Abstract

2012 Annual Meeting of the California-Nevada Section of the APS

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W2AGZ Technologies

Possible Quantum Transport in (RE)$Ba_2Cu_3O_{7-y}$ Perovskites

4. - 4. Condensed Matter Physics and Materials Science

C - Computational

ORAL

For y $\approx$ 0, the crystal structure of the ``1-2-3'' family of rare earth perovskites displays a curious ``porosity'' feature, namely, along the b-axis direction of a region usually termed the ``CuO chains,'' one observes a dramatically wide ``channel'' bounded within a Ba-Cu-O tube. The cross-sectional area of these channels is roughly that of a single-wall carbon nanotube, suggesting the former may manifest Buettiker-Landauer quantum conductance similar to that observed in the latter. Moreover, by employing various ratios of Pr/Y for the RE component of the host system, the bulk electrical properties of the surrounding host can be tailored from completely insulating to metallic. We test our conjecture predicting ballistic transport down the ``Ba-Cu-O channel'' using density functional theory and report our initial findings here. We also discuss possible experimental embodiments which could lead to nano-controllable gate structures.

Submitter

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GR166160

USA

Possible Quantum Transport in $(RE)Ba_2Cu_3O_{7-y}$ Perovskites

Session H4: Condensed Matter IV: Atoms and Molecules
Talk H4.00001, 2:00 PM, Saturday, 3 November 2012

Paul Michael Grant

APS Senior Life Fellow
Staff Associate, JPL/CalTech
IBM Research Staff Member Emeritus
EPRI Science Fellow (Retired)
Principal, W2AGZ Technologies

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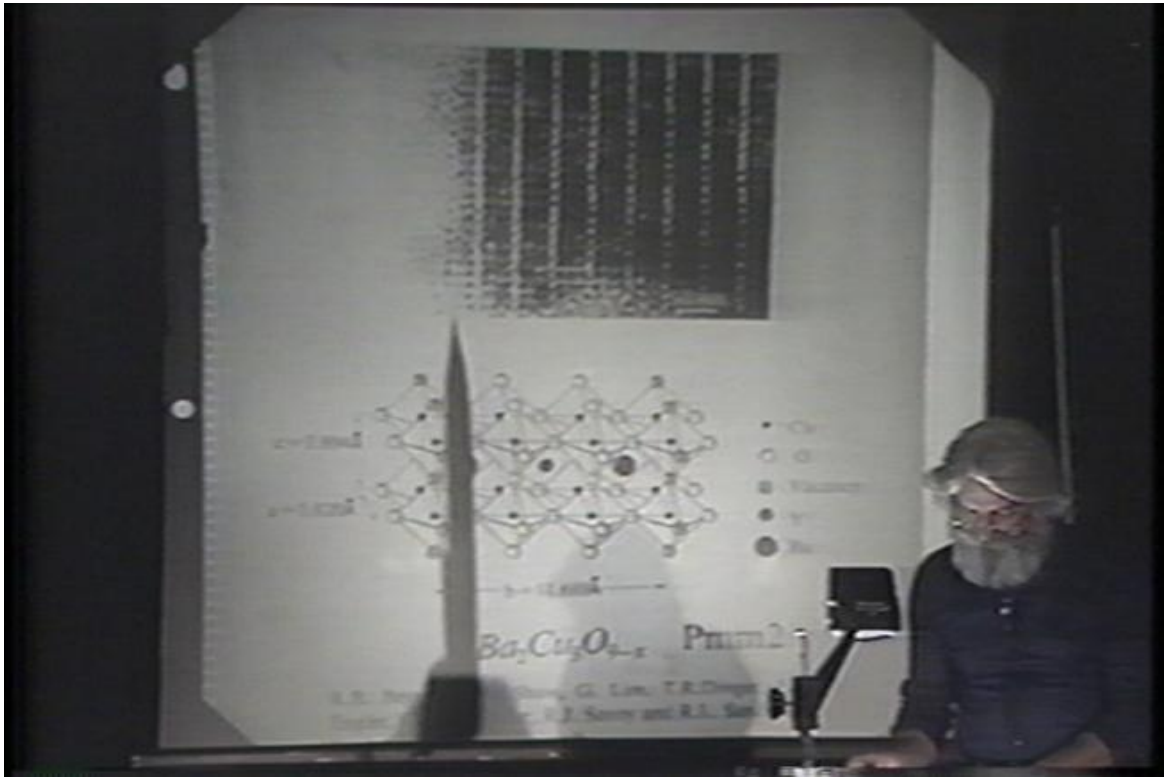
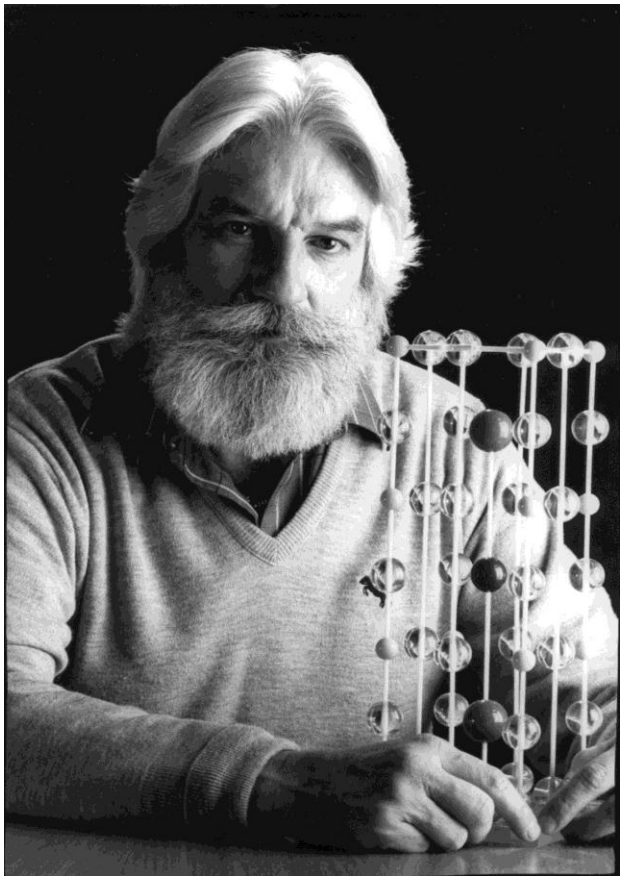
Paul Michael Grant

Aging IBM Pensioner

(research supported under the IBM retirement fund)



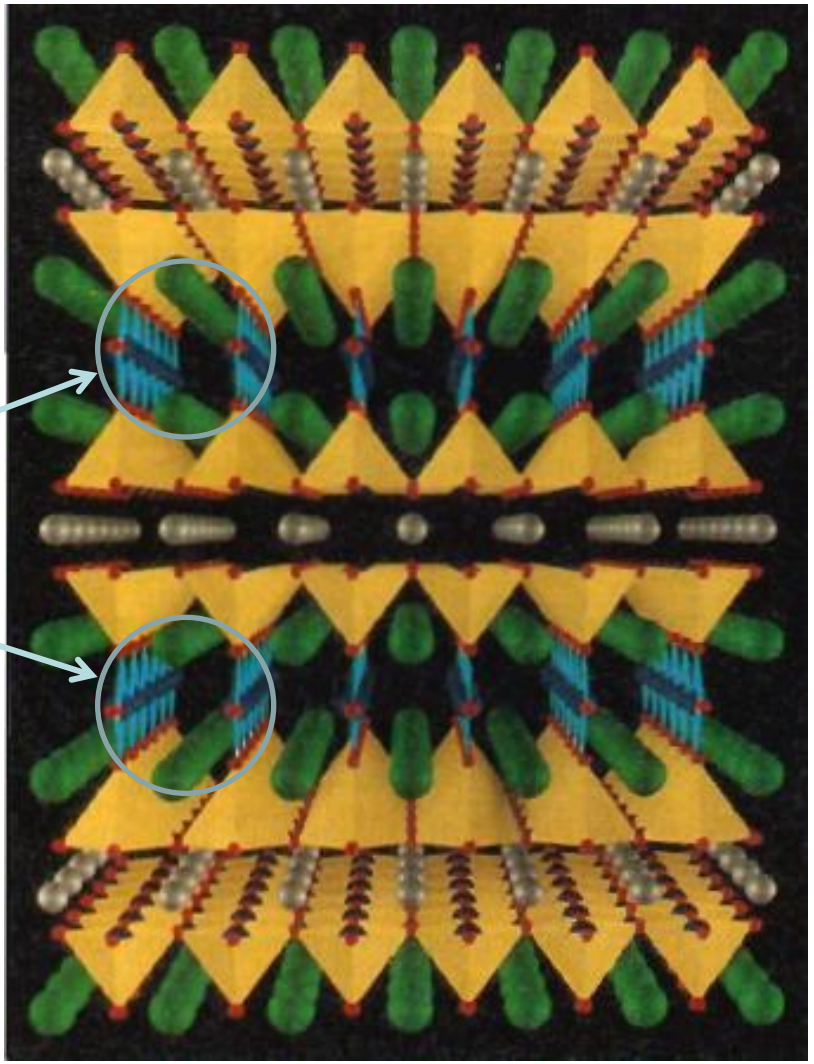
Woodstock of Physics



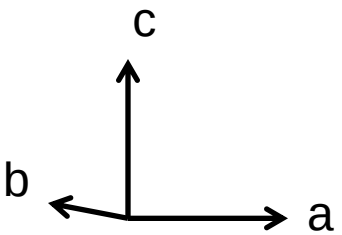
17 March 1987
Revealing the Structure of “1-2-3”

“We Band of Brothers (and a Sister!)”
- IBM Almaden, March 1987 -

PMG, Adv. Mater. 2 (1990) No. 5 p. 236
RE-1237 (RE = Y, Pr, Nd...whatever)

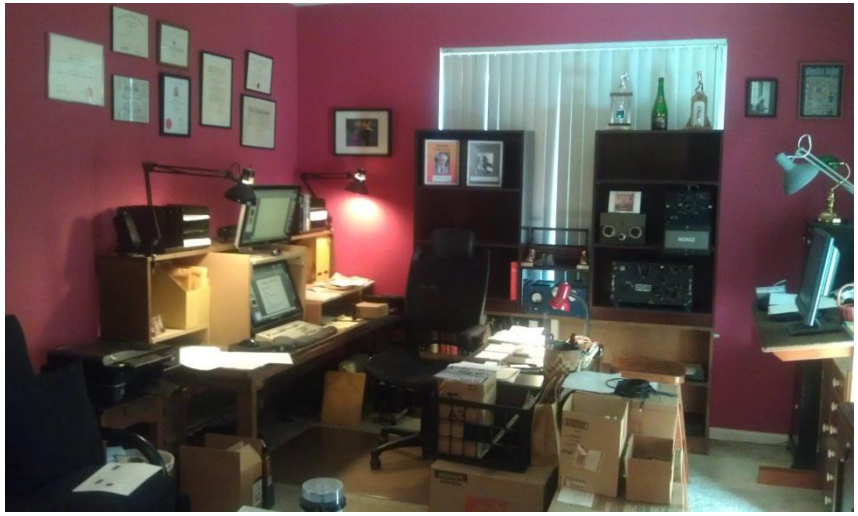


Ba – Cu – O Channels



RE - Silver
Ba - Green
Cu - Blue
O - Red

“Gadgets in My Tool Box”



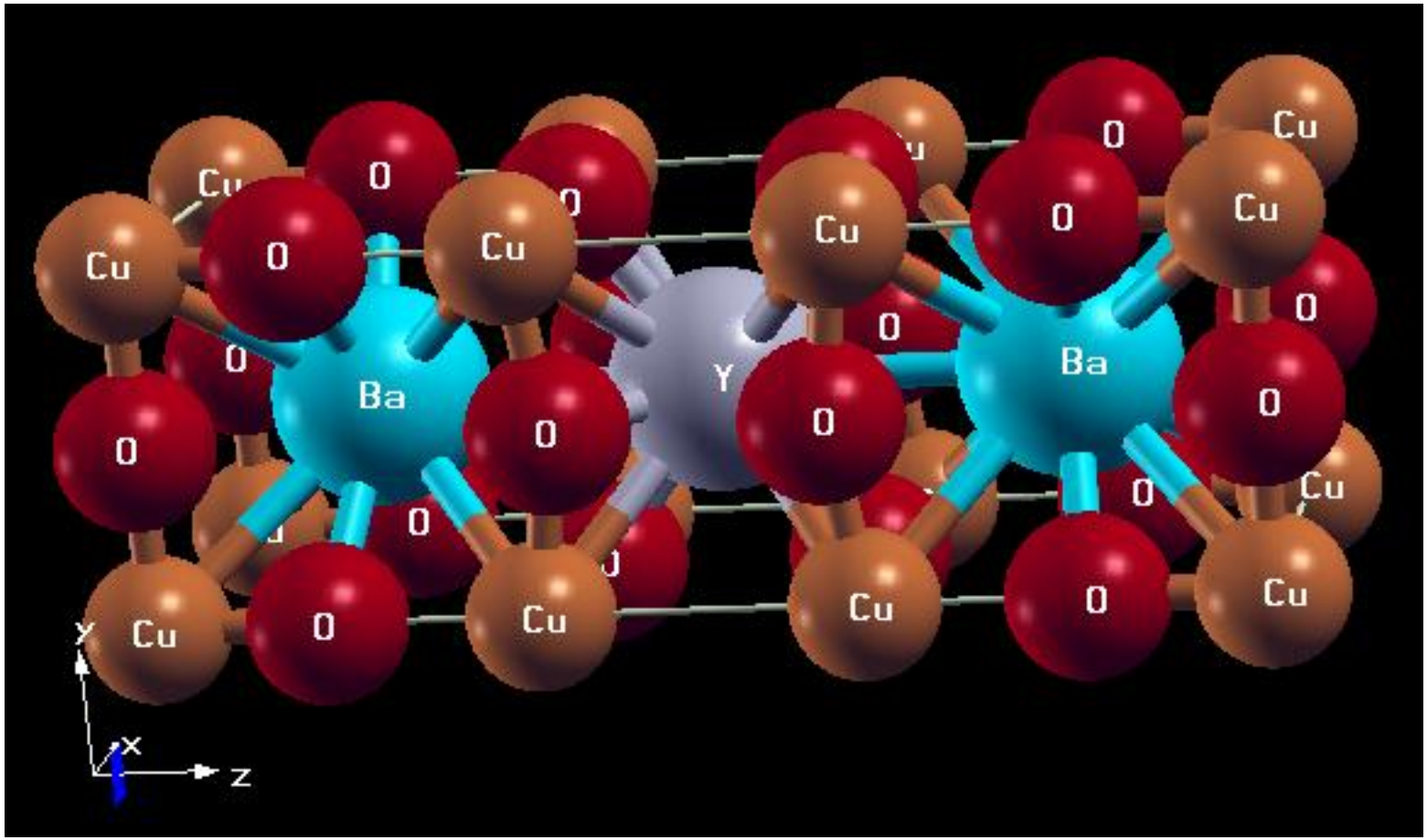
- Graphics/Visuals
  - jMol
  - XCrySDen (Kokalj)
- DFT Table Top Calculators (Kubuntu)
  - PWscf (Giannozzi)
  - PWcond (Smogunov)
  - Wannier90 (Mostofi)
- *All available for free from Quantum-Espresso and Java!*

“Power Machines in My Garage”

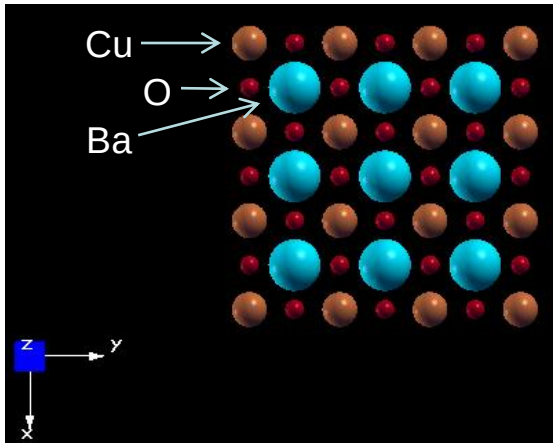
- Antpile Cluster at JPL/NASA/CalTech

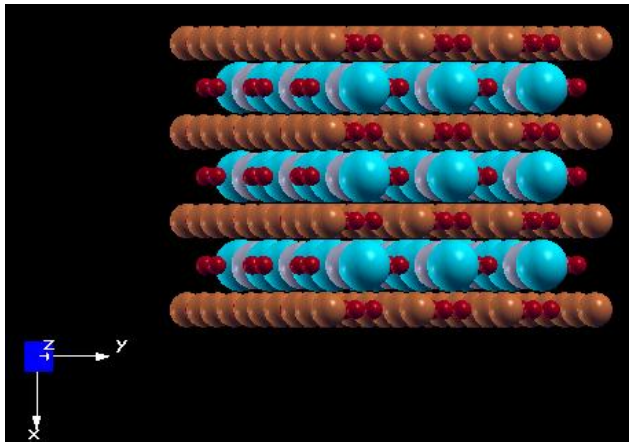
Many Thanks
to
Paul von
Allmen

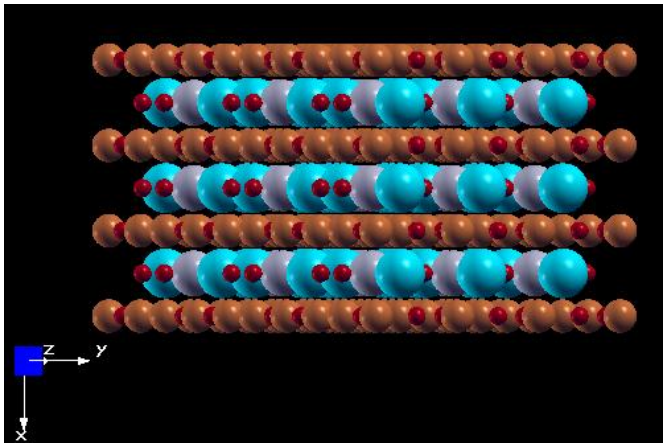
1-2-3
“The Object of My Affection”

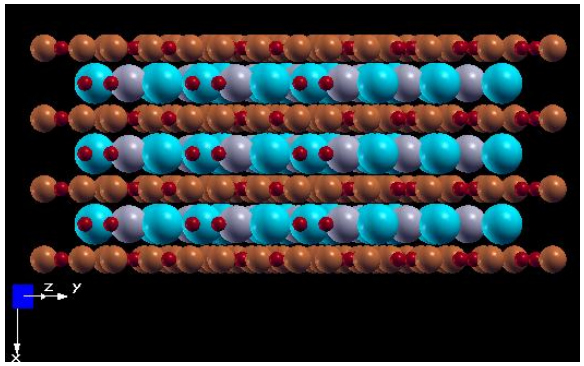


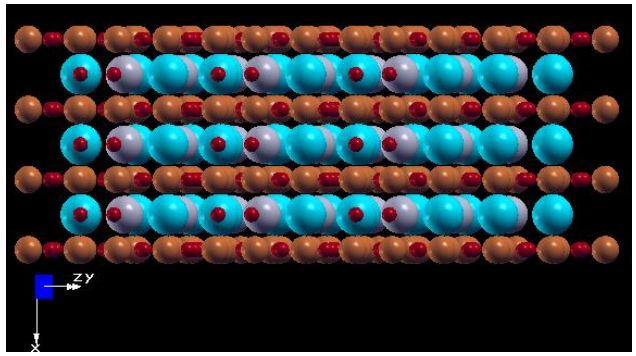
“The abc’s (xyz’s) of RE-123”

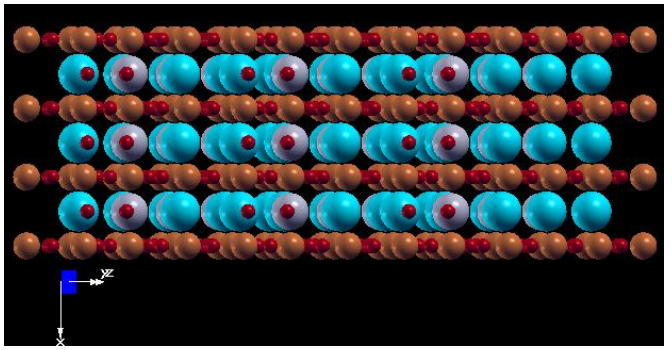


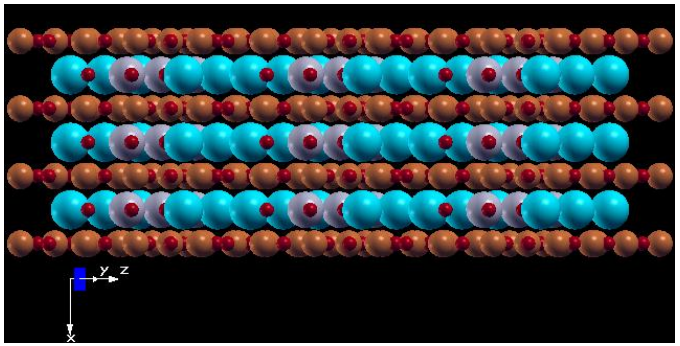


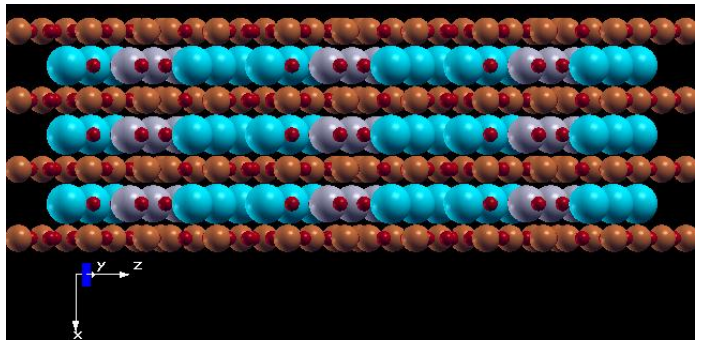




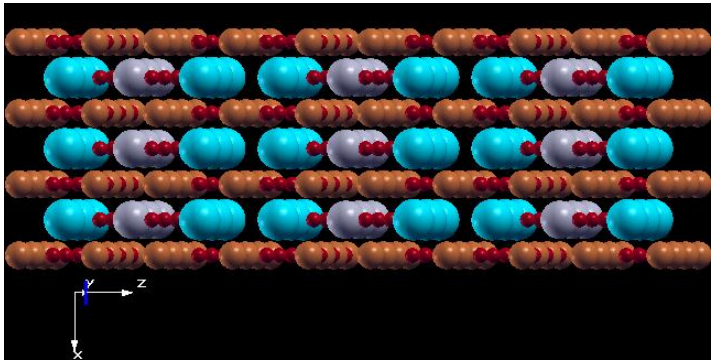


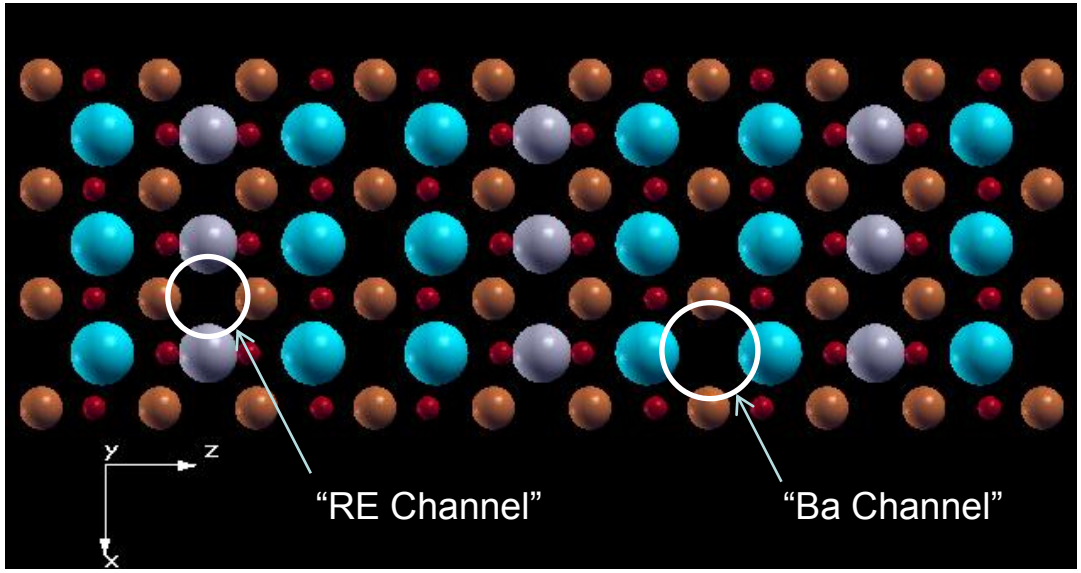




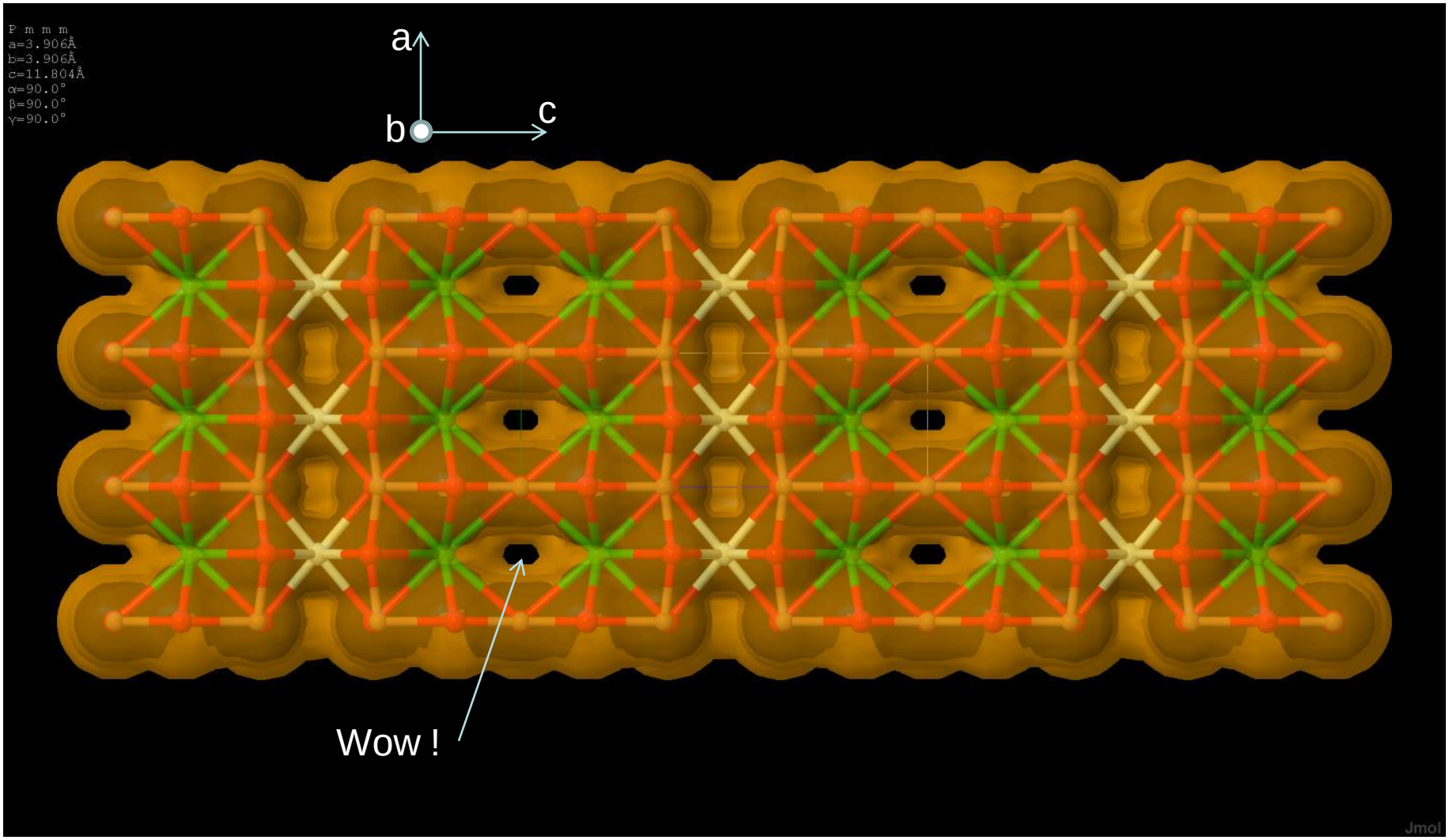


“...and Finally...”



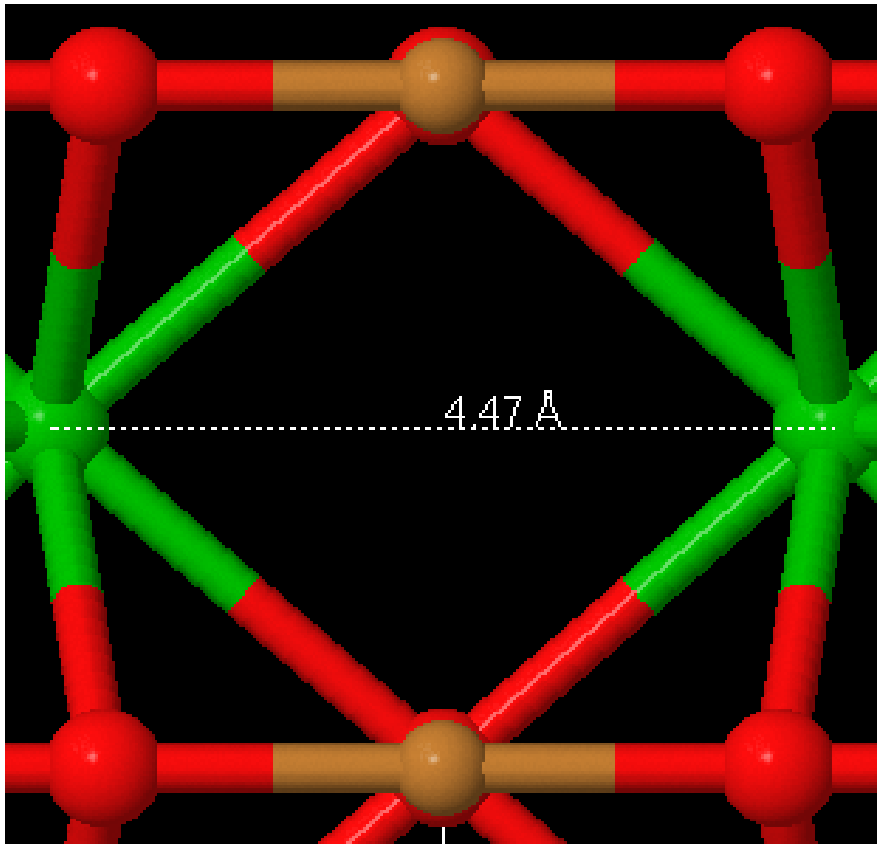


Van der Waals Surface for RE-123

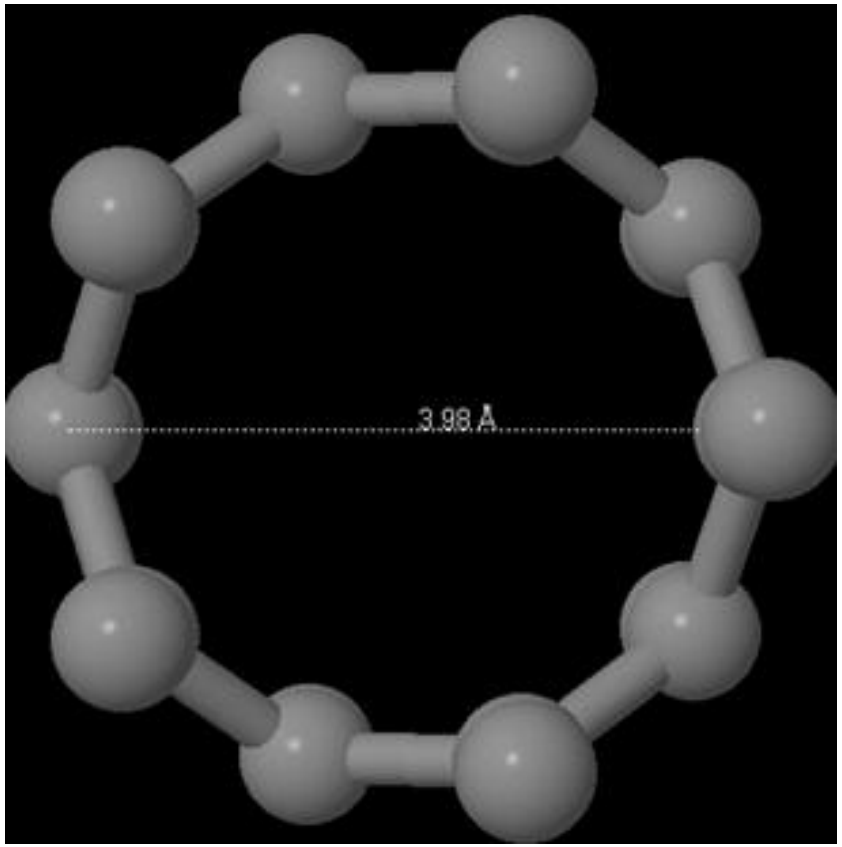


Channel Structure Comparisons

PBCO



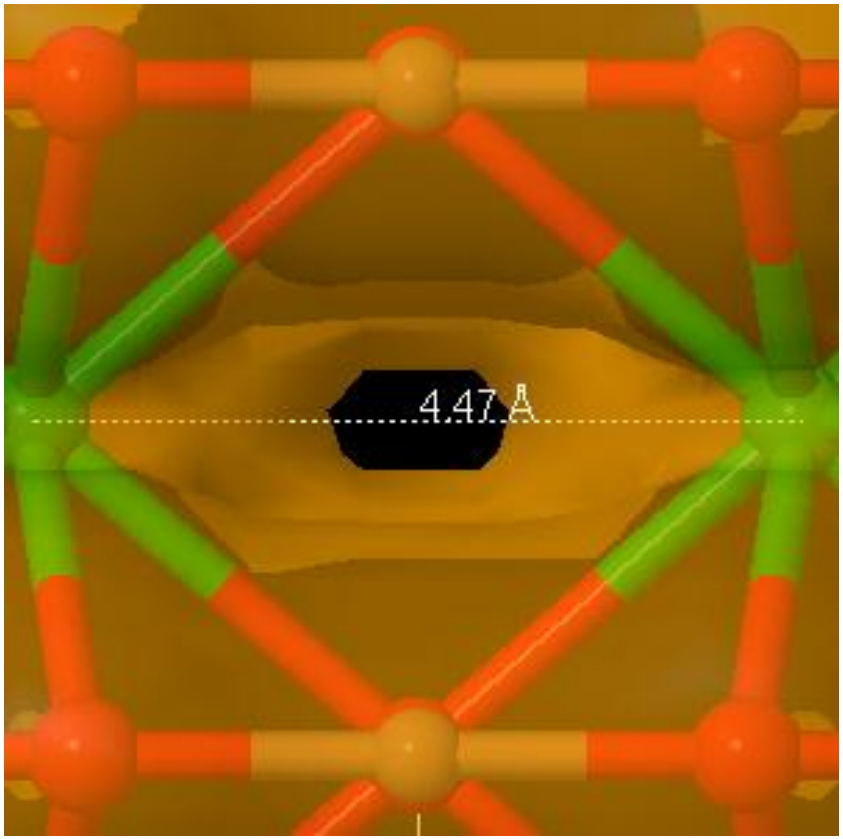
CNT-5,0



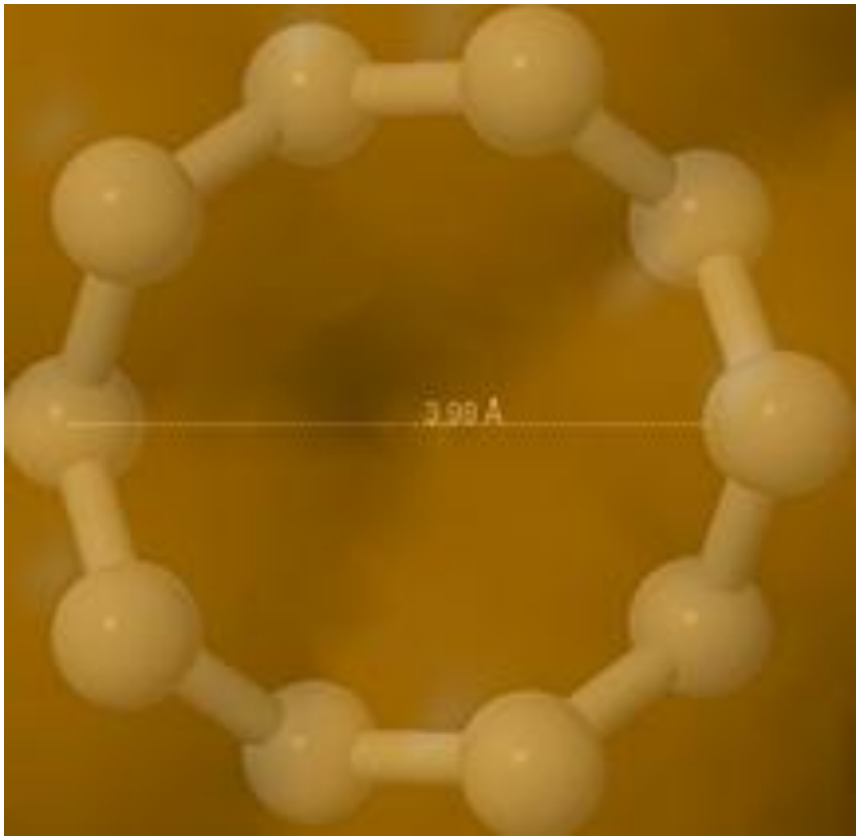
NB: Relative Dimensions Approximate

Van der Waals Surfaces

PBCO



CNT-5,0



NB: Relative Dimensions Approximate

Landauer-Buettiker Formalism

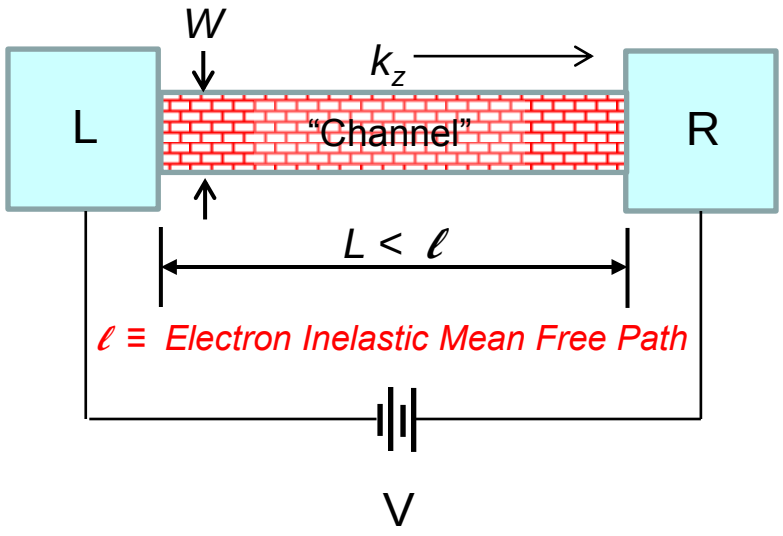
$$I_{L\to R} = \frac{2e}{h}\int_{E_{F_R}}^{E_{F_L}} T(E)[f_L(E) - f_R(E)]dE$$

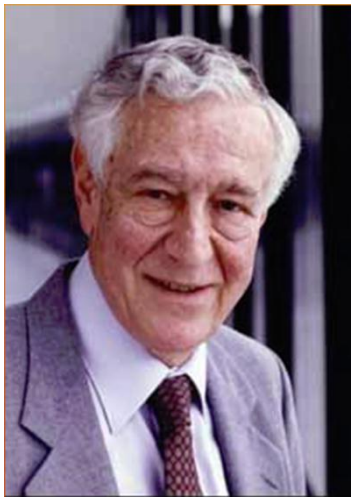
$$f_{L/R} = [1 + \exp((E - \mu_{L/R})/kT)]^{-1}$$

$$\mu_L - \mu_R = e\delta V$$

For δV small, $G = \frac{I_{L\to R}}{\delta V} = \frac{2e^2}{h}T(E_F)$,

Where $T(E_F) = \sum_{i,j} t^R_{i,j}(E_F)$, and i, j indexes the right-traveling transfer integrals of the relevant eigenstates.





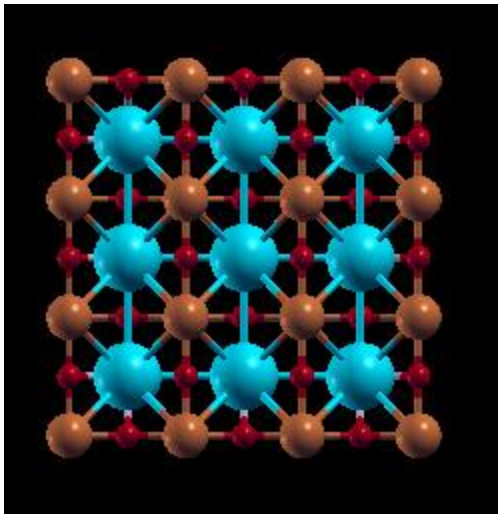
Rolf Landauer (1927-1999)

Note:

1. If $L > \ell$, then $T(E_F)$ reverts to Ohm's Law
2. If not, ballistic boundary conditions apply, a la Landauer, and $T(E_F)$ can scale from 1 to >20, depending on the number of channels (eigenstates) available for transport, times $2e^2/h = 7.75 \times 10^{-5}$ siemons = 1/12.9 $k\Omega$
3. $T(E_F)$ can be calculated using the PWcond tools with the Quantum-Espresso DFT package
4. The following calculations for RE-123 assume only one unit cell in the "channel."

YBCO-c

trans.ybcobulk



T ($2e^2/h$)

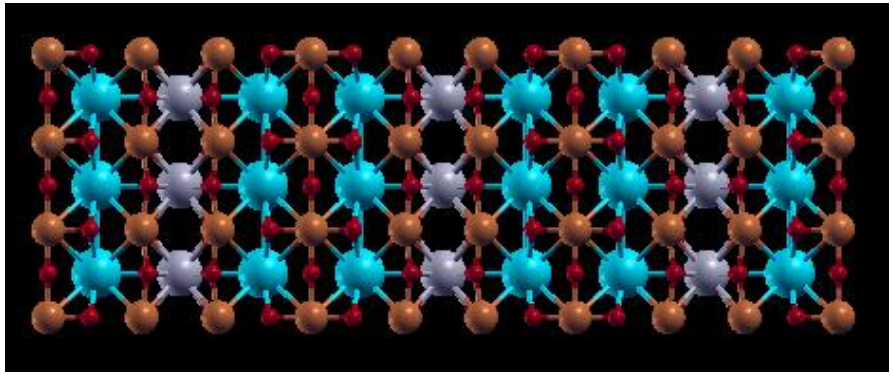
20
15
10
5
0

-6
-4
-2
0
2

E-E_f (eV)

YBCO-a

trans.ybcobulk

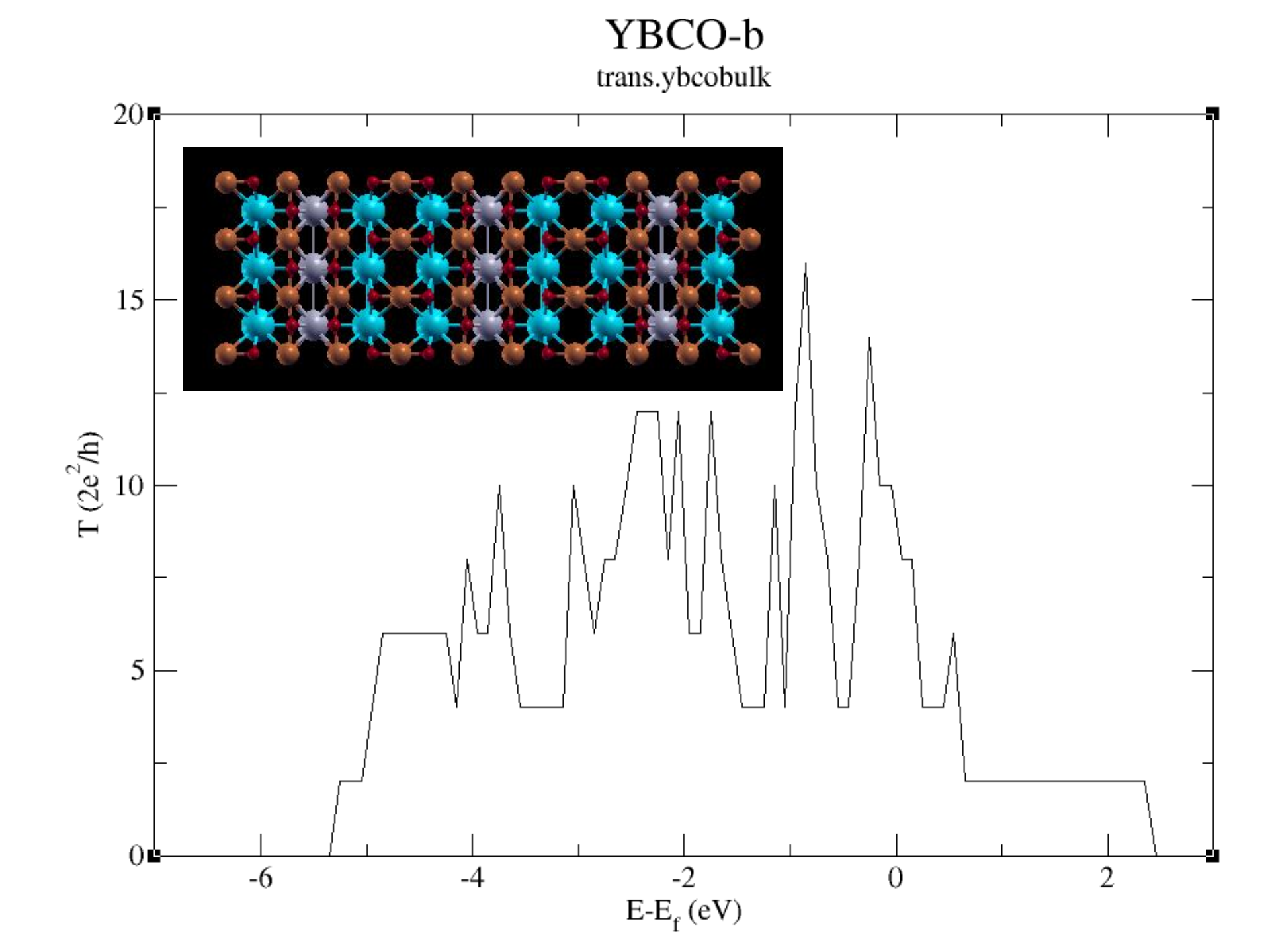


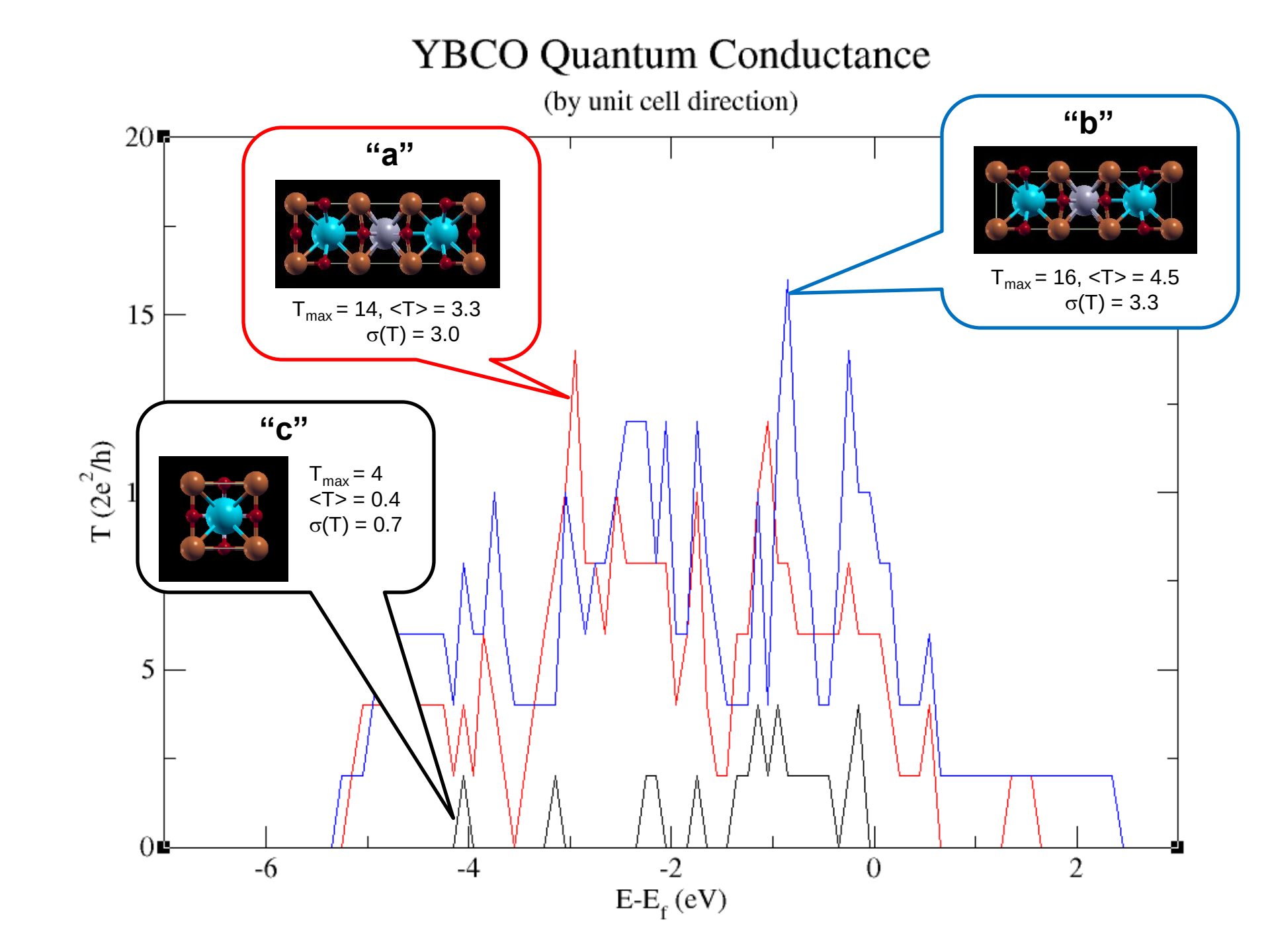
T ($2e^2/h$)

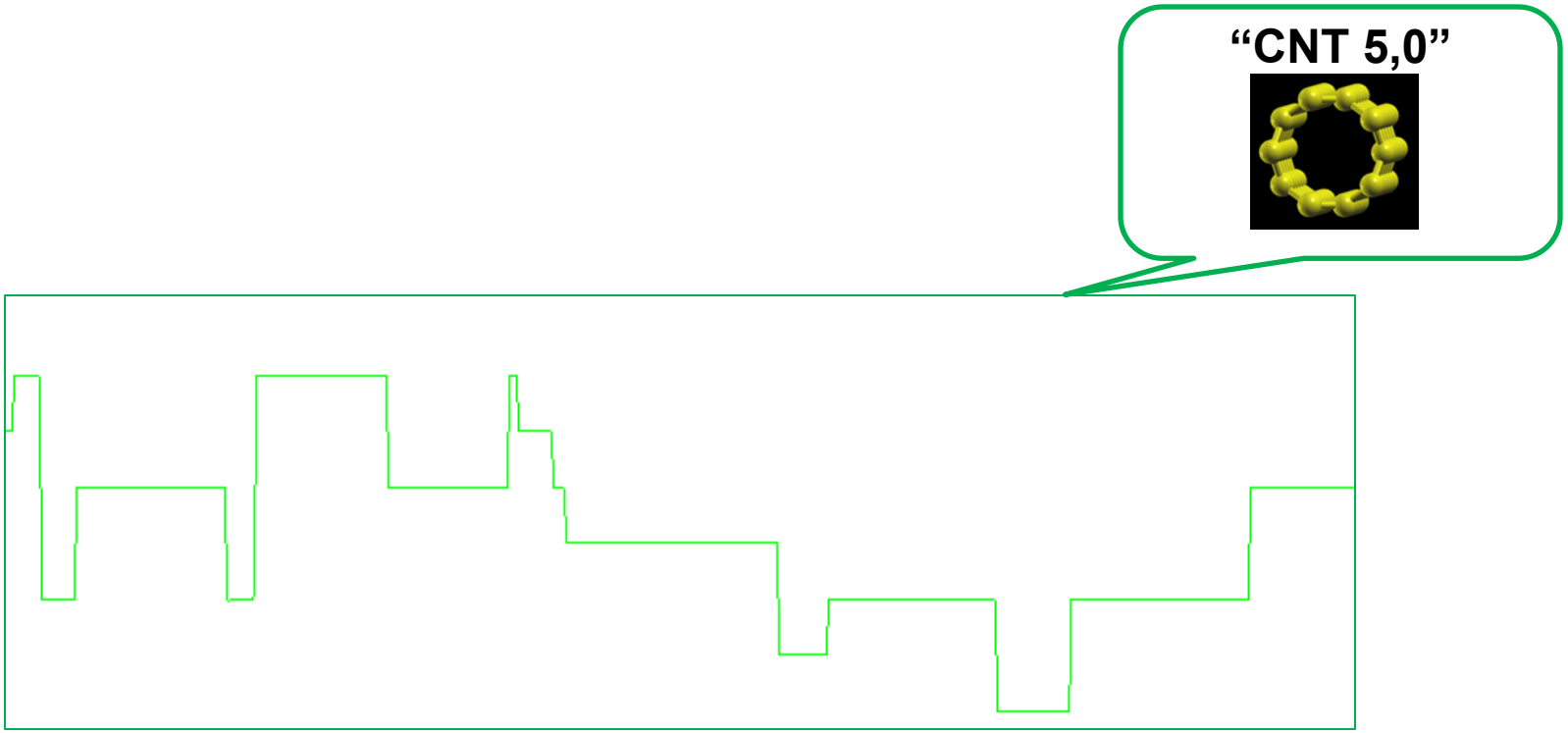
20
15
10
5
0

-6
-4
-2
0
2

E-E_f (eV)

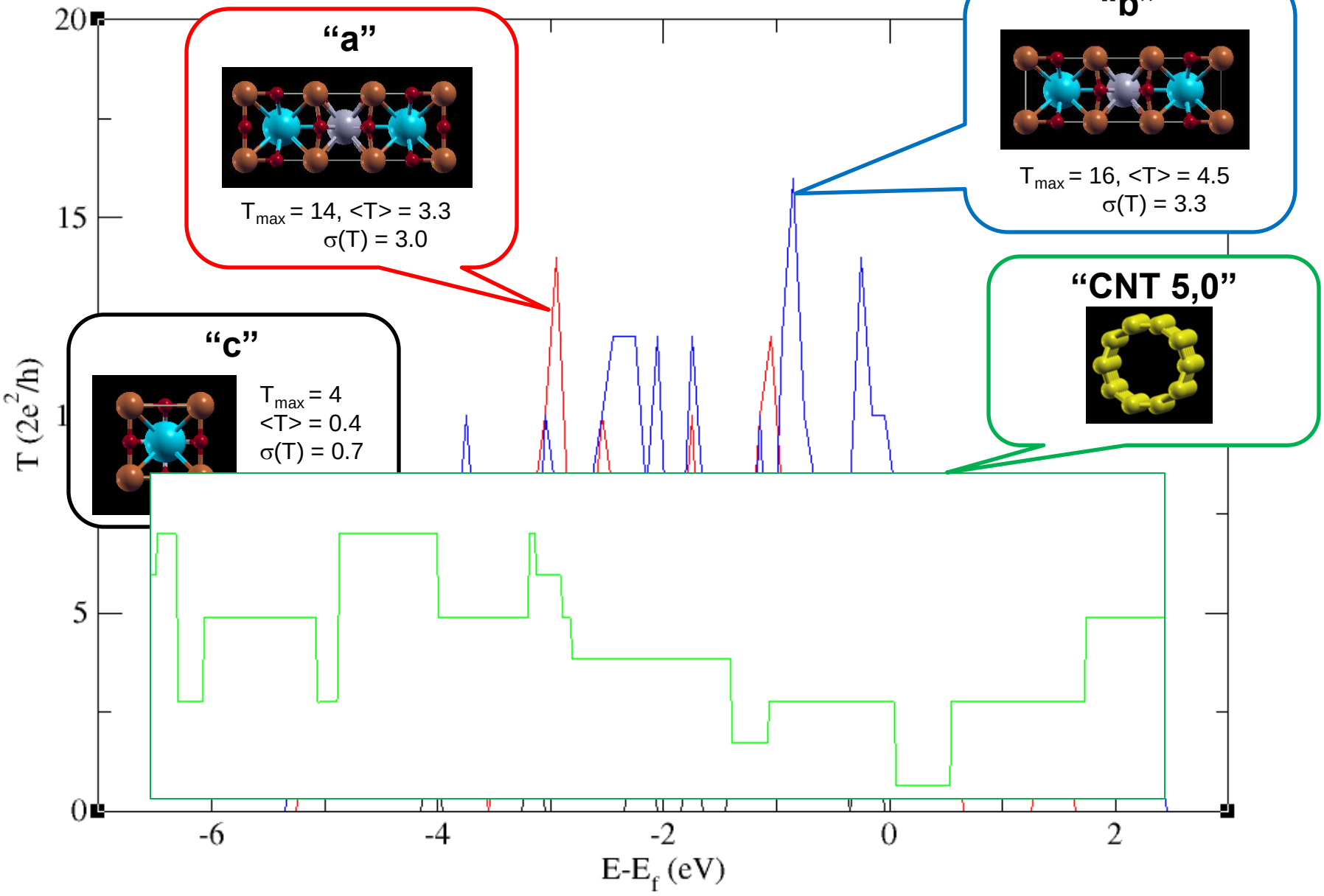

YBCO-b
trans.ybcobulk
20
15
10
5
0
T (2e²/h)
-6
-4
-2
0
2
E-E_f (eV)


YBCO Quantum Conductance
(by unit cell direction)
"a"
T_{max} = 14, <T> = 3.3
σ(T) = 3.0
"b"
T_{max} = 16, <T> = 4.5
σ(T) = 3.3
"c"
T_{max} = 4
<T> = 0.4
σ(T) = 0.7
T ($2e^2/h$)
E-E_f (eV)
20
15
1
5
0
-6
-4
-2
0
2


“CNT 5,0”

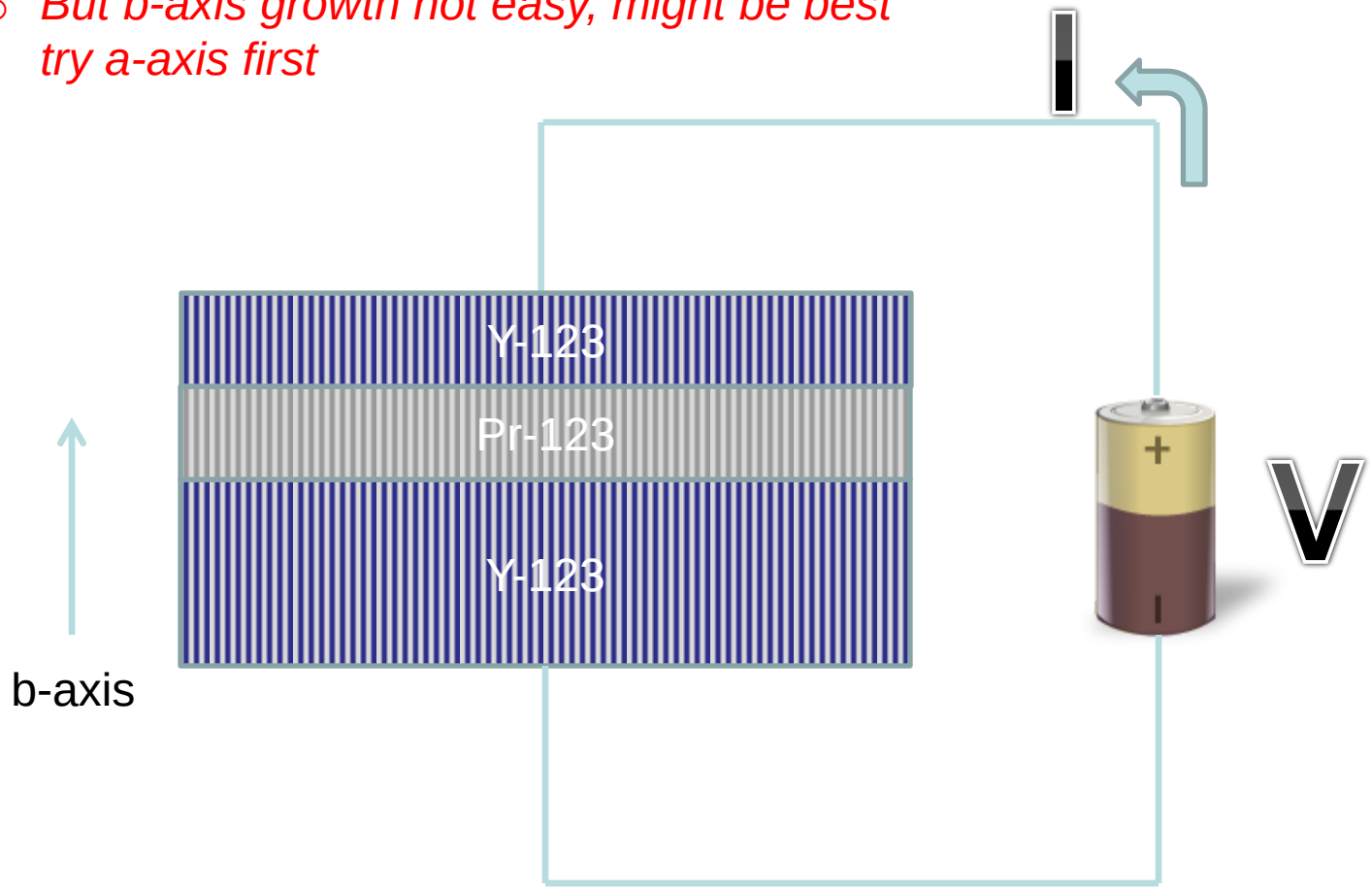
YBCO Quantum Conductance

(by unit cell direction)



“Need to Test by Experiment”

- Y-123 Conducting
- Pr-123 Insulating (10 monolayers, ~ 50 Å)
- Can be made by MBE
  - *But b-axis growth not easy, might be best try a-axis first*



“The Last Word(s)”

- Quantum Conductance in the a, and especially b, directions of RE-123 appears plausible.
- Coulomb correlation (aka “Hubbard U”) needs to be taken into account.
- Experimental verification is required.
- Can the effect be exploited for FET gate applications? Or maybe something completely new?
  - Stay tuned
  - *Attend my talk at the 2013 APS March Meeting (see you in Baltimore)*