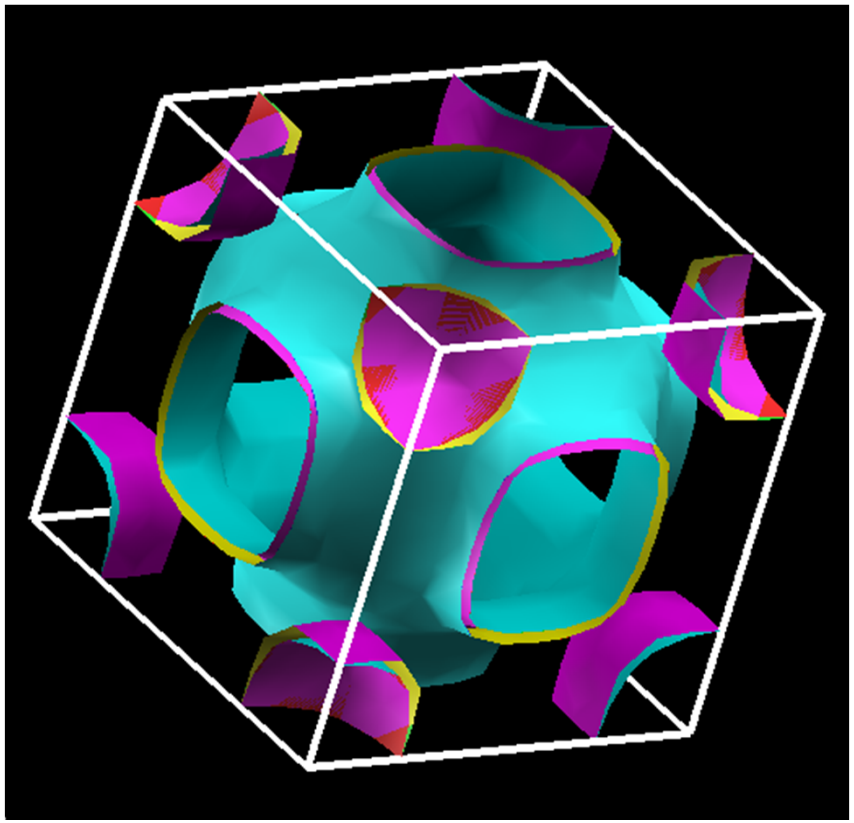

25.196
22.378
E
19.559
16.741
13.923
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16
Band Widths

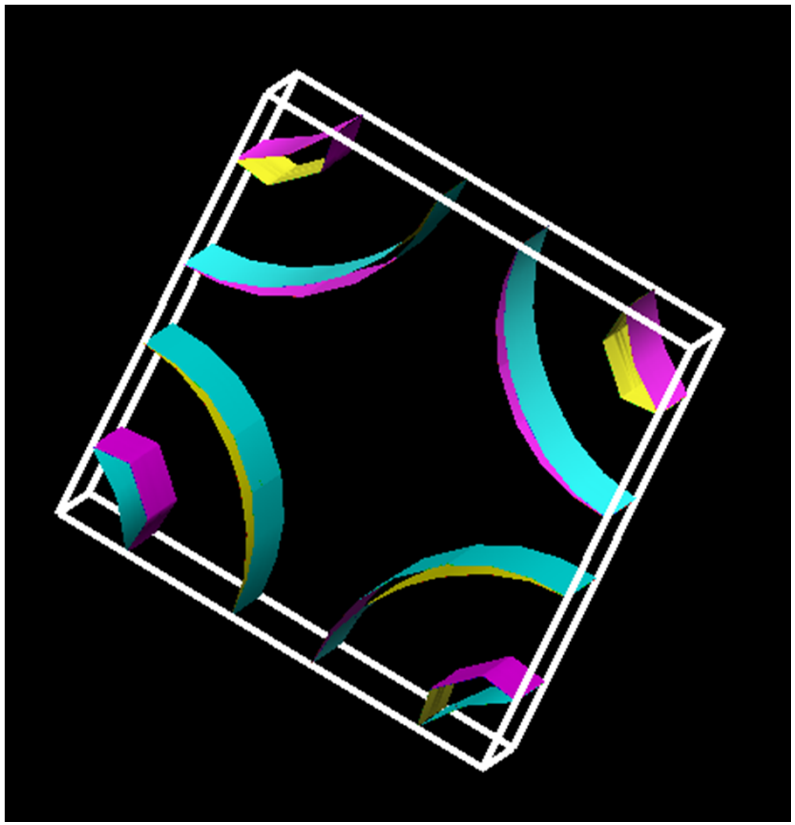
“Films”


2.951
1.219
E
-0.514
-2.247
-3.980
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16
Band Widths

“Rocks”

“Films”

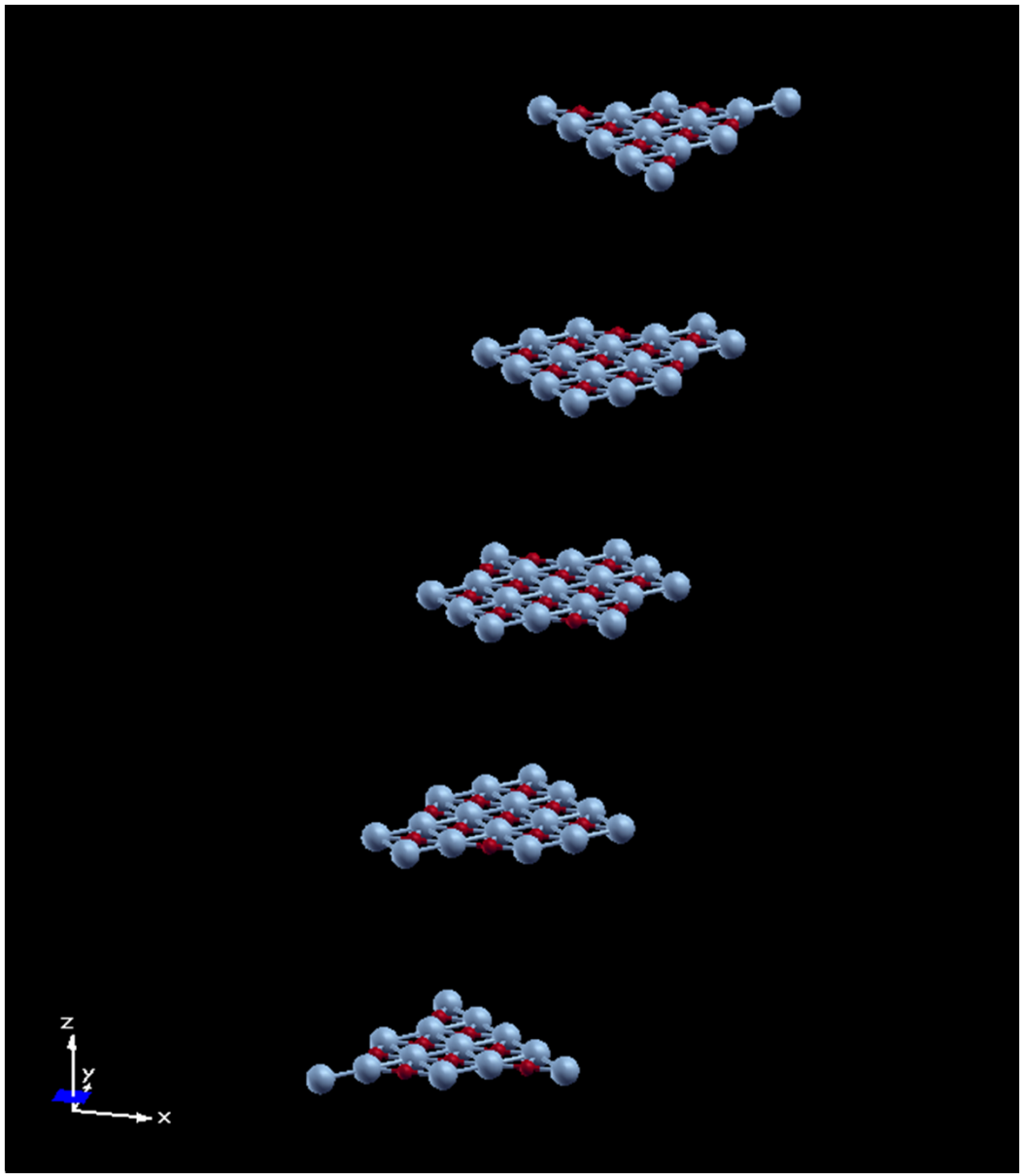




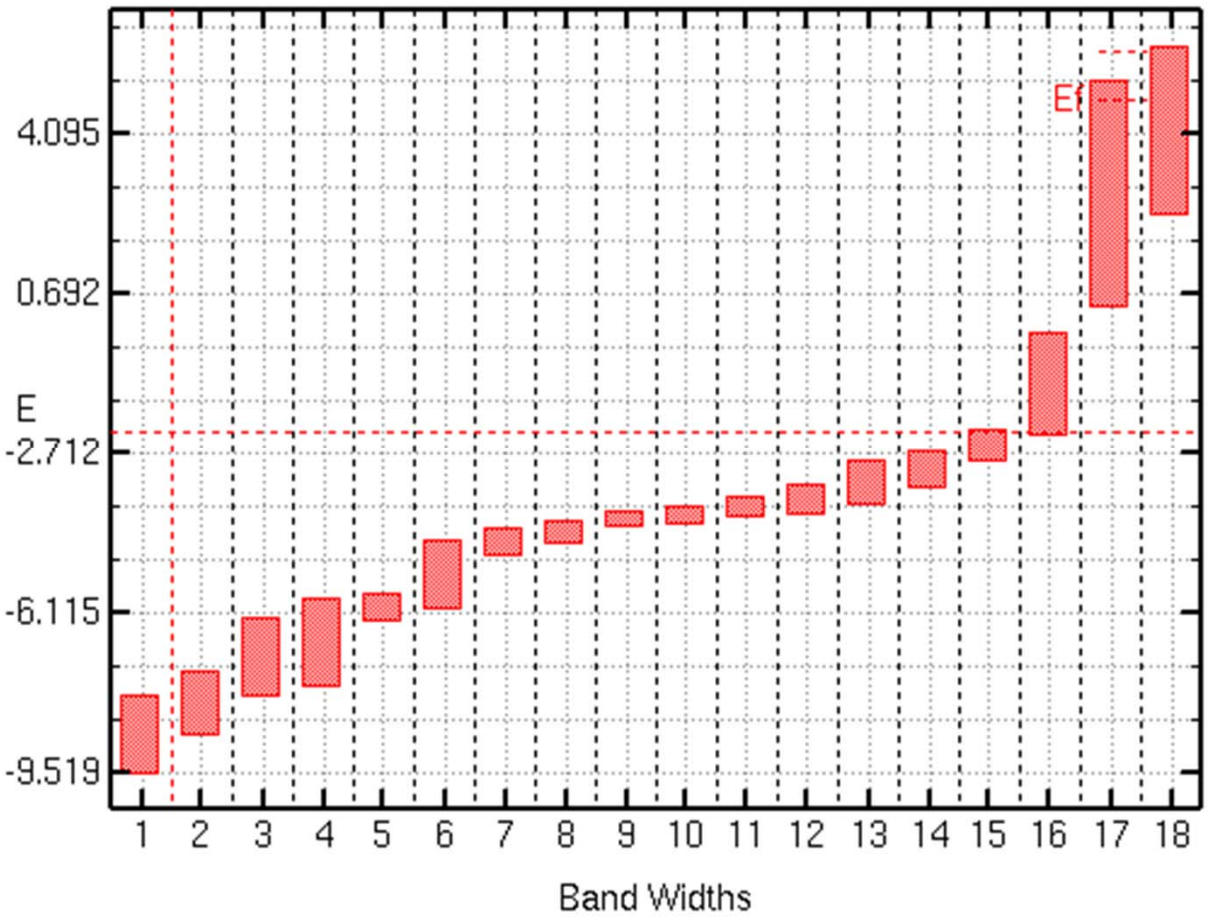
“Jahn – Teller”

“Nesting”

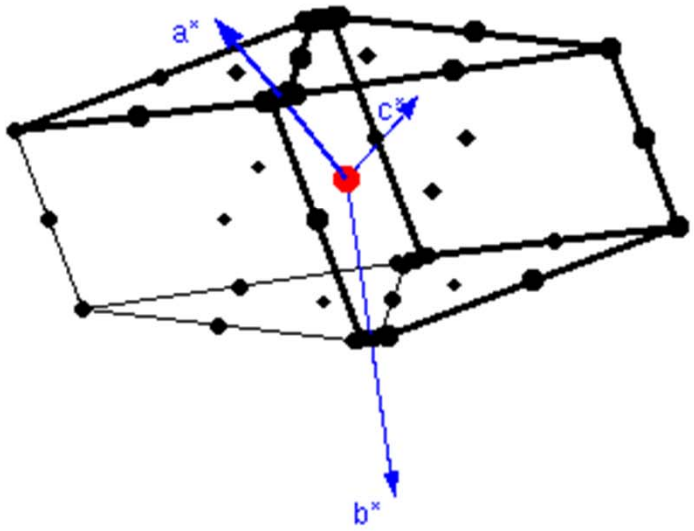
af-CuO c=6*a U~0.001 eV

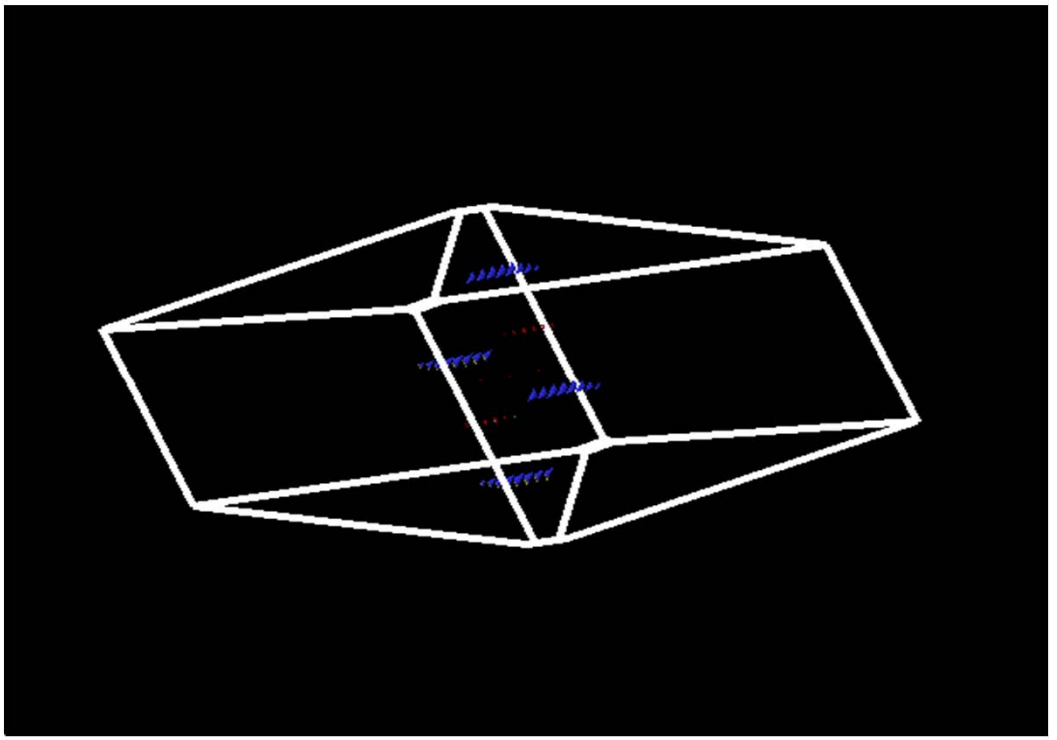


af-CuO c=6*a U~0.001 eV

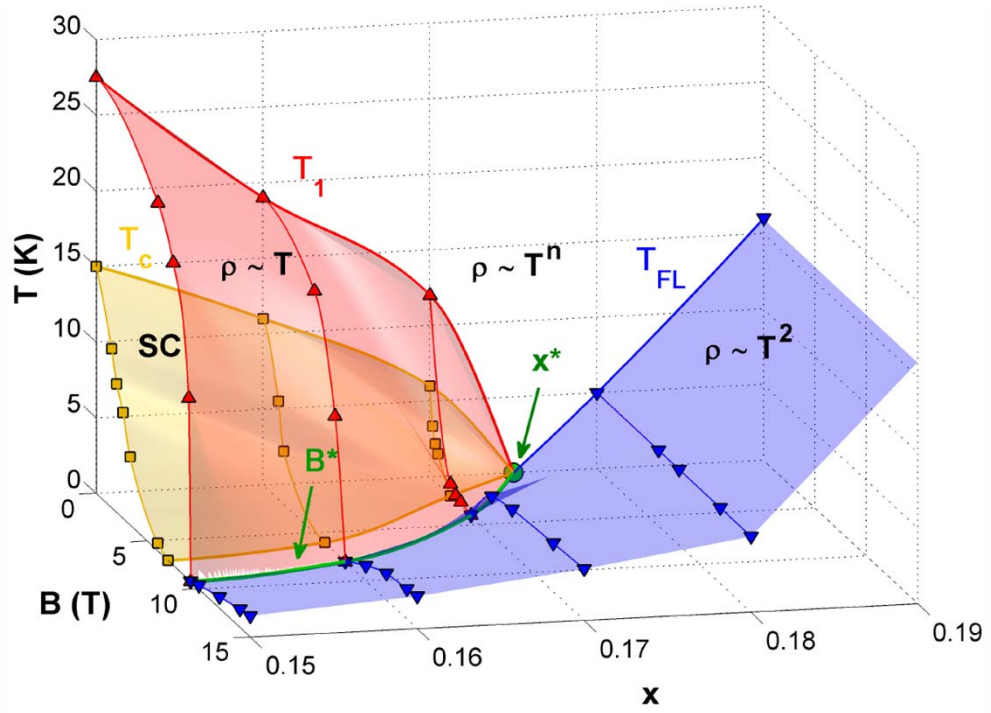


af-CuO c=6*a U~0.001 eV





Shakes & Spins
Copacetic, Competitive or Conundrum?
That is the question…*anon*



3D phase diagram of overdoped La2-*x*Ce*x*CuO4 with 0.15 ≤ *x* ≤ 0.19.

Pairing associated with quantum critical energy scales in superconducting electron-doped cuprates

K. Jin, N. P. Butch, K. Kirshenbaum, J. Paglione, and R. L. Greene*

-submitted to Nature-

*will answer *all* questions…

Bottom Line:

Can studying CuO proxies with DFT
+ LDA+U
+ phonons
provide the answer?

I say "Yes," but…
How to compute λ(SDW)?
Size Matters…
…and I need a…
BIGGER COMPUTER!