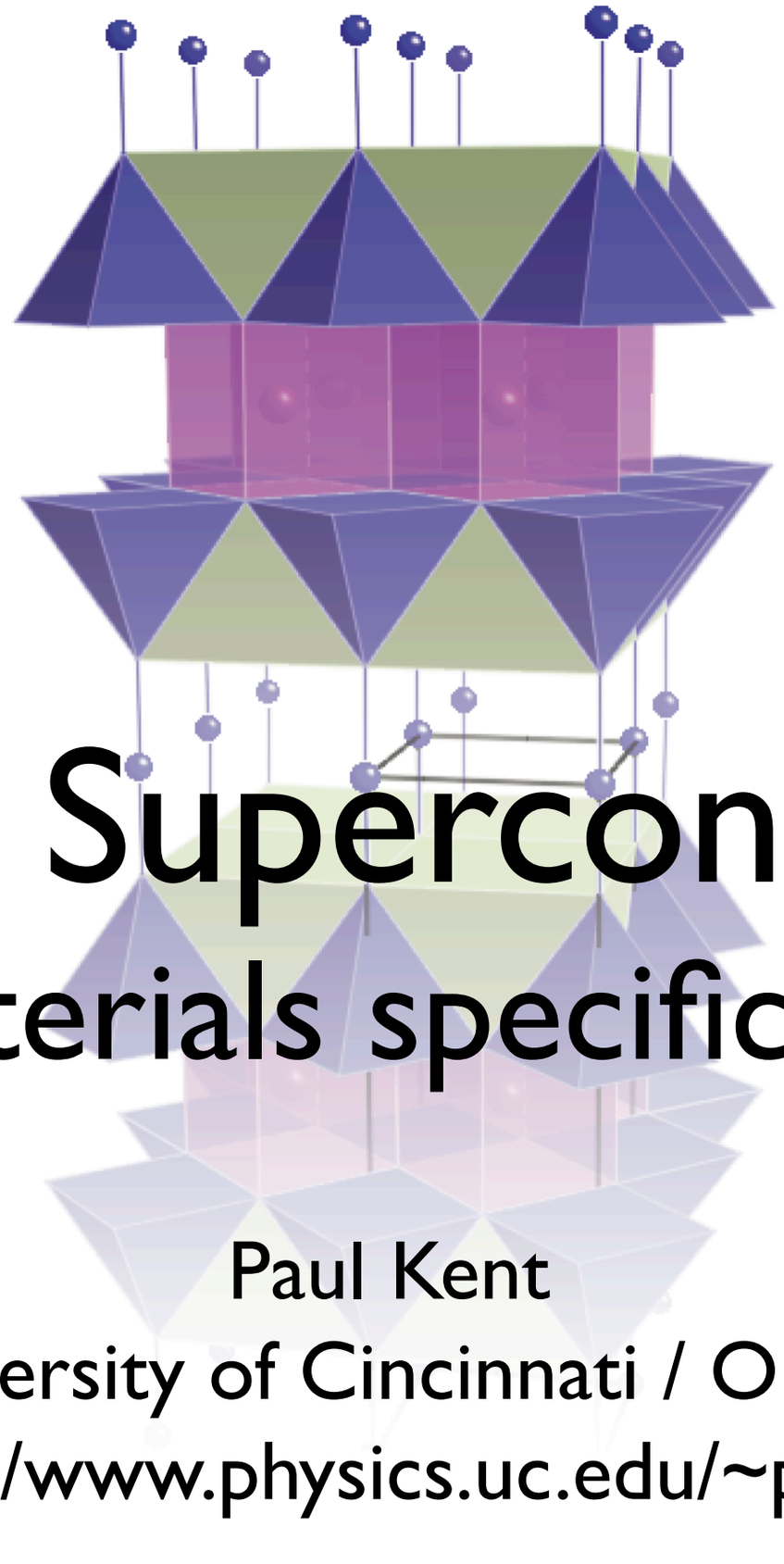

Cuprate Superconductors:
Towards materials specific calculations

Paul Kent
University of Cincinnati / ORNL
http://www.physics.uc.edu/~pkent

Acknowledgements

Collaborators:

Mark Jarrell, Alexandru Macridin / UC

Thomas Maier, Thomas Schulthess / ORNL

Ole K. Andersen, Tanusri Dasgupta, Ove Jepsen / MPI Stuttgart

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DOE / CMSN

Computer time:

Cray X1 / ORNL

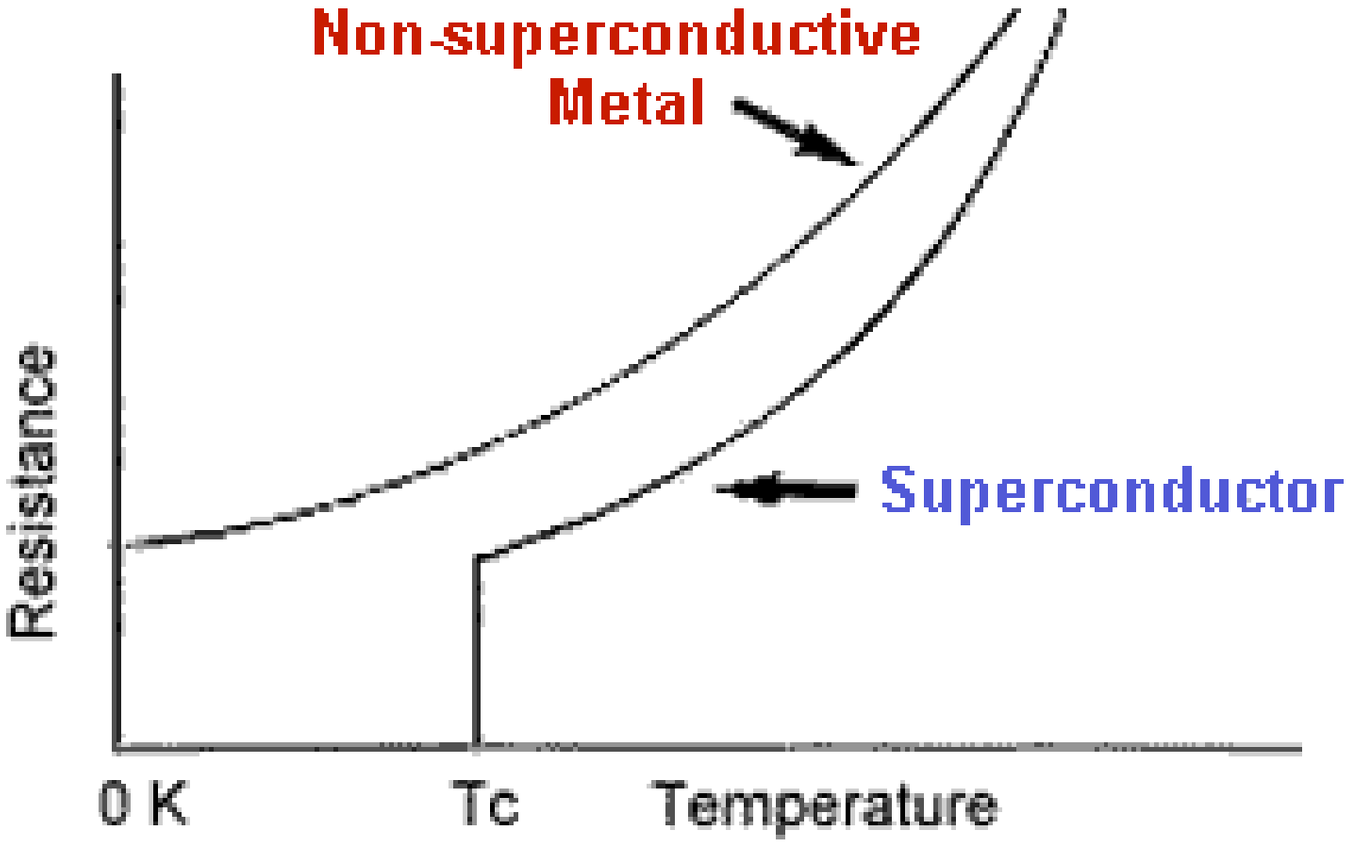
Figures:

superconductors.org
DOE
APS

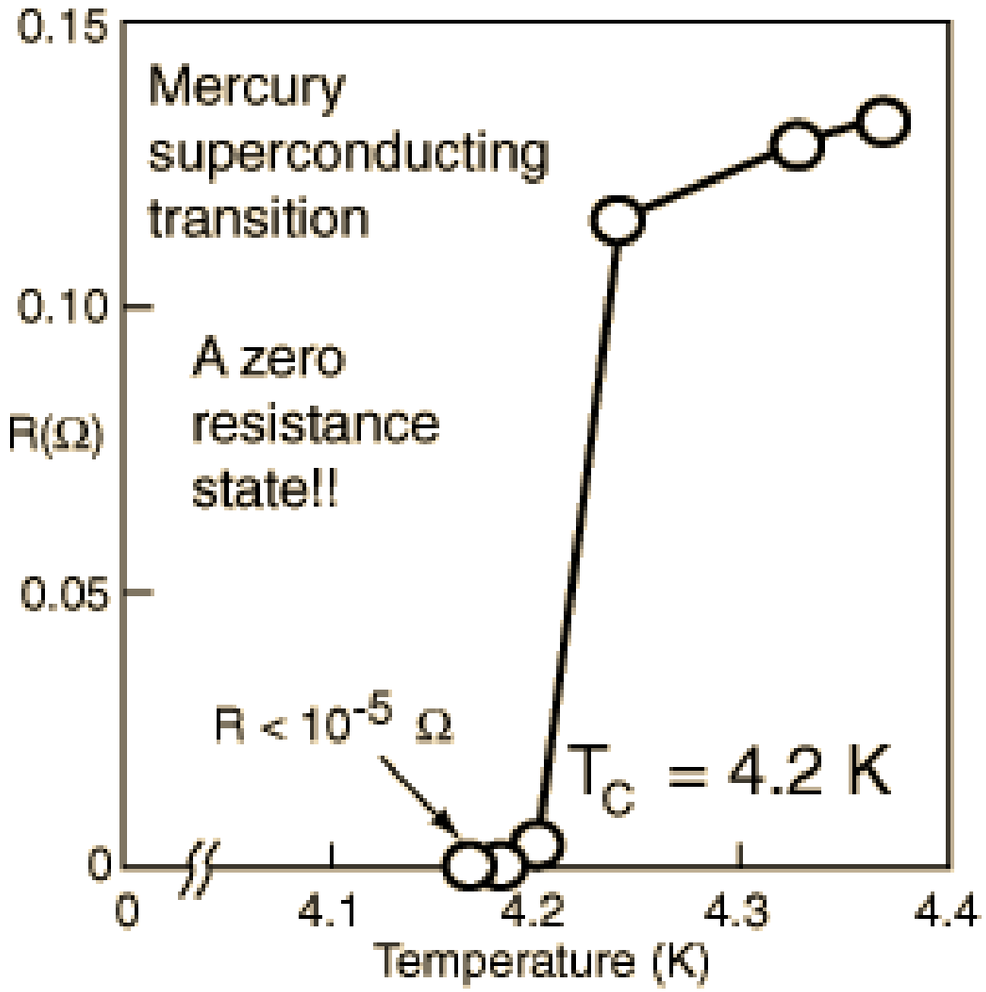
Outline

1. Superconductivity Background
2. Model theories (?)
3. Materials specific simulation (?)
4. Next Steps and Summary

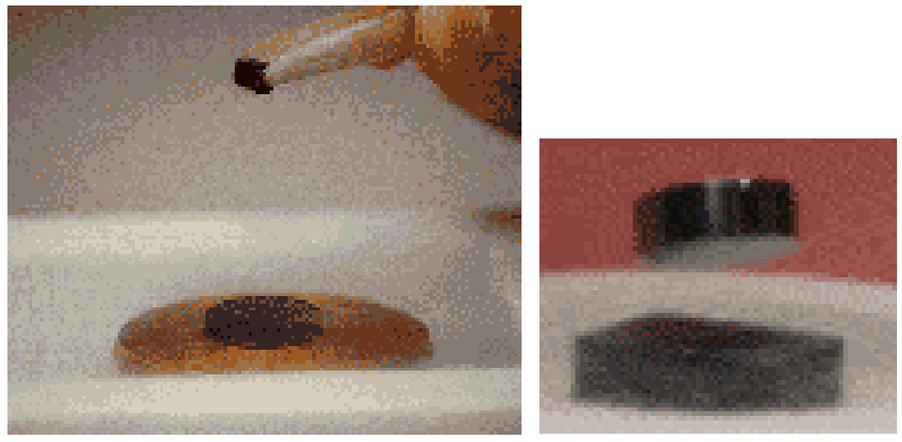
Superconductivity



Superconductivity in Mercury

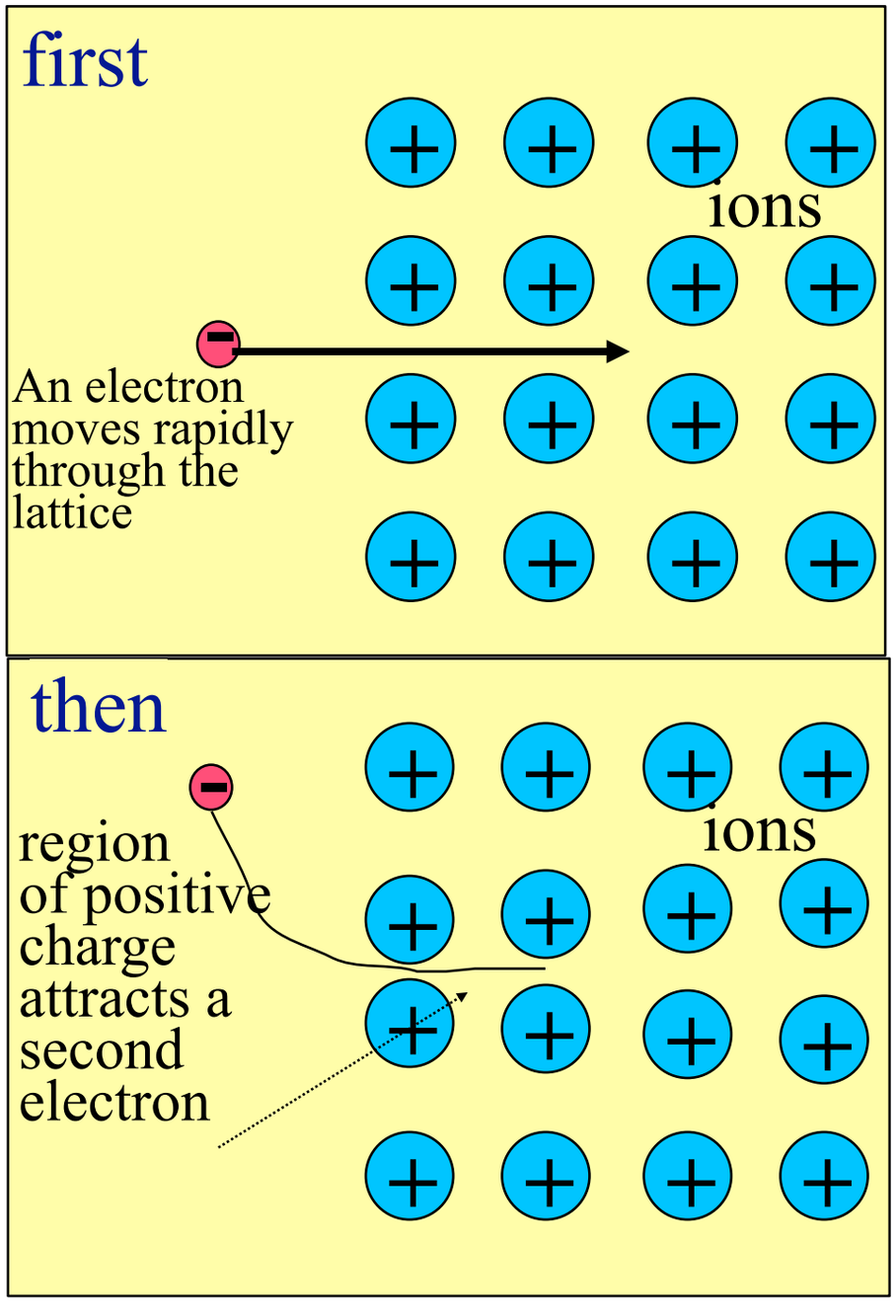


H.K. Onnes, Commun. Phys. Lab. **12** 120 (1911).



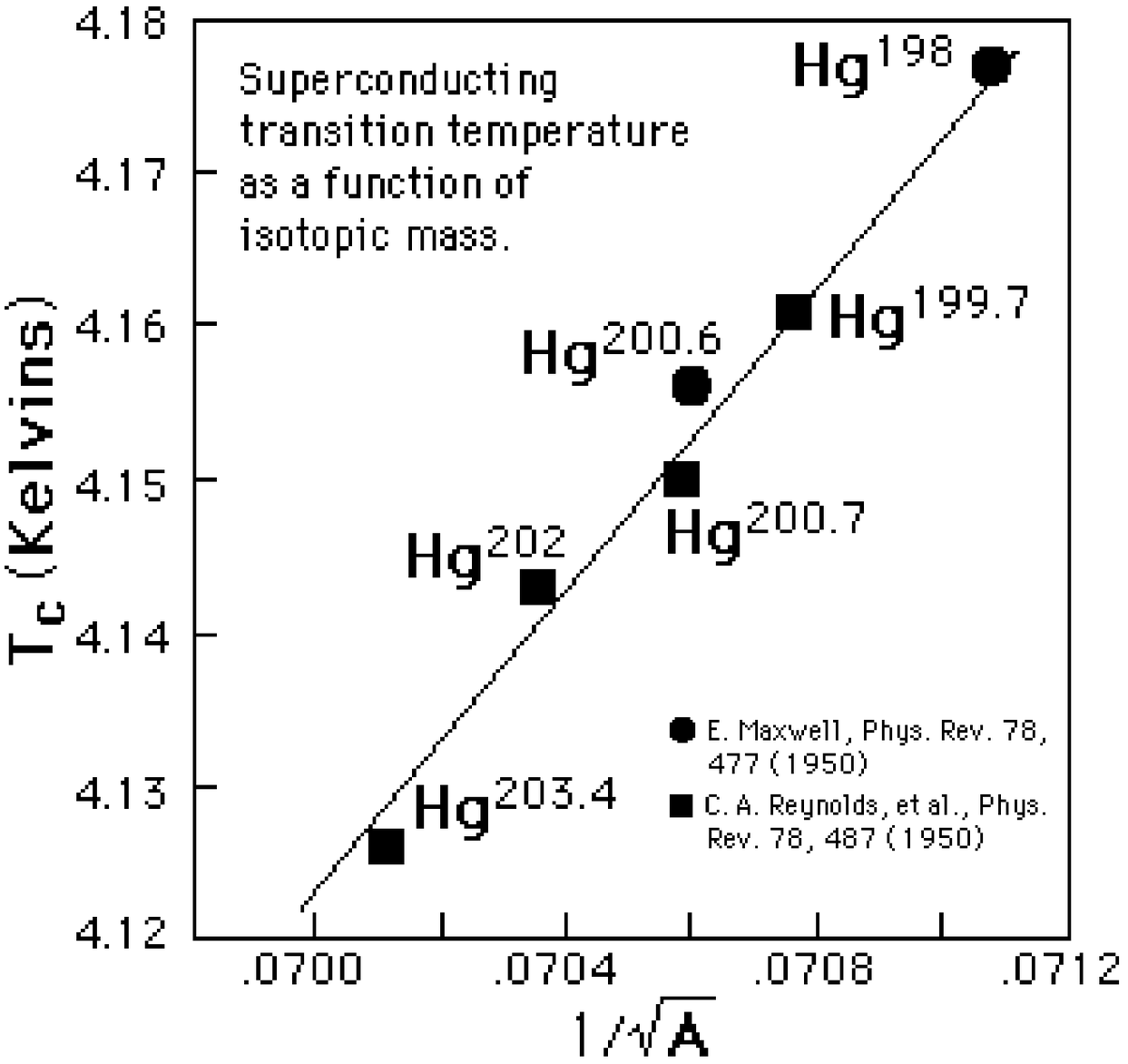
H. K. Onnes
1913 Nobel Prize (He)

Conventional Superconductors

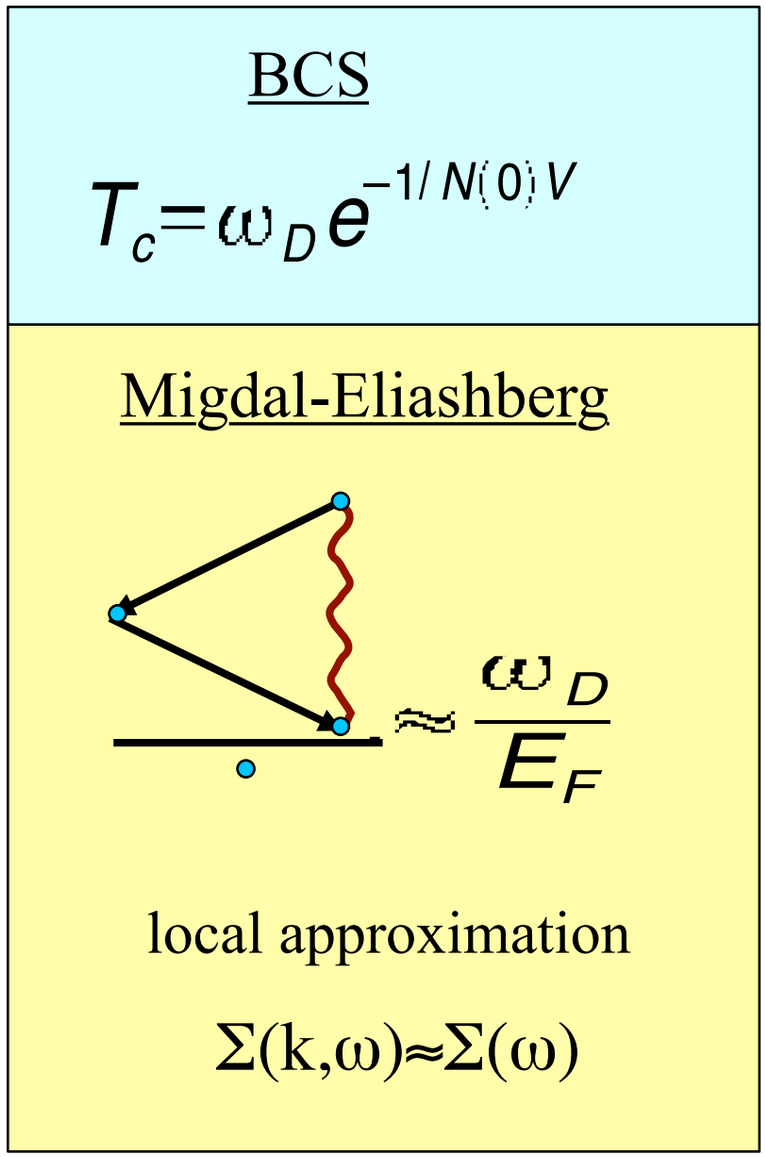


- Pairing due to phonon-mediated pairing potential
- Fermi-liquid Normal State
- Moderately Correlated Systems
- s-wave

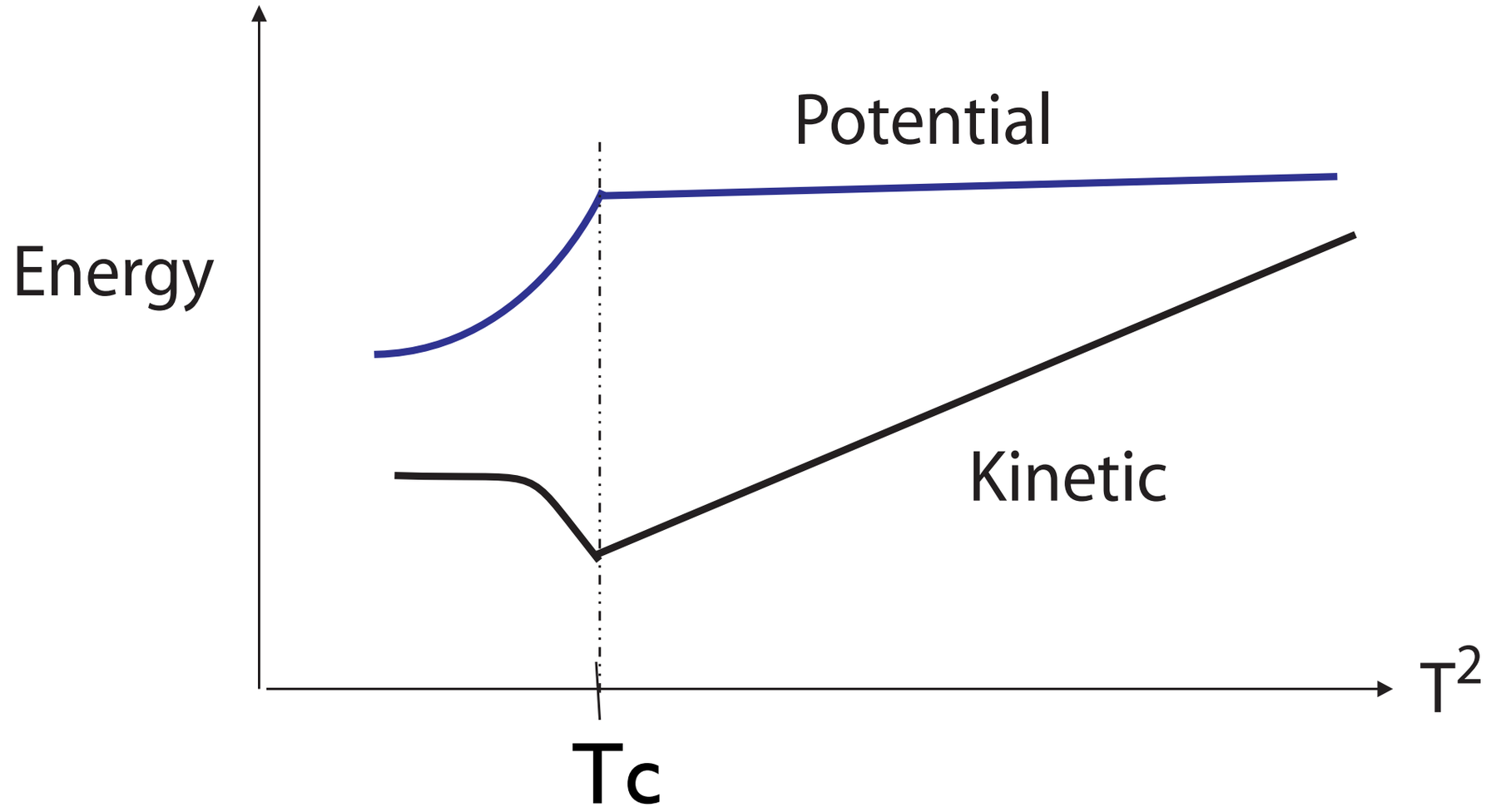
The Isotope Effect (the smoking gun)



BCS



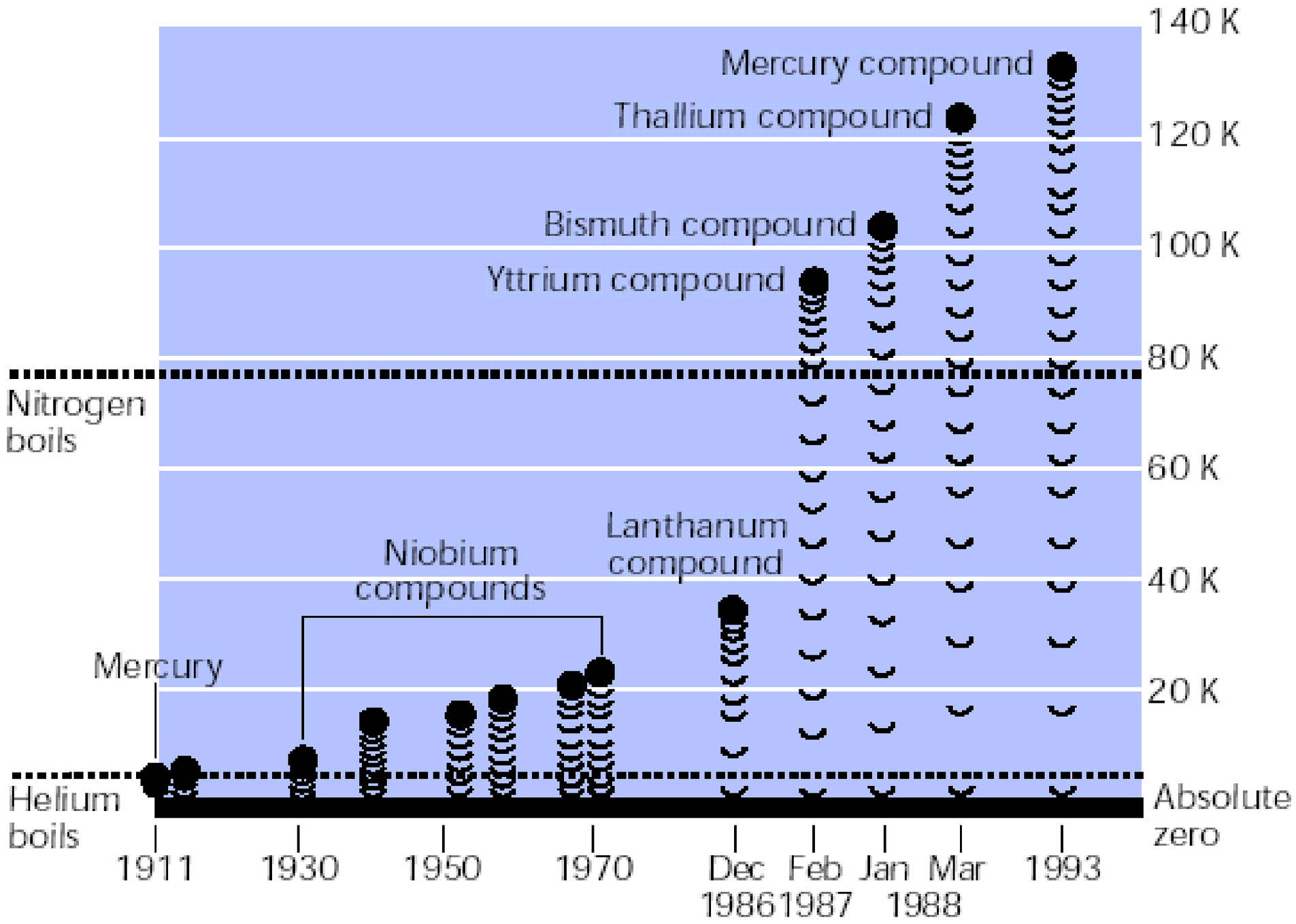
Pairing is due to potential energy recovery



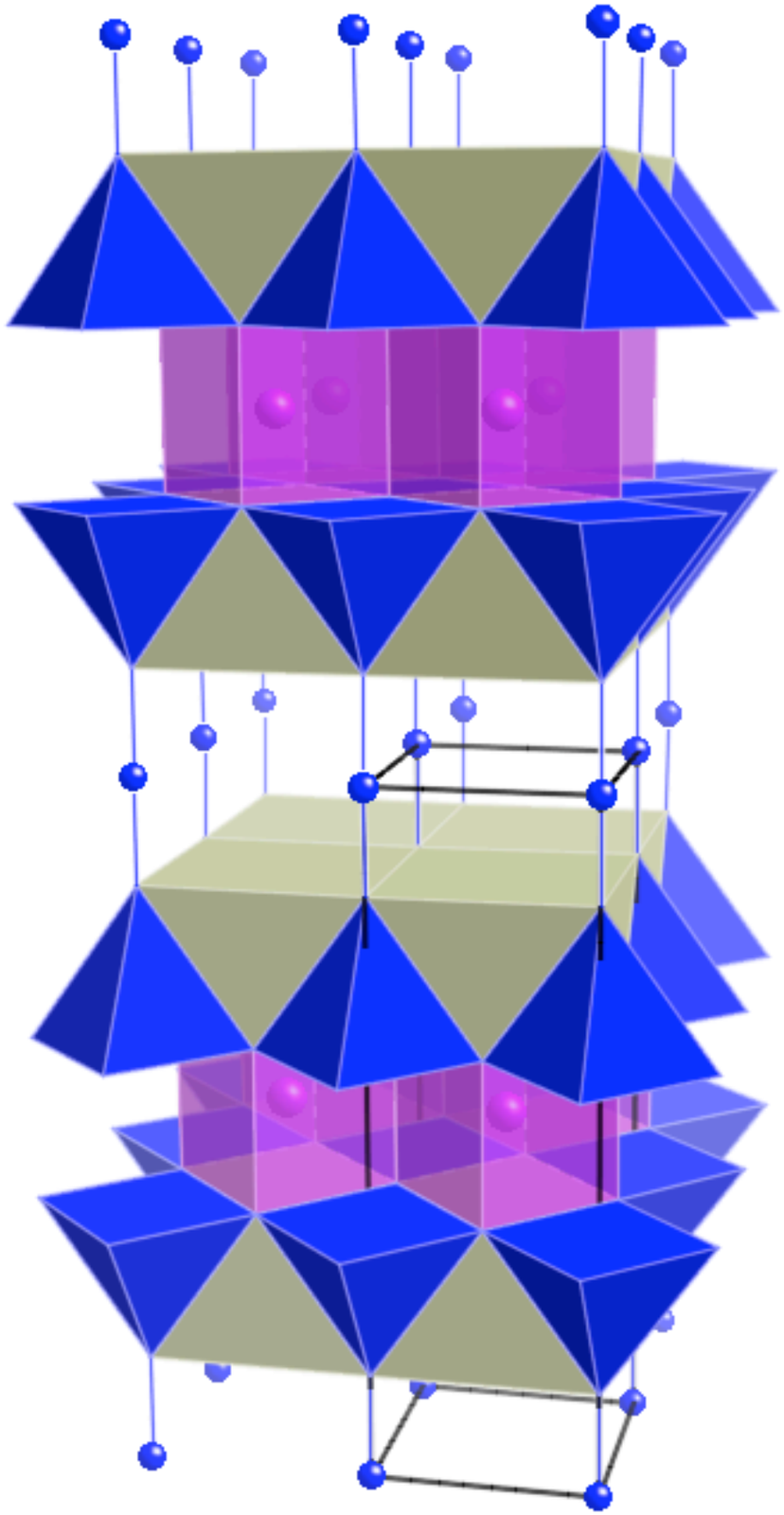
System recovers substantial potential energy by forming pairs. However, paired electrons must occupy states outside the Fermi sea, i.e. states with an increased kinetic energy.

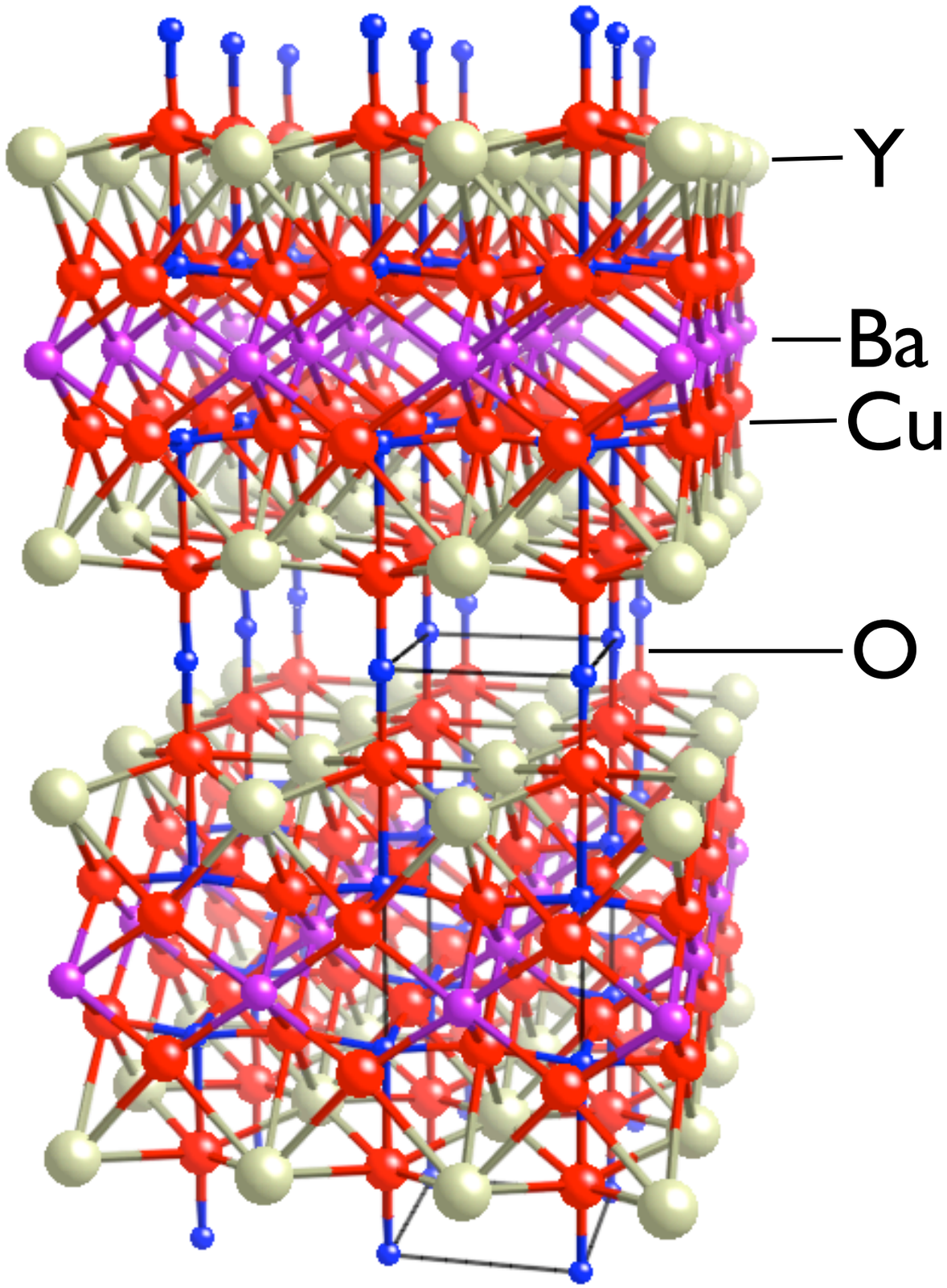
New superconductors ('86)

Pressure
168K



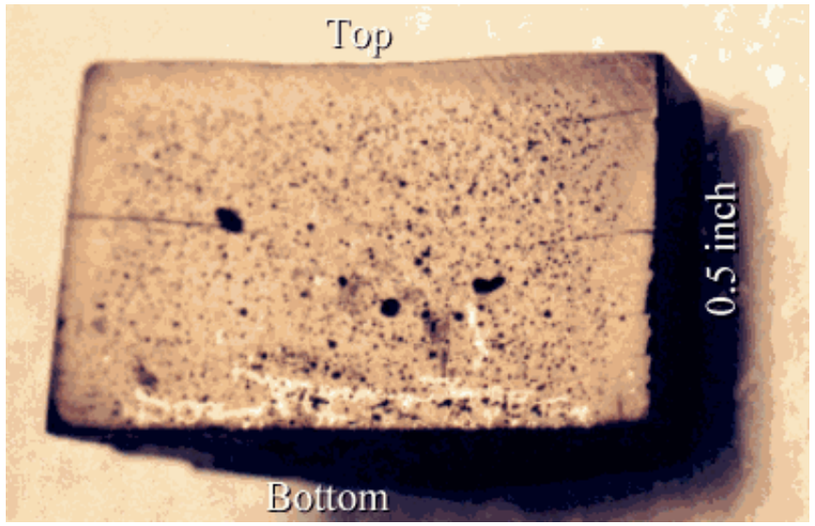
DOE figure



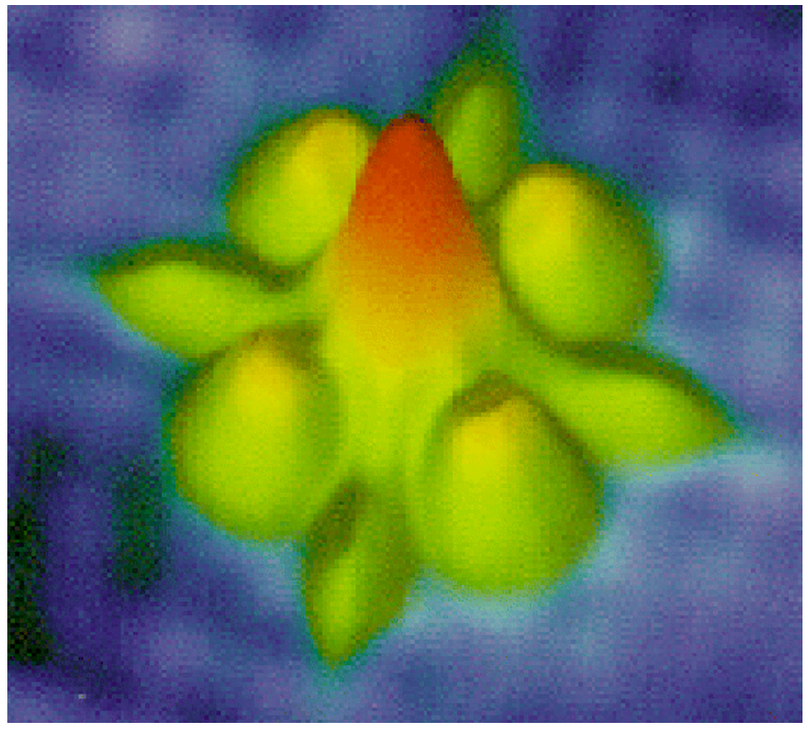


YBa2Cu3O6

Cuprates: Unusual Superconductors



Ceramic material



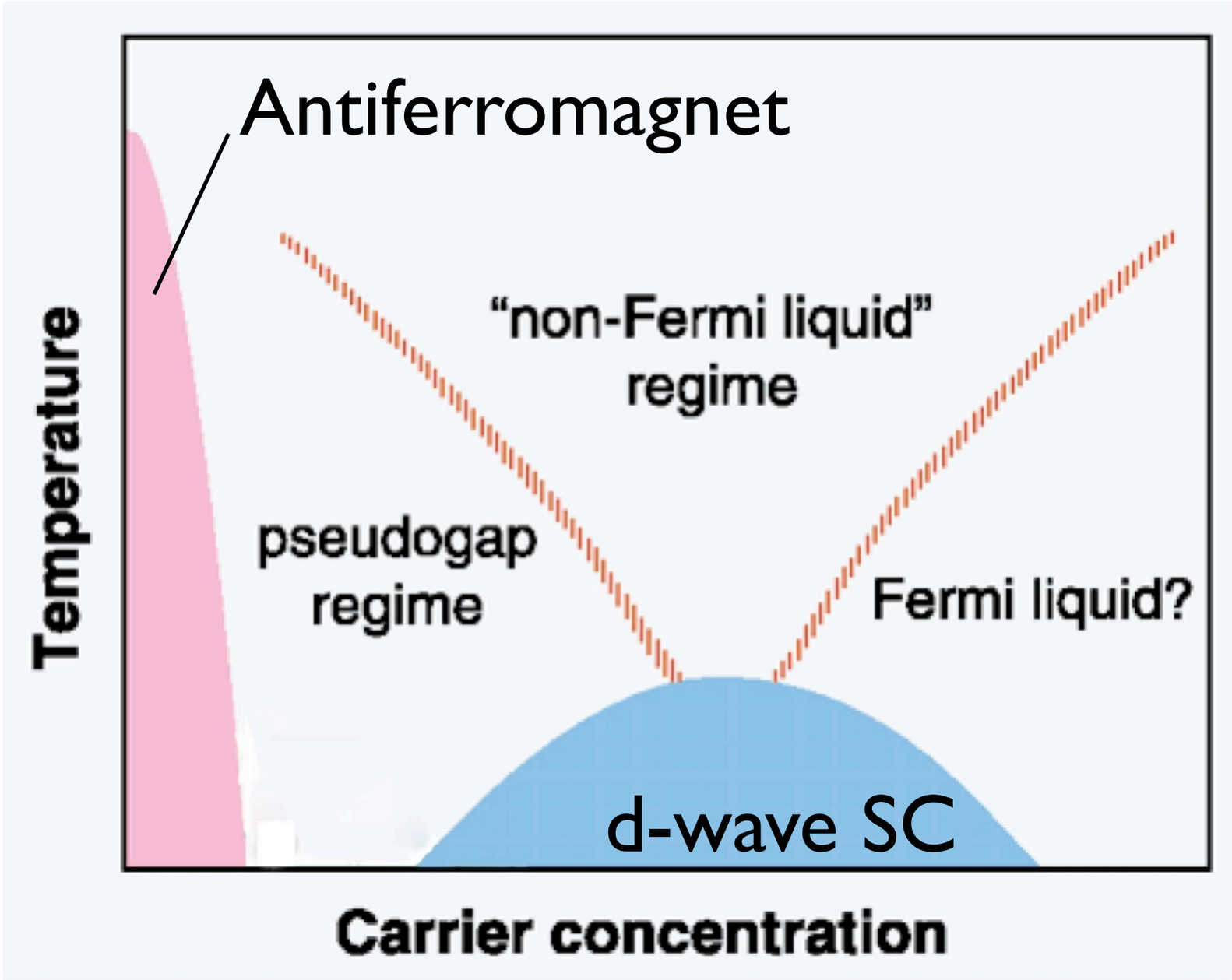
S. Pan, dI/dV at resonance

- No BCS-like phonon/isotope "smoking gun"
- Mechanism?
- Non-Fermi liquid underdoped normal state (pseudogap)
- Doped Mott insulator
- d-wave
- Kinetically Driven Pairing

Alex Müller and Georg Bednorz
1987 Nobel Prize

Complex phase diagram

Unlike BCS, must dope to ~15% holes for highest Tc

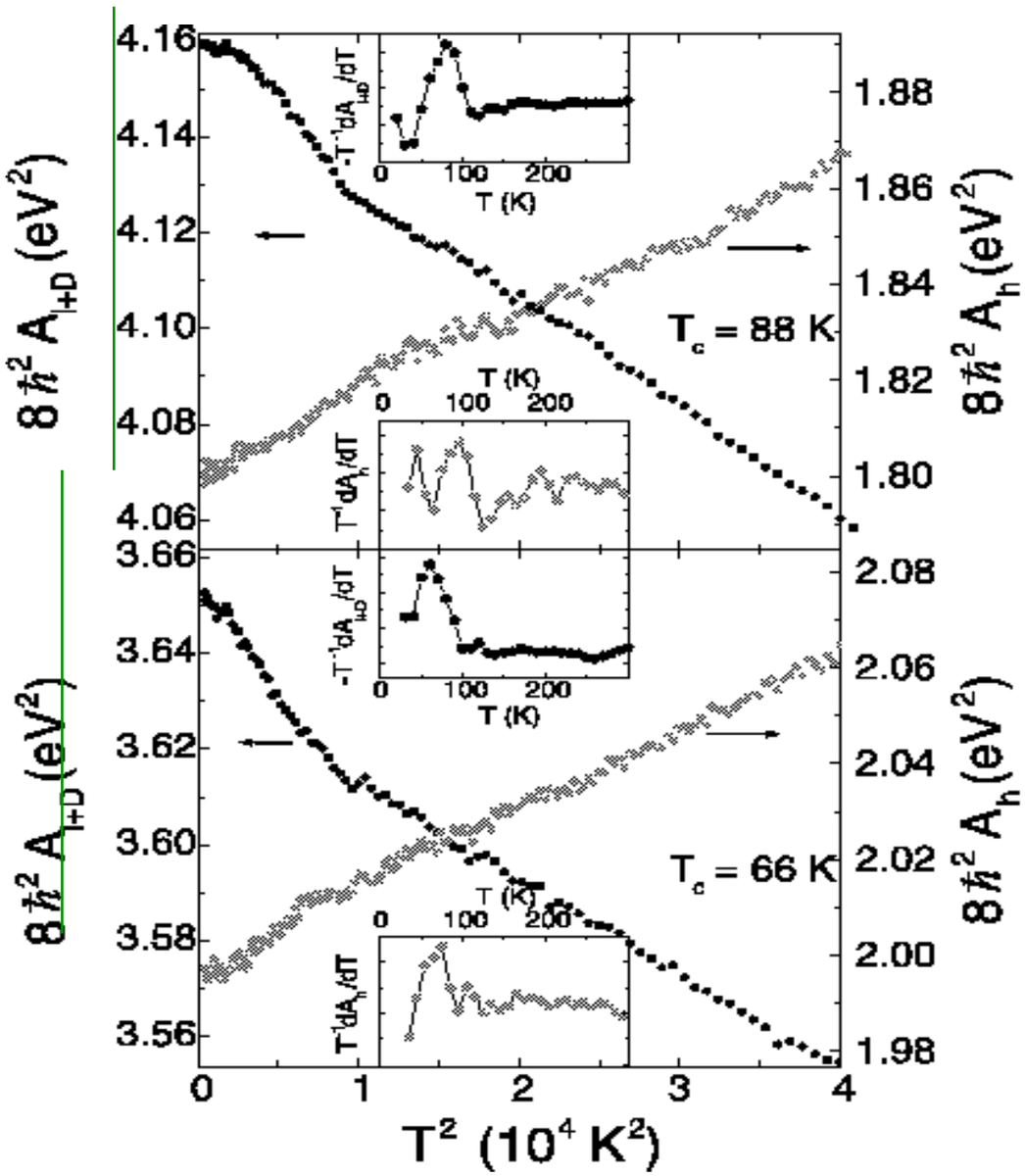


Kinetic Energy Reduction (opposite of BCS)

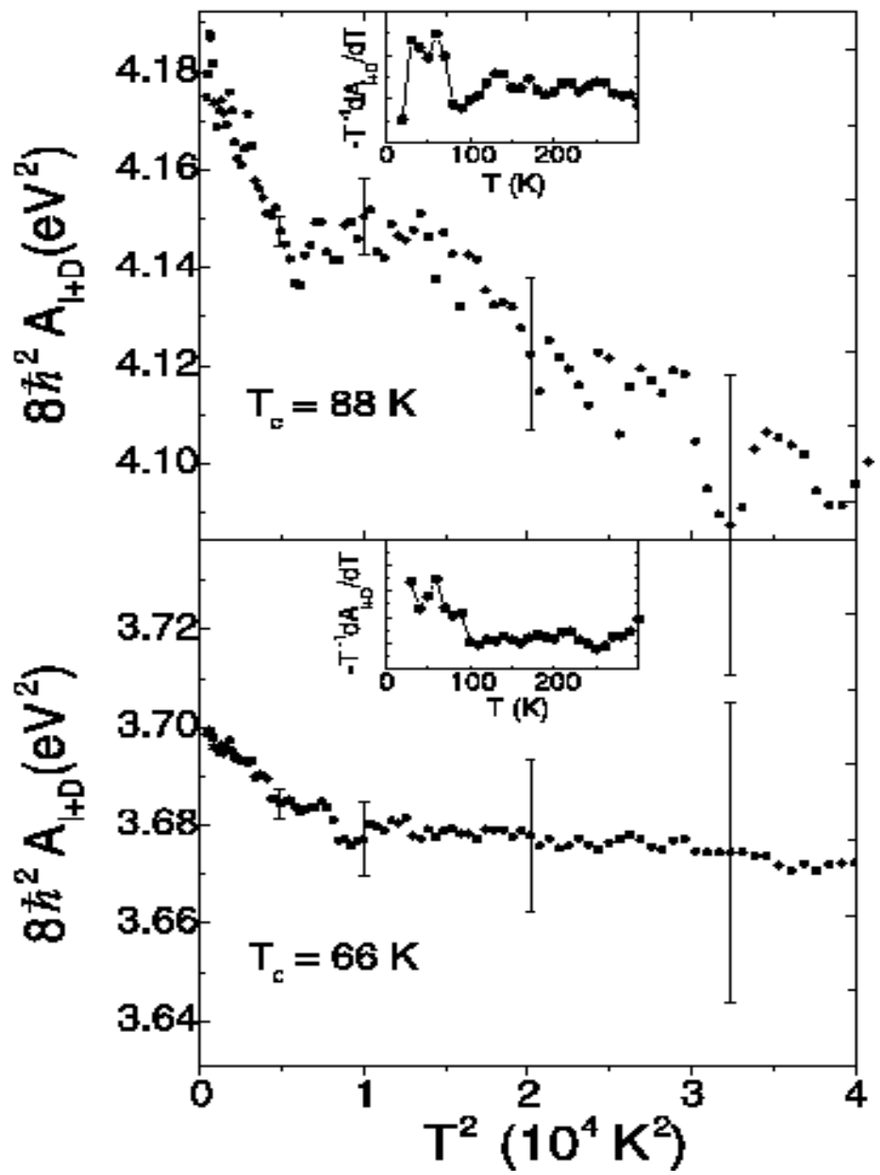
From spectroscopic ellipsometry. Bi2Sr2CaCu2O8 samples. Molegraaf Science **295** 2239 (2002)

A_{1+D}= - kinetic energy

Fit to Drude-Lorentz Osc.



Kramers-Kronig



Kinetic Energy reduction is roughly 1meV > condensation energy!

Meanwhile...

(Back in the real world)

American Superconductor

http://www.amsuper.com/

Google

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Wind Energy

Search Go

American Superconductor Announces Continued Rapid Advancement in 2G Technology

Industrial manufacture of HTSC wires, power machinery (motors, generators) exploiting high current densities achievable

Outstanding questions
(19 years later)

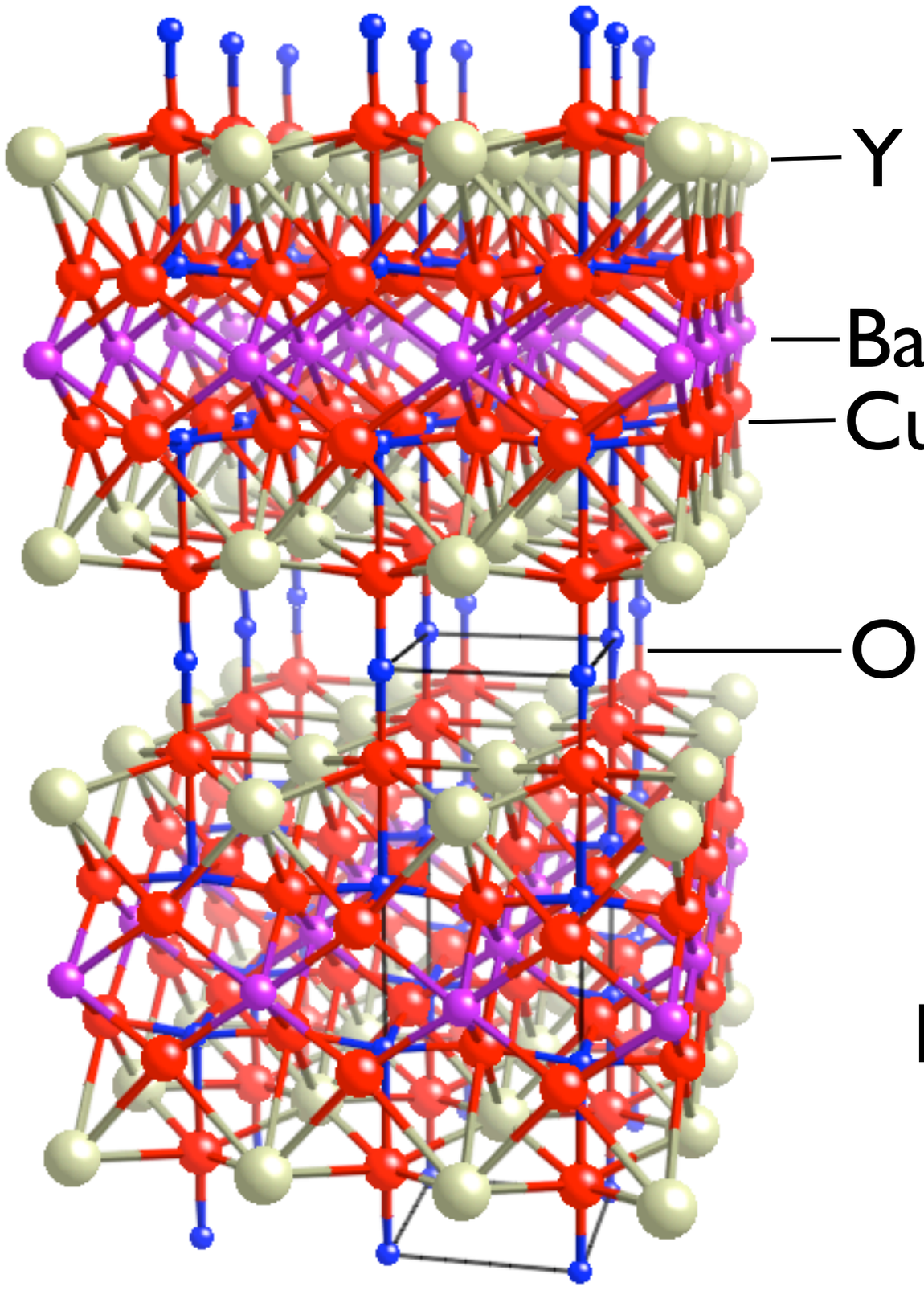
- What is the principal mechanism?
  - Electrons? Phonons? Both? Other?
  - Does material A, B, or C have higher Tc?
  - Influence of pressure, magnetic fields?
  - Other materials with same mechanism?

    c.f. new BCS-like MgB2 in 2001, 39K
  - ...many others

Outline

1. Superconductivity Background
2. Model theories
    a. Hubbard model
    b. DCA simulations
3. Materials specific simulation
4. Next Steps and Summary

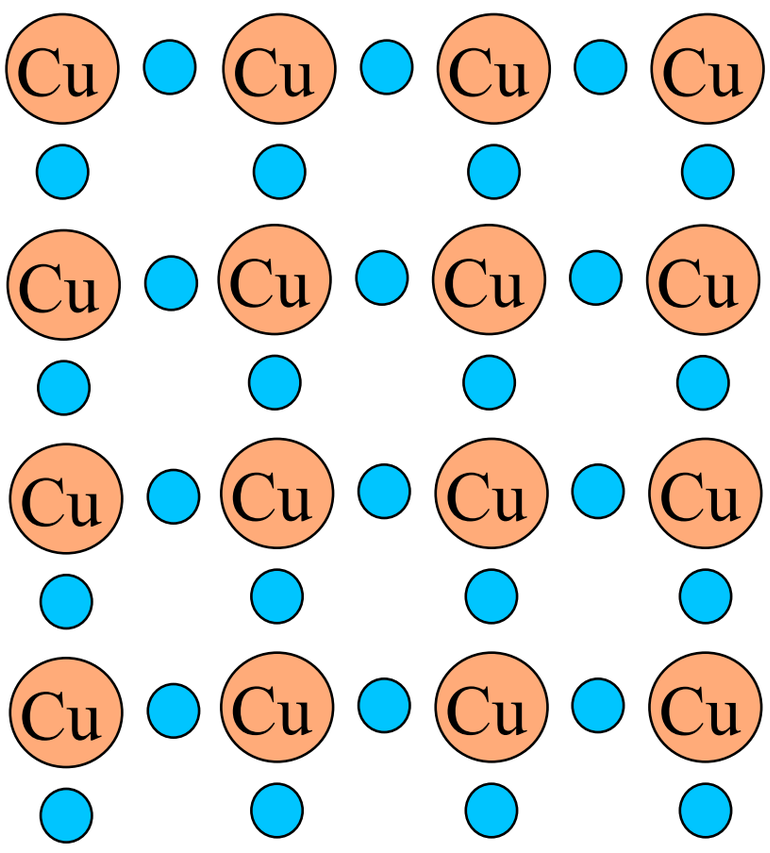
Focus on Cu-O layers



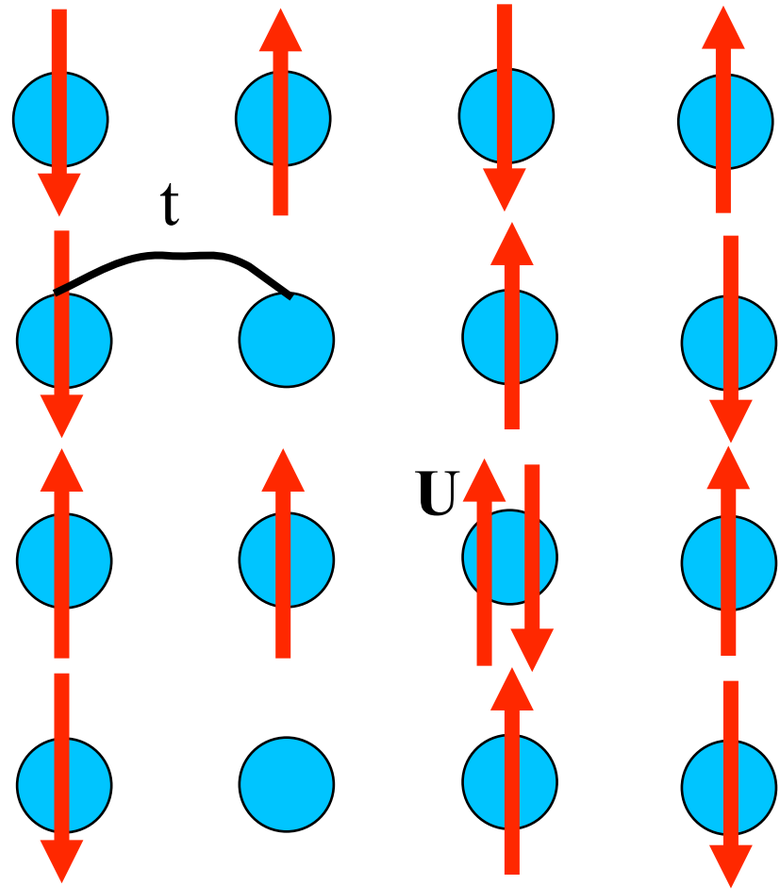
Focus here

Quasi 2D system
SC is in plane
Half-filled when undoped
Antiferromagnet

The Hubbard Model of the Cuprates



CuO_2 Planes

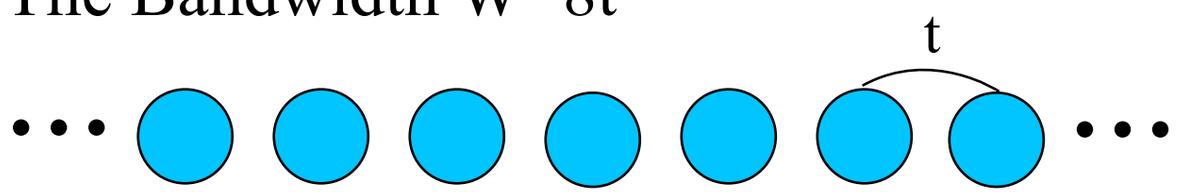


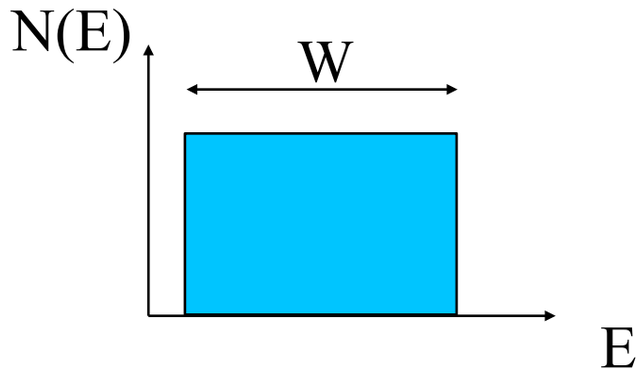
Hubbard Model with $8t = W \approx U$
Anderson 87, Zhang-Rice 88

Note: A few model parameters (t,U) fit to experiment

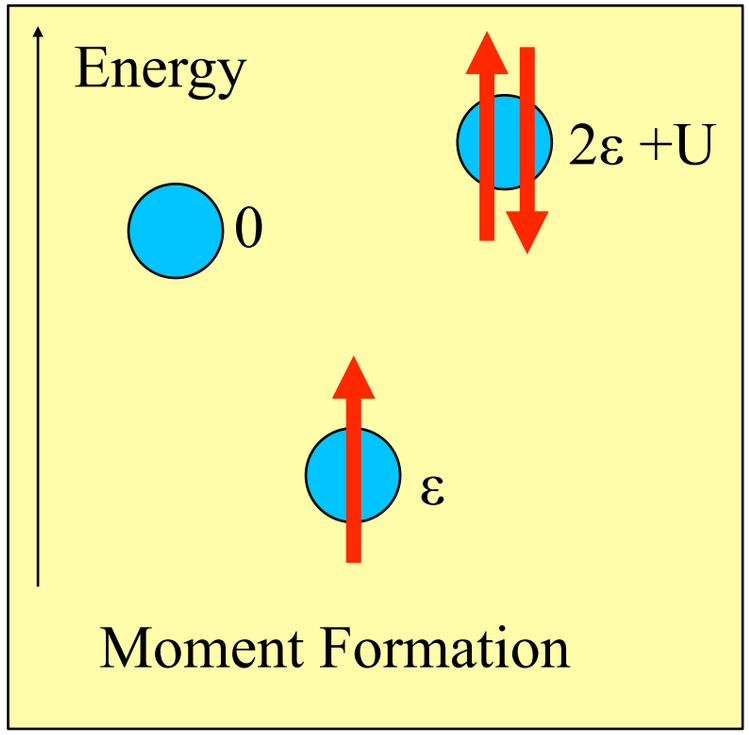
The Energy Scales in the Hubbard Model

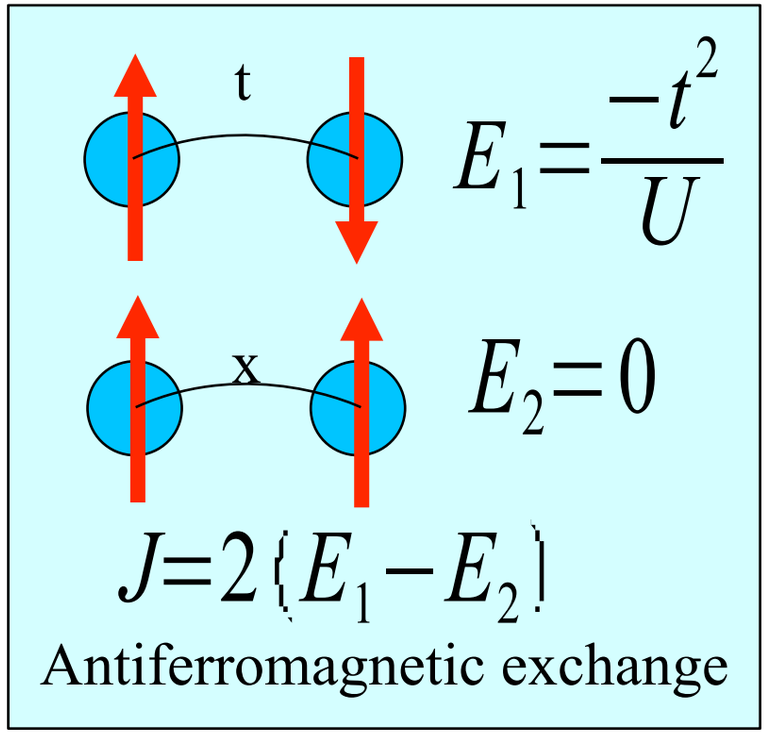
The Bandwidth W=8t





The local Coulomb repulsion U

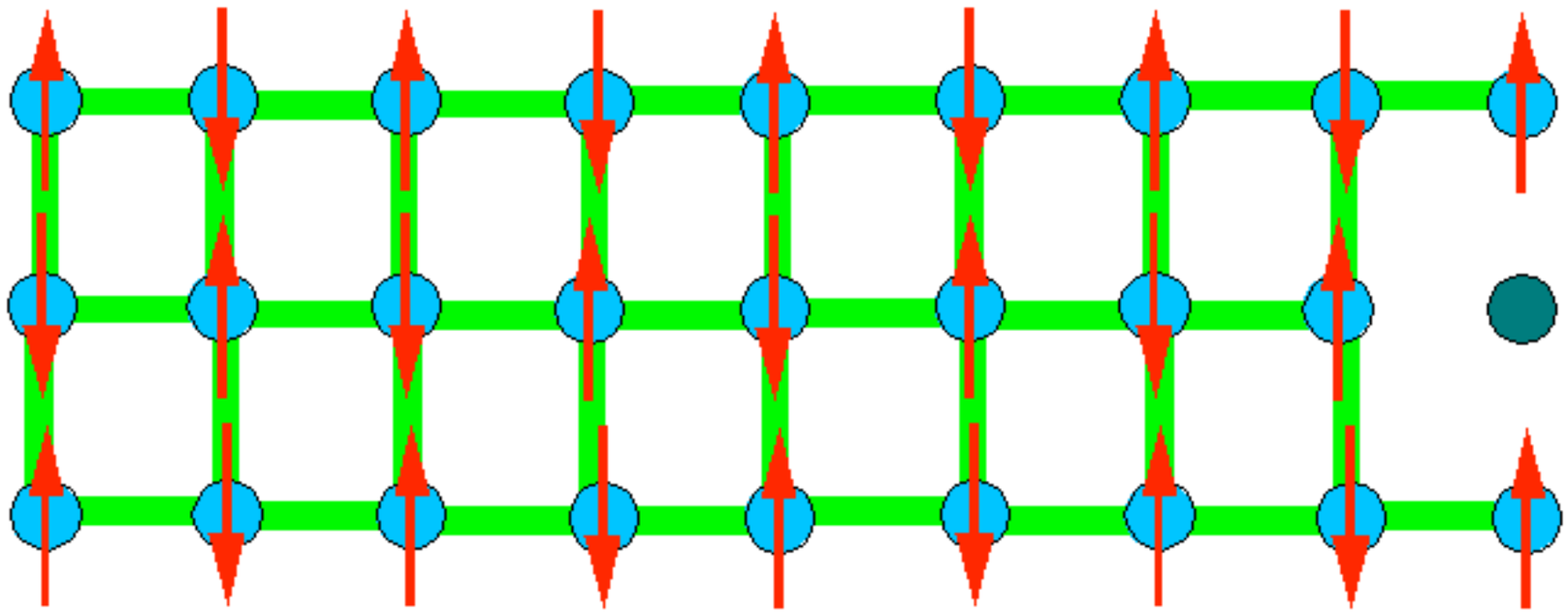




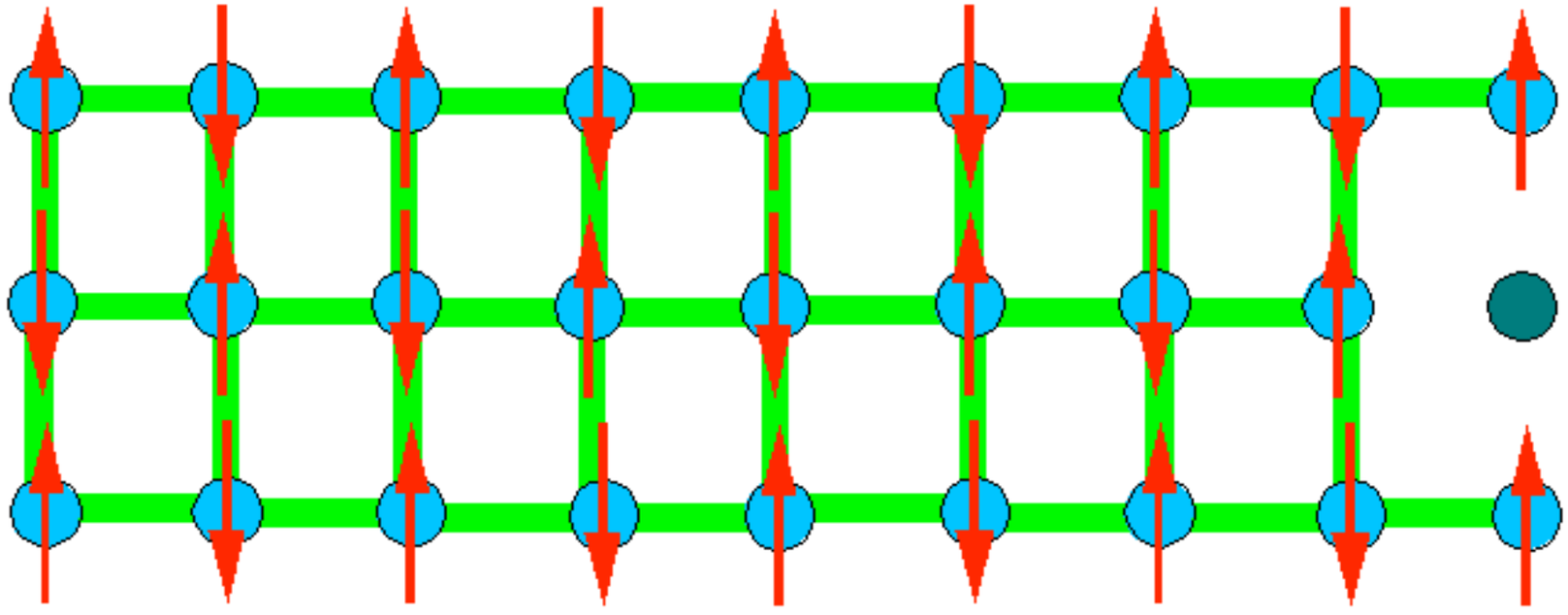
Note: A few model parameters (t,U) fit to experiment

Pairing Mechanism: Holes in AF background

One hole motion breaks AF bonds



A bound second hole restores the AF bonds



Brinkman 1970, Bonca 1989, Hirsch Science 2002

Pseudogap due to SRO or pre-formed pairs, Pairing due to kinetic energy gain

Outline

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    a. Hubbard model
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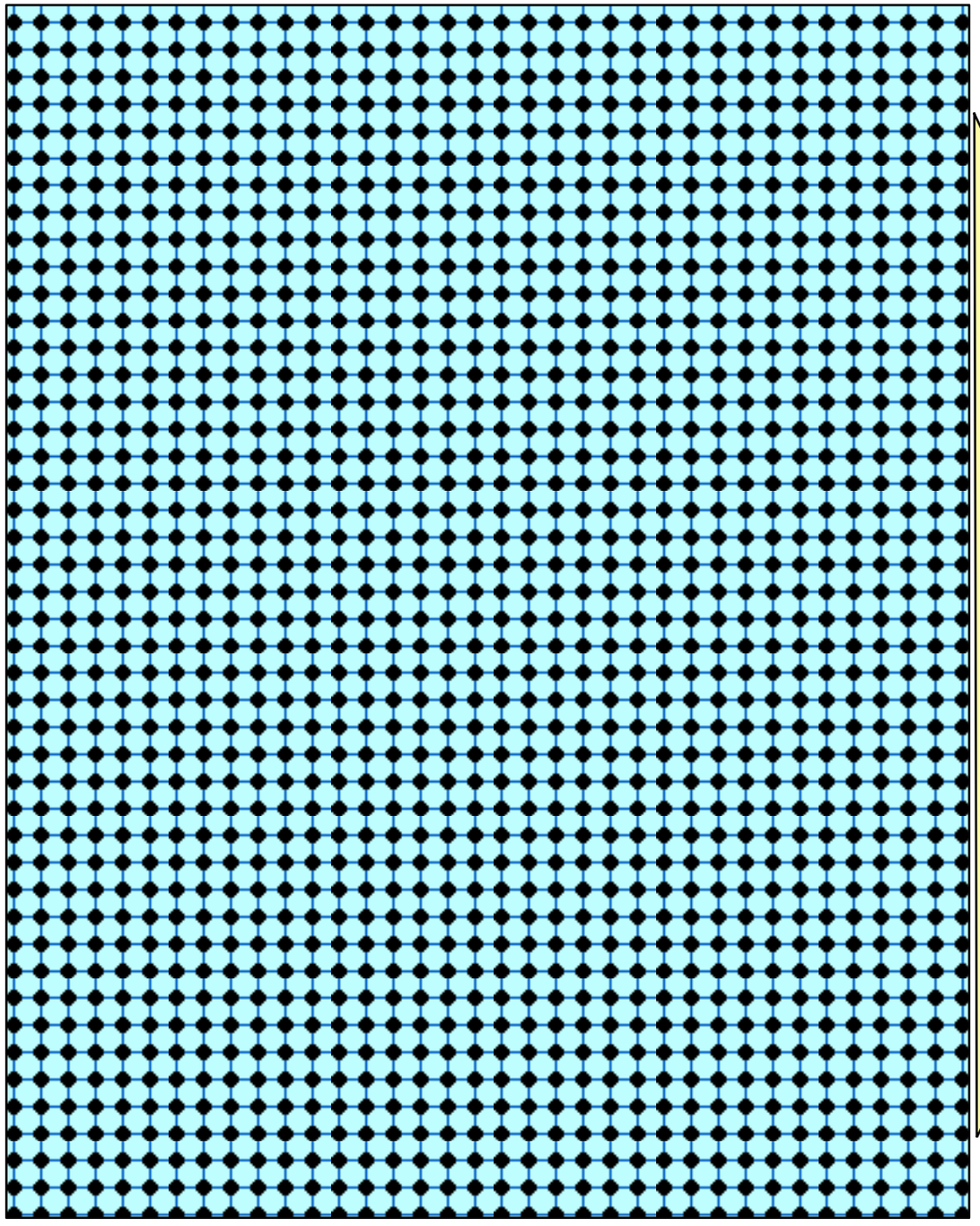
Periodic Lattice

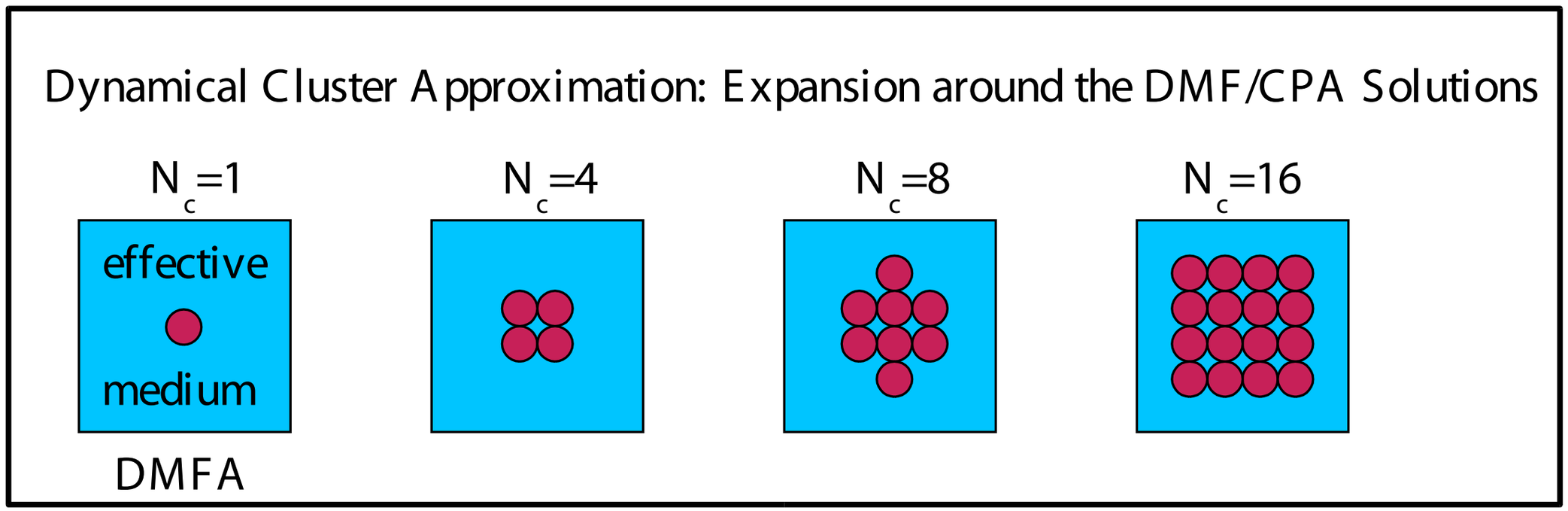


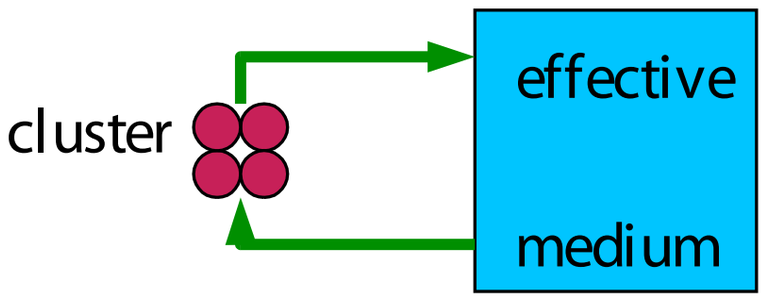
Difficult to solve accurately directly

Dynamical Cluster Approximation

Solve self-consistently

Cluster Approximations

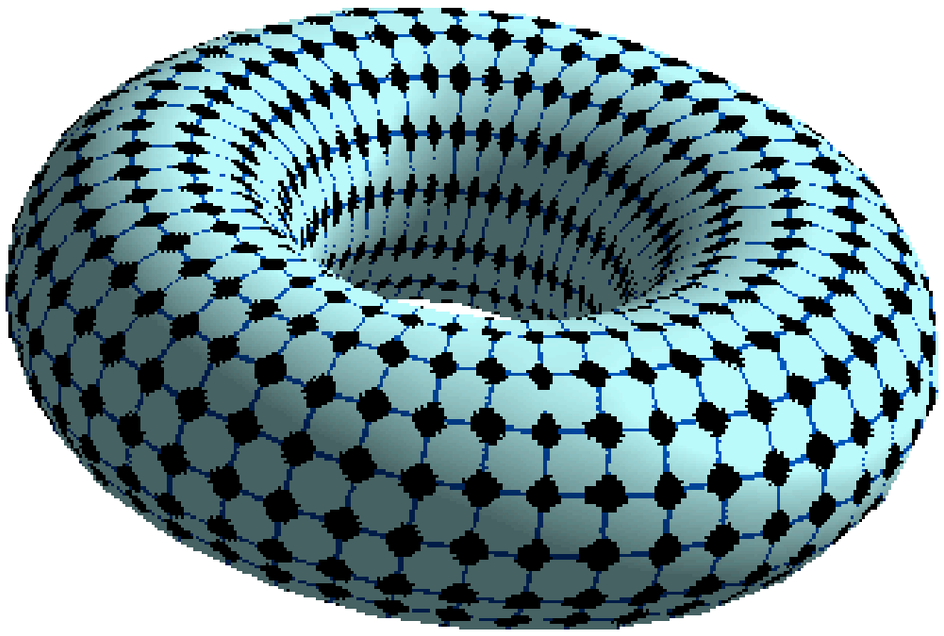




$$\Sigma_{\text{lattice}} \simeq \Sigma_{\text{cluster}}$$

DCA papers http://www.physics.uc.edu/~jarrell

We Solve The Cluster Problem with Quantum Monte Carlo (QMC)

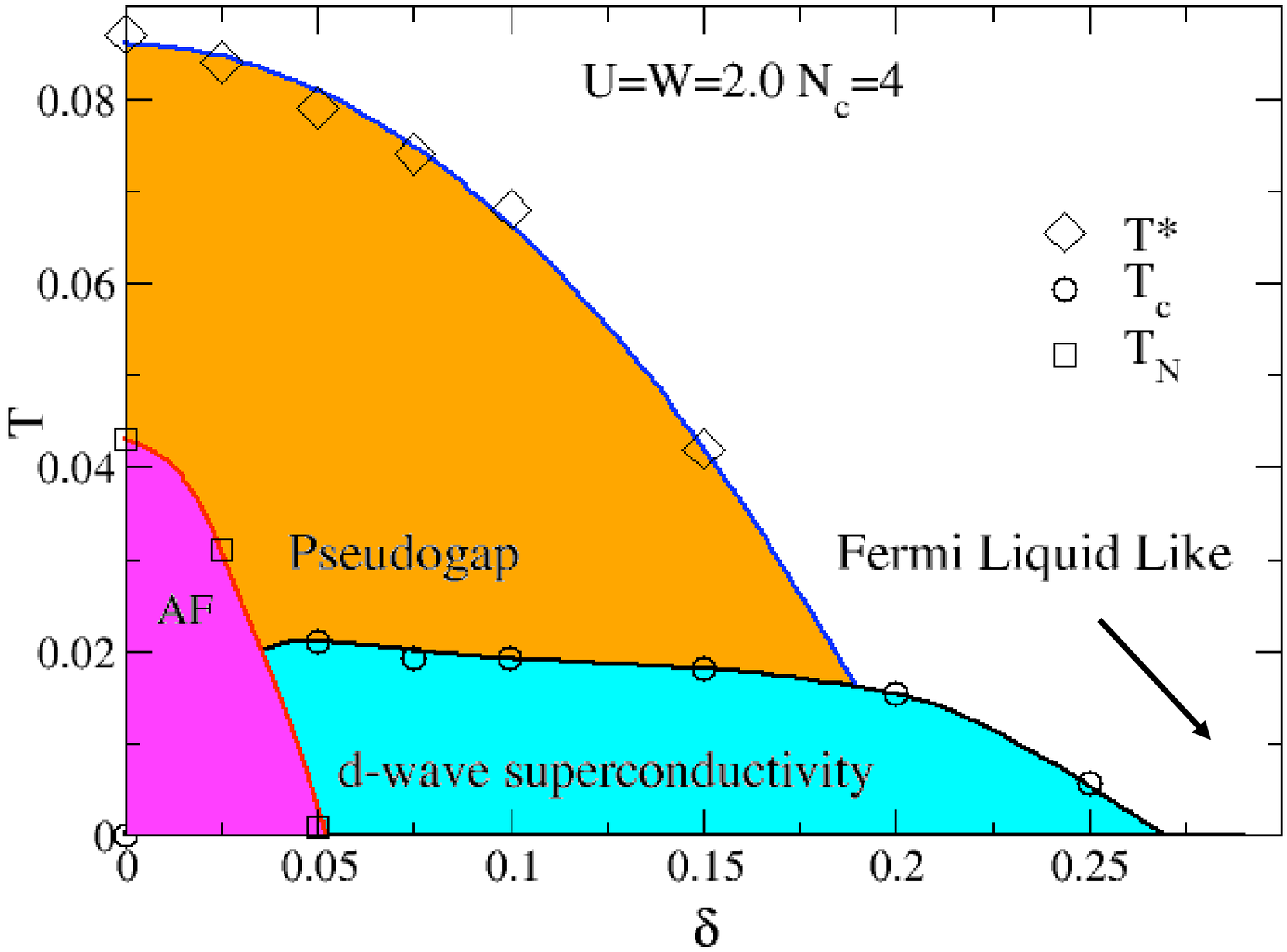


ORNL/CCS and
OSC CRAY X1

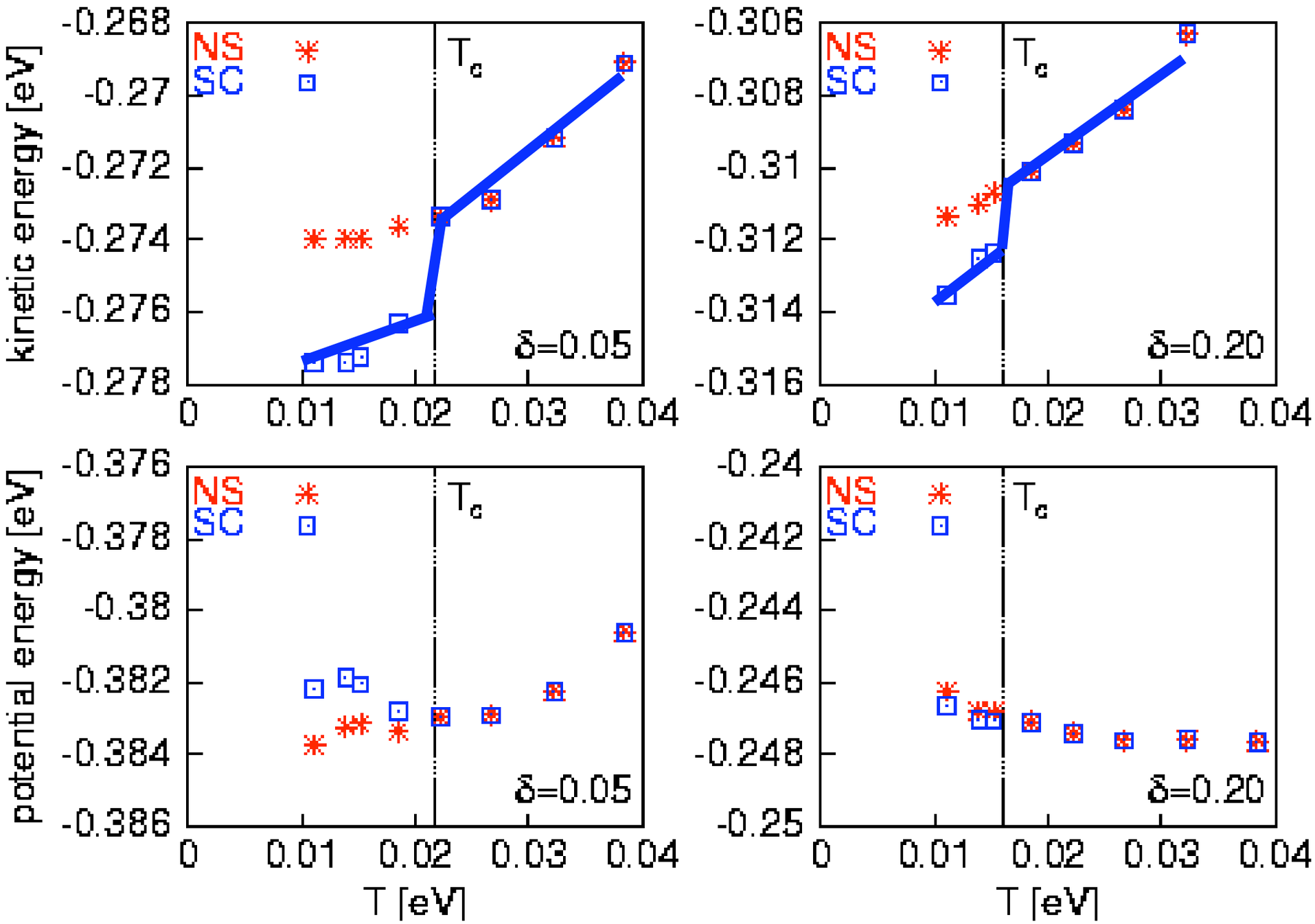
Expensive! 1-1000+ cpu hours per temperature and doping
Many temperatures and dopings per phase diagram

Small cluster results

Phase Diagram N_c=4



Energies for $T<T_c$



Kinetic energy reduction entering SC phase

Small cluster DCA Hubbard calculations display key features of cuprate phase diagram

Outline

1. Superconductivity Background
2. Model theories
3. Materials specific simulation
4. Next Steps and Summary

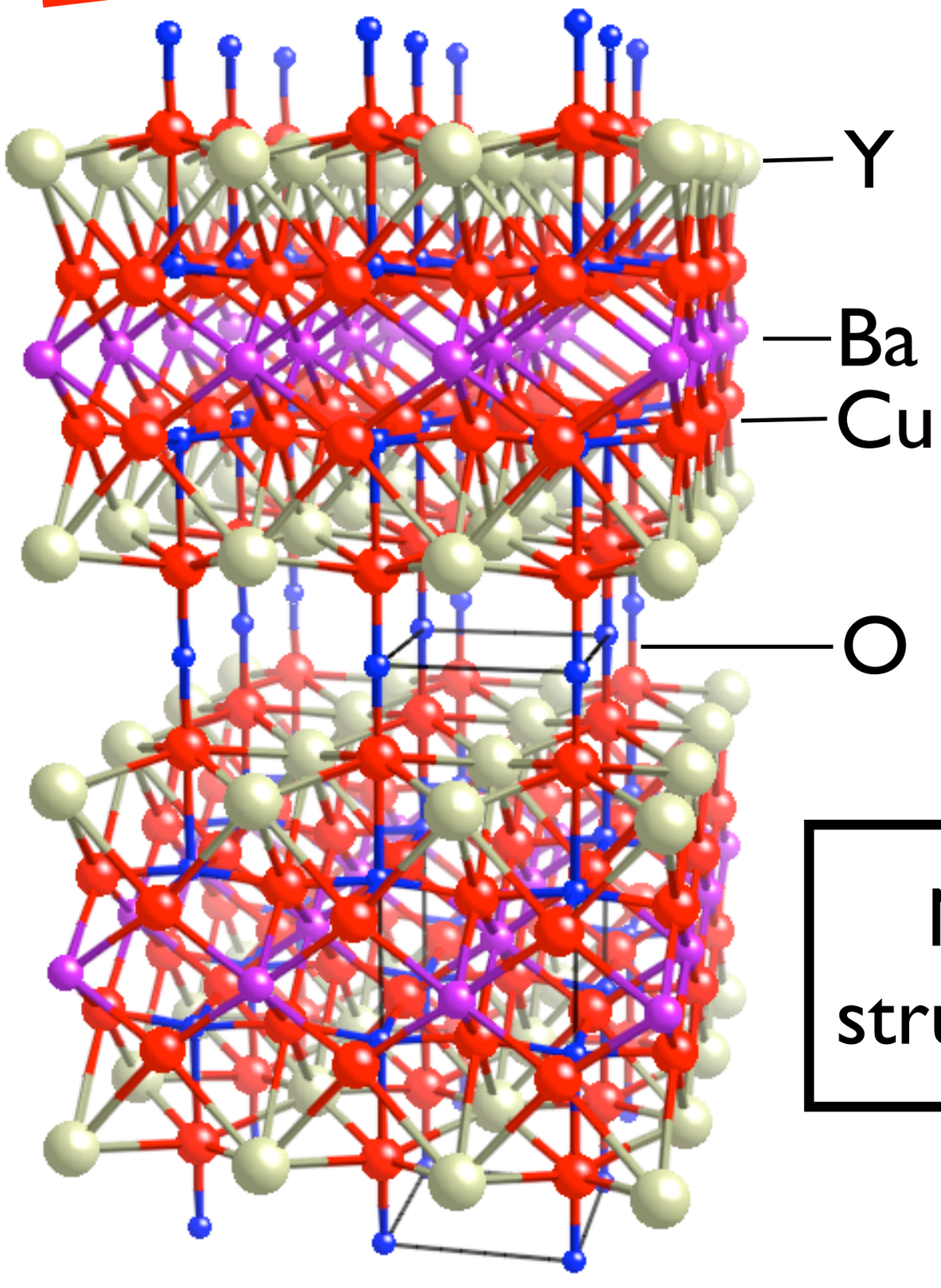
Outstanding questions
(19 years later)

- What is the principal mechanism?
  - Electrons? Phonons? Both? Other?

    Mostly electronic

- Does material A, B, or C have higher Tc?
- Influence of pressure, magnetic fields?
- Other materials with same mechanism?
  - c.f. new BCS-like MgB2 in 2001, 39K

~~Focus on Cu-O layers~~

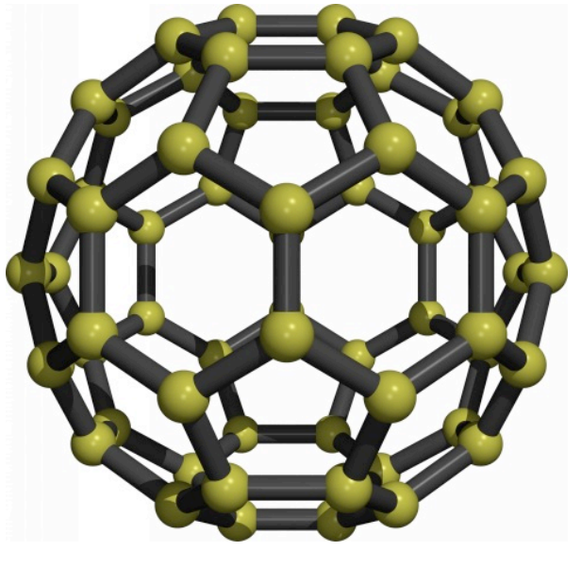


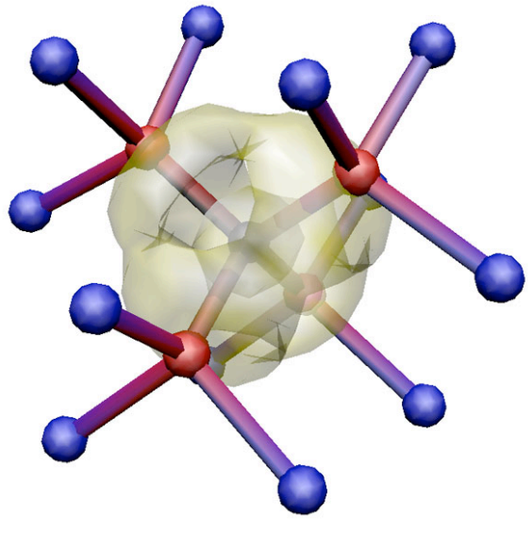
Need to include entire structure, additional orbitals

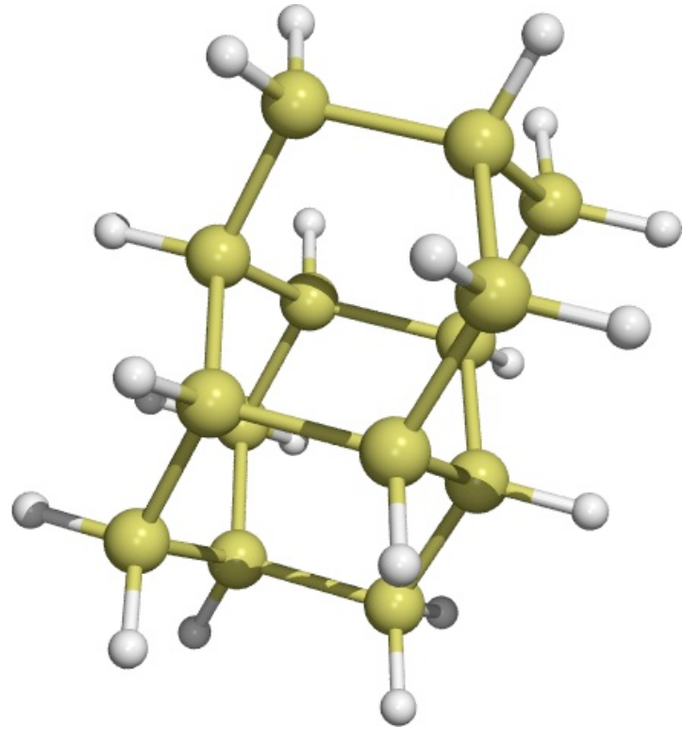
First-principles calculations

Use zero-temperature LDA density functional calculations for structure and bonding

Although these band-structure methods "fail", structure and bonding are close to experiment: hope/look for trends.

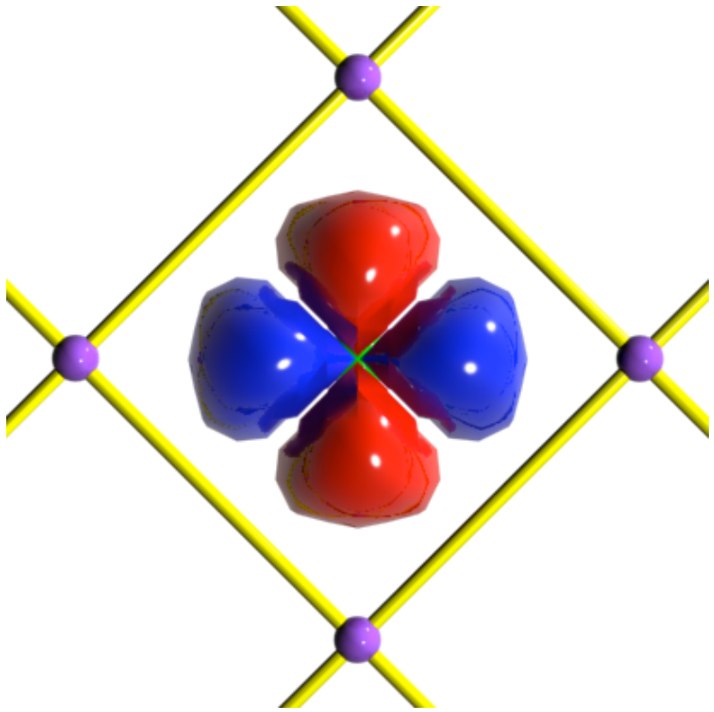






Method

$n(\mathbf{r})$

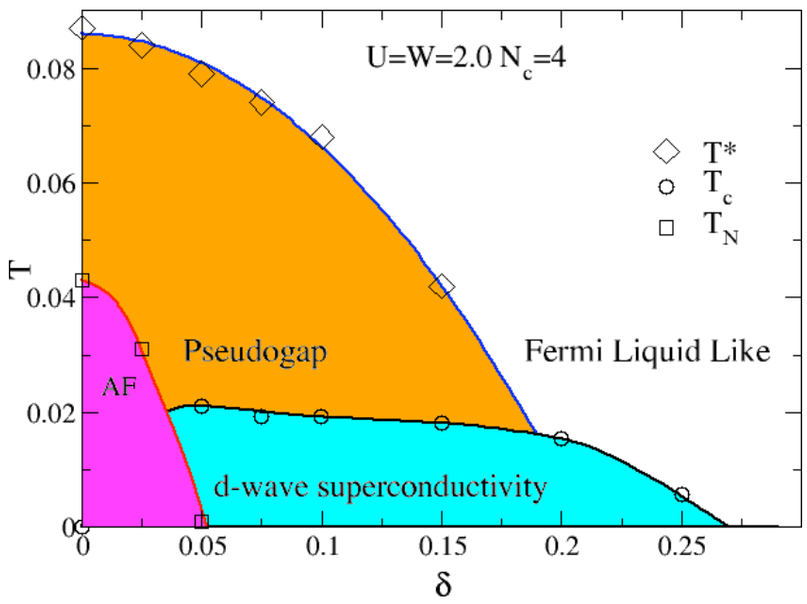


1. DFT LDA ground state

Obtain parameters

2. Multi-band Hubbard Hamiltonian

DCA

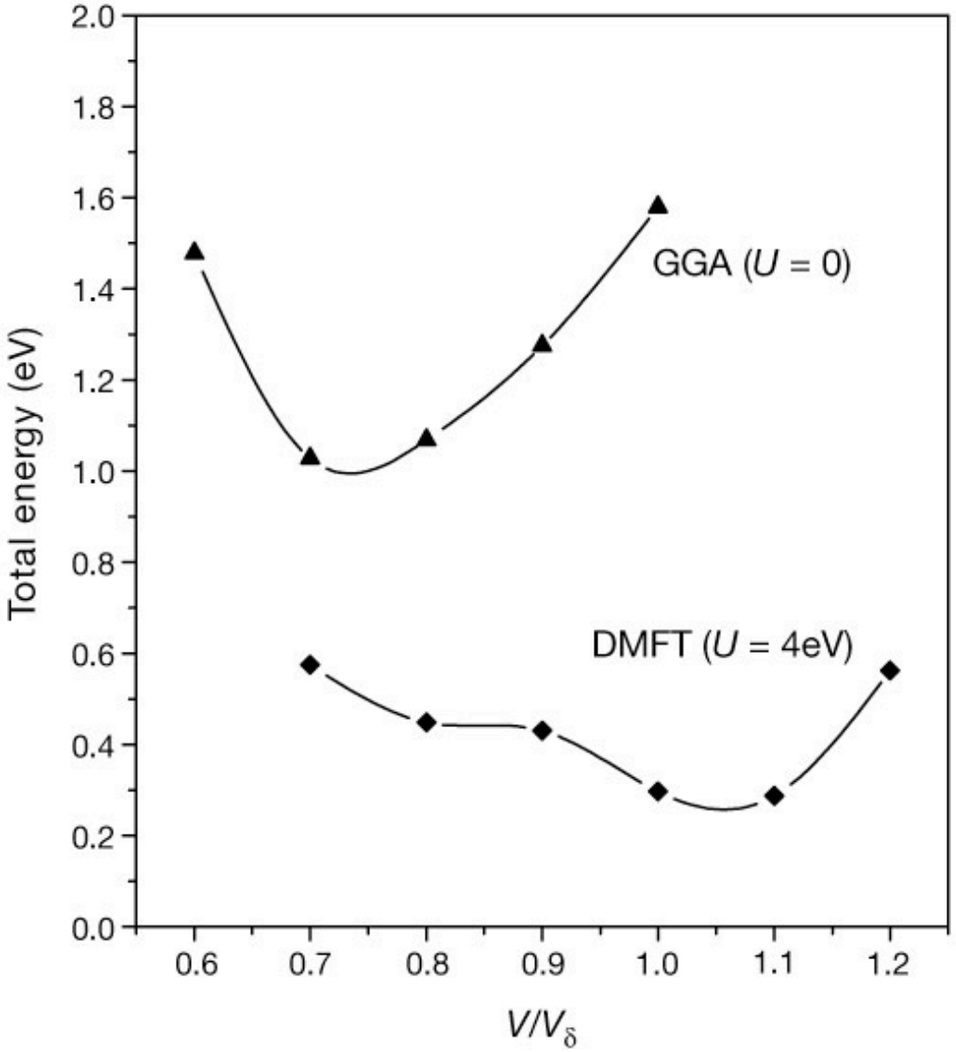


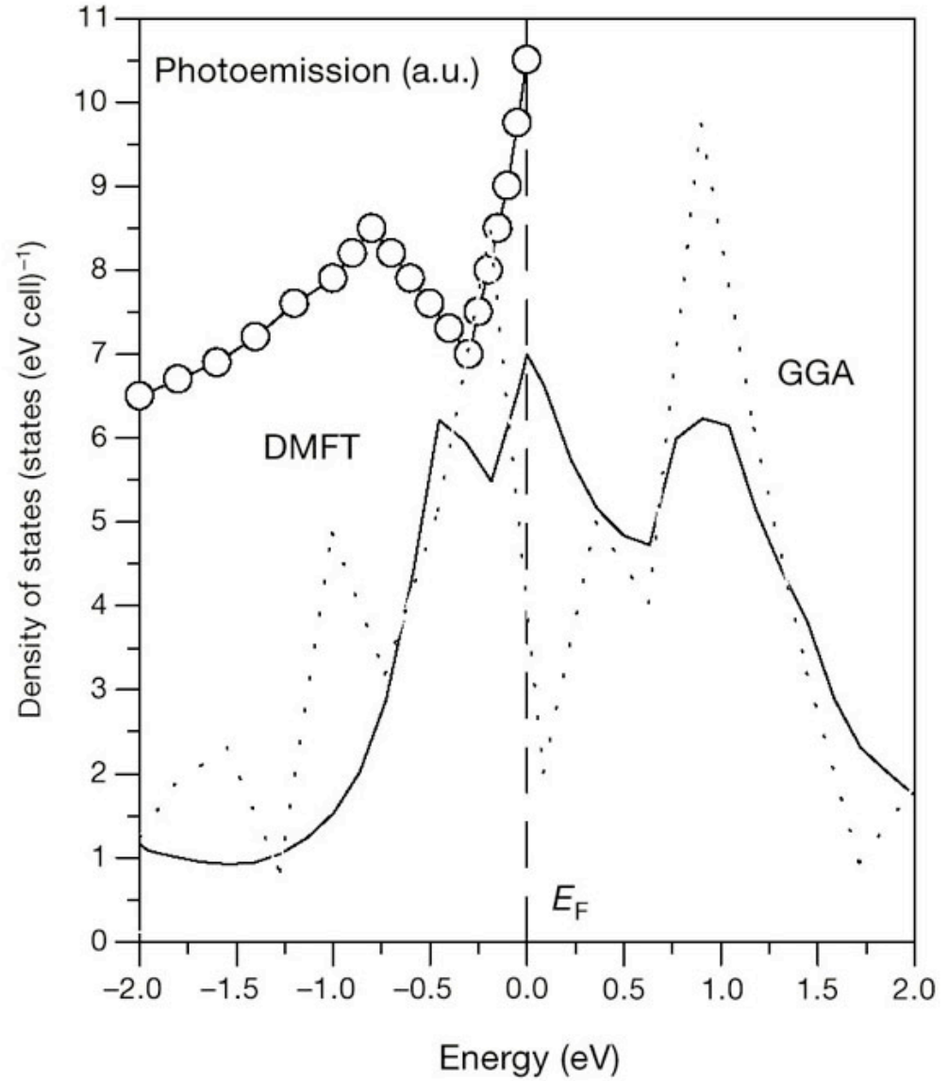
3. Phase Diagram

Can this work?

LDA+DMFT

Similar method recovers structural phase transition in Pu

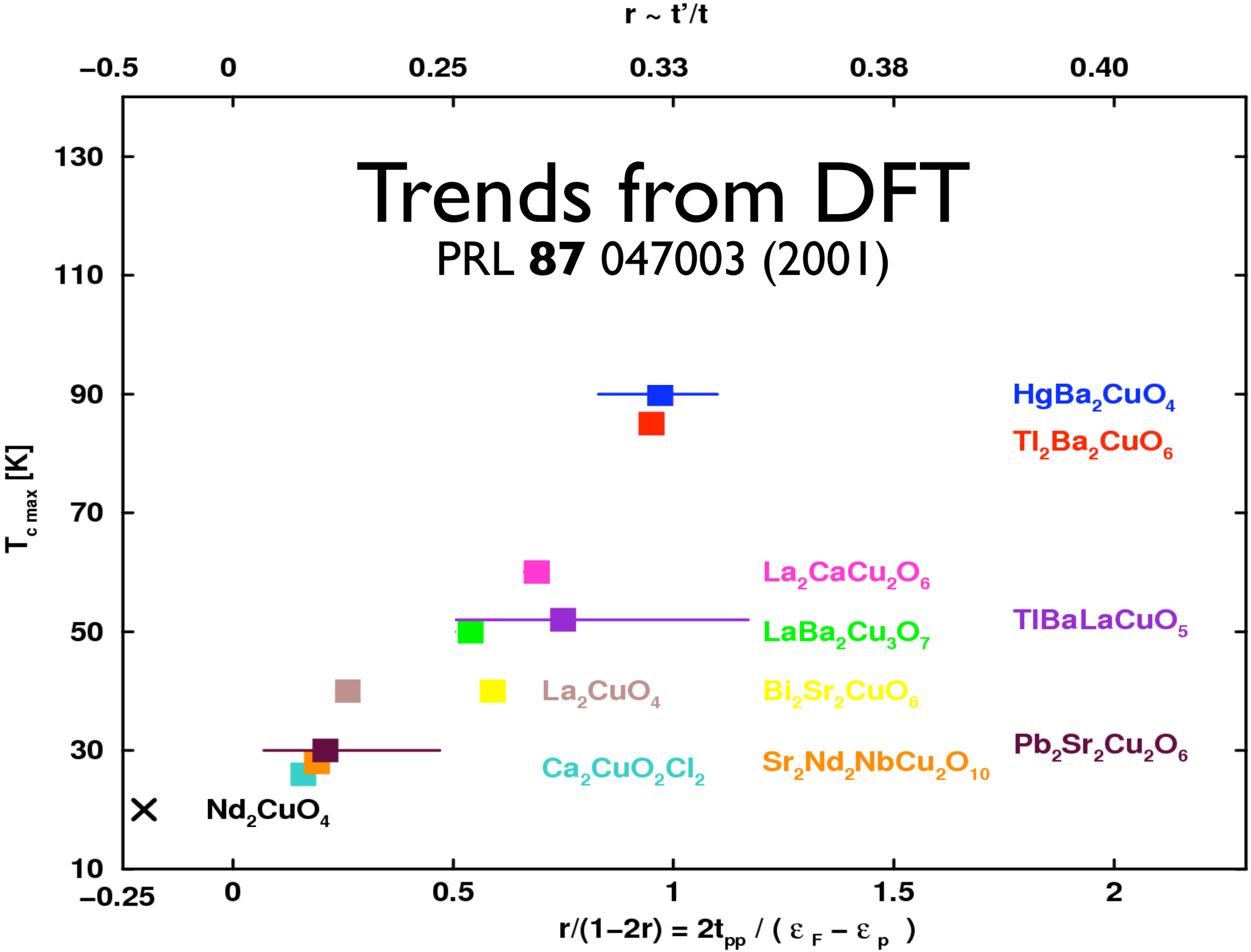




Kotliar Nature **410** 793 (2001)

Trends from DFT

PRL **87** 047003 (2001)



r ~ t'/t

–0.5 0 0.25 0.33 0.38 0.40

$HgBa_2Ca_2Cu_3O_8$

$HgBa_2CaCu_2O_6$

$Tl_2Ba_2Ca_2Cu_3O_{10}$

$Tl_2Ba_2CaCu_2O_8$

$YBa_2Cu_3O_7$

$HgBa_2CuO_4$

$Tl_2Ba_2CuO_6$

$Pb_2Sr_2YCu_3O_8$

$La_2CaCu_2O_6$

$TlBaLaCuO_5$

$LaBa_2Cu_3O_7$

La_2CuO_4

$Bi_2Sr_2CuO_6$

$Pb_2Sr_2Cu_2O_6$

$Sr_2Nd_2NbCu_2O_{10}$

$Ca_2CuO_2Cl_2$

Nd_2CuO_4

$T_{c\,max}$ [K]

130 110 90 70 50 30 10

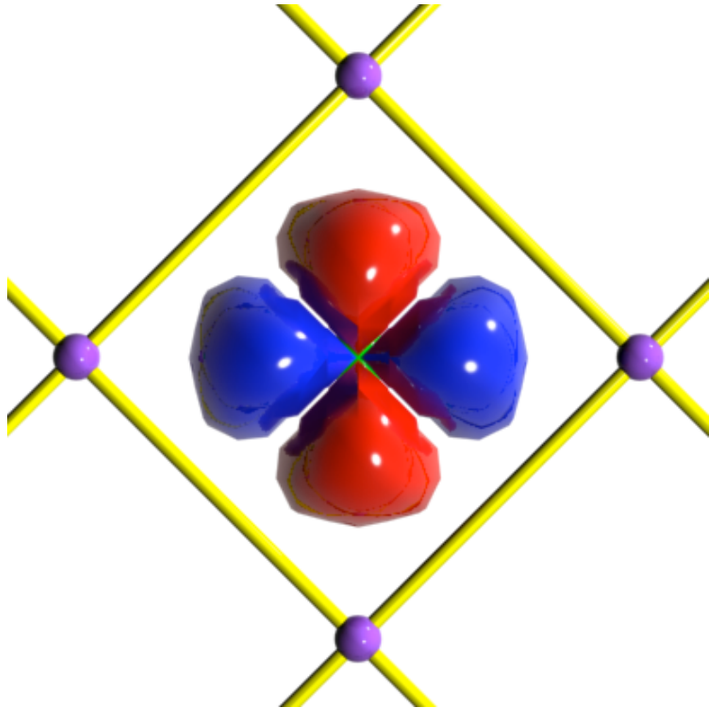
–0.25 0 0.5 1 1.5 2

$r/(1-2r) = 2t_{pp} / (\varepsilon_F - \varepsilon_p)$

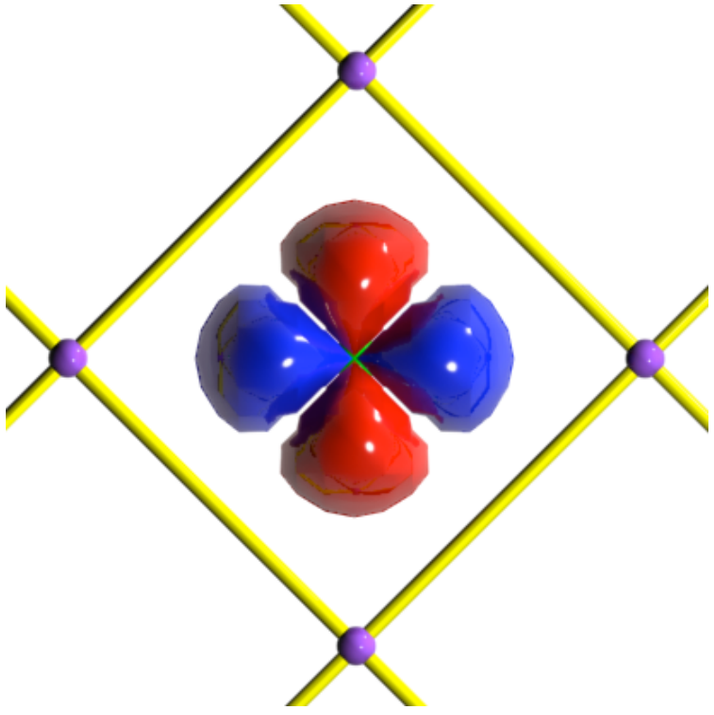
DFT Orbitals

Well-localized Cu d orbital obtained: small materials differences.

O px, py: strong hybridization.



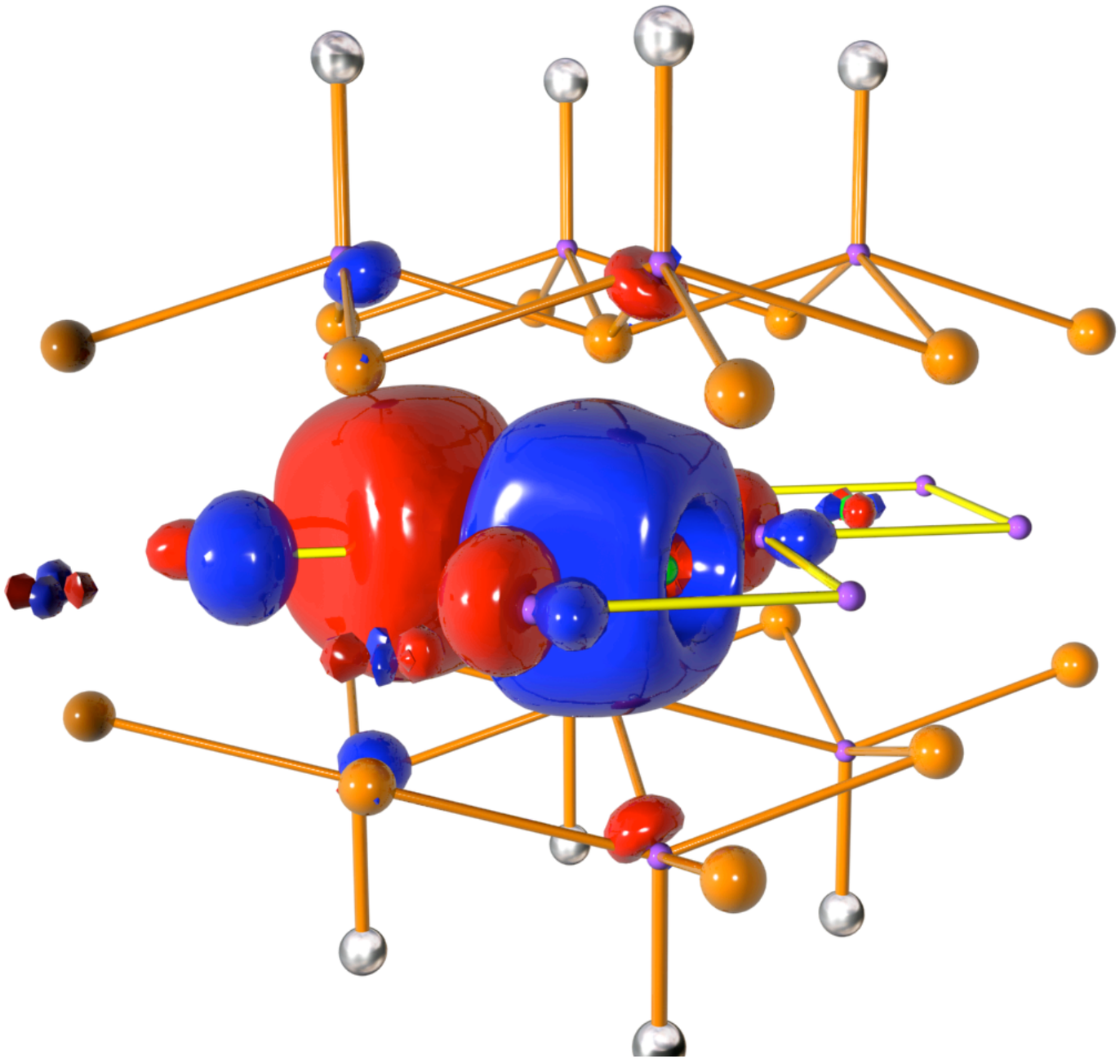
La2CuO4

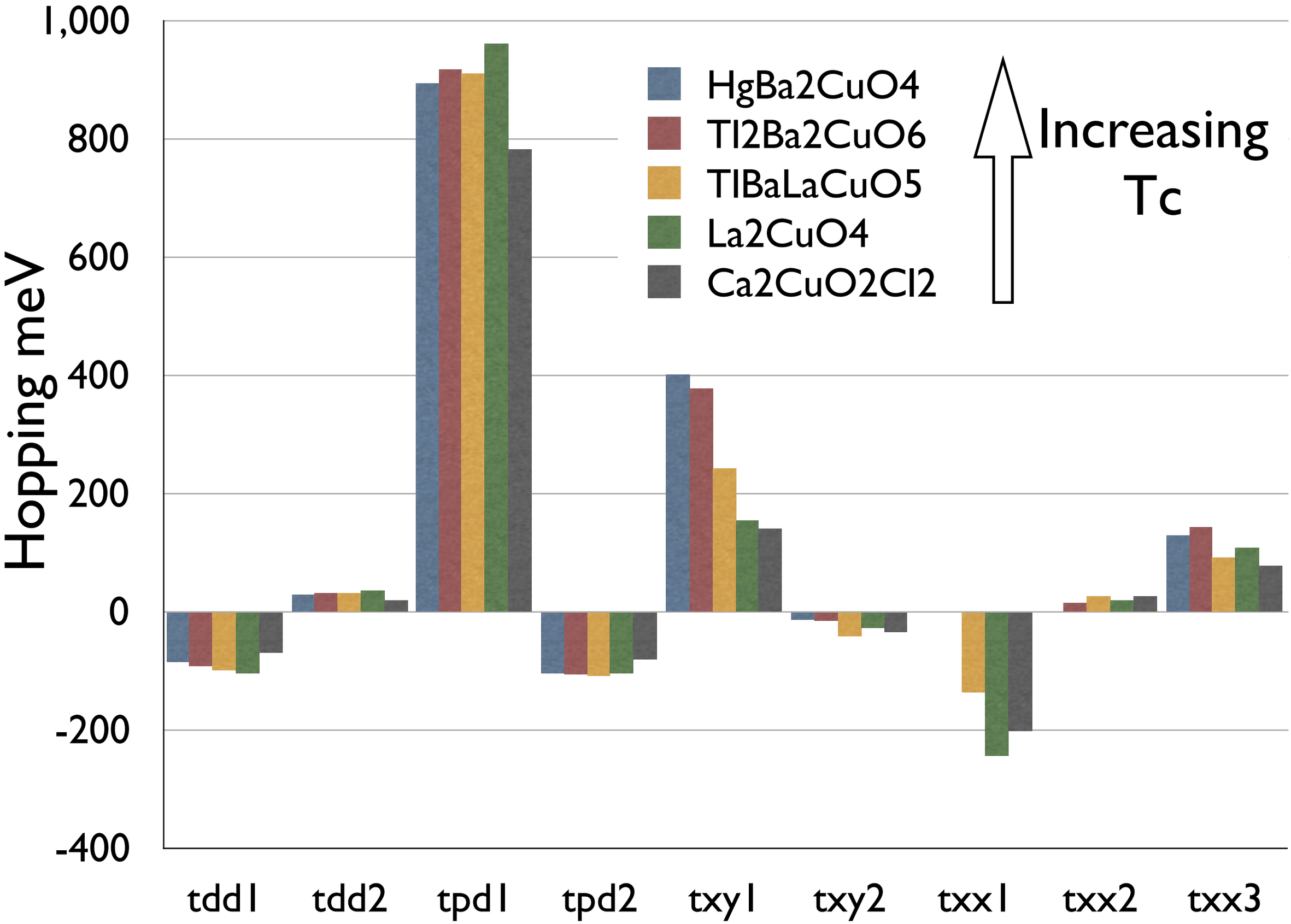


HgBa2CuO4

DFT Orbitals

Some far from atomic picture



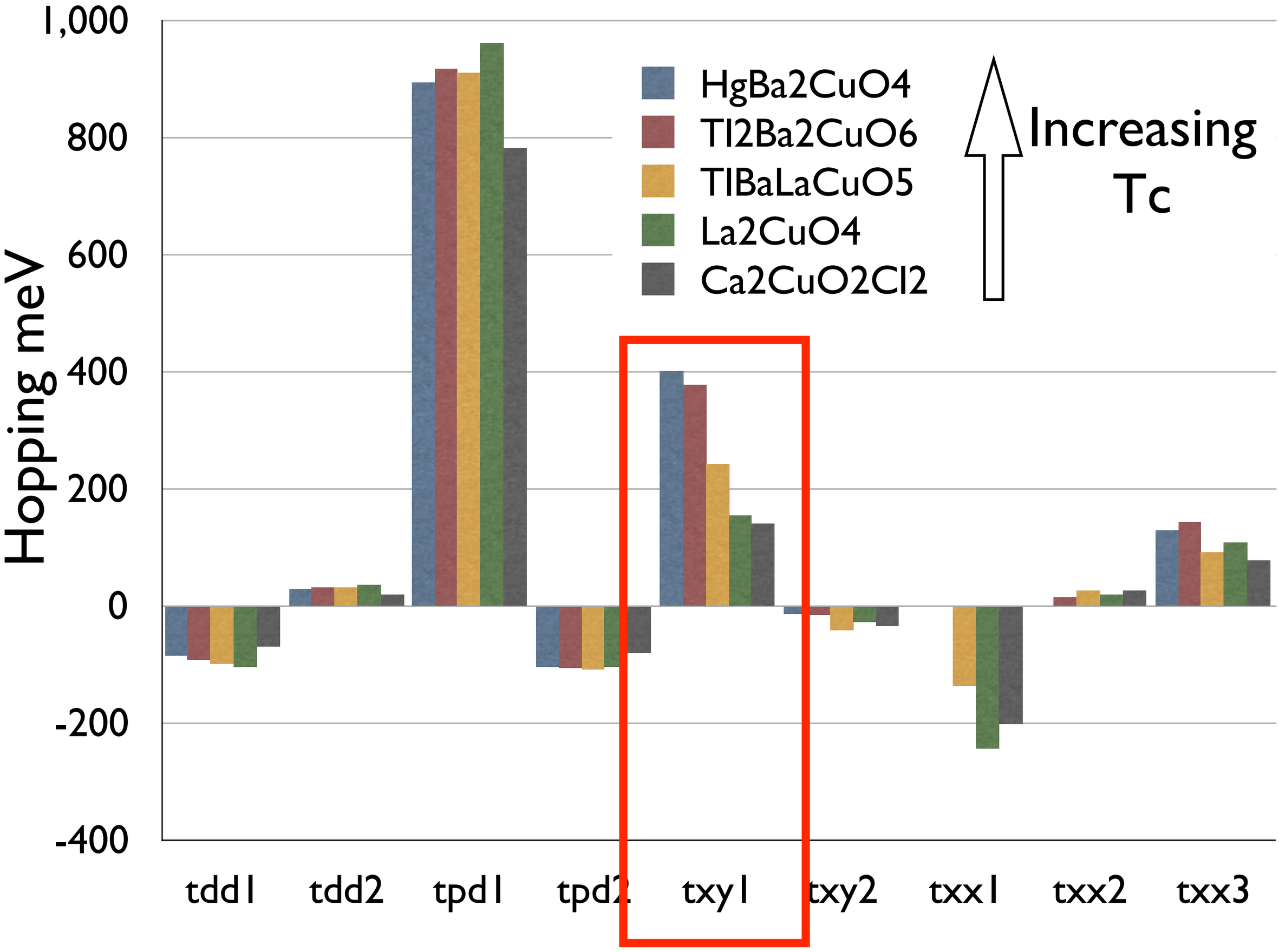

1,000
800
600
400
200
0
-200
-400
Hopping meV
HgBa2CuO4
Tl2Ba2CuO6
TlBaLaCuO5
La2CuO4
Ca2CuO2Cl2
Increasing Tc
tdd1
tdd2
tpd1
tpd2
txy1
txy2
txx1
txx2
txx3

DFT Results

- ~6 terms appear significant, in this basis

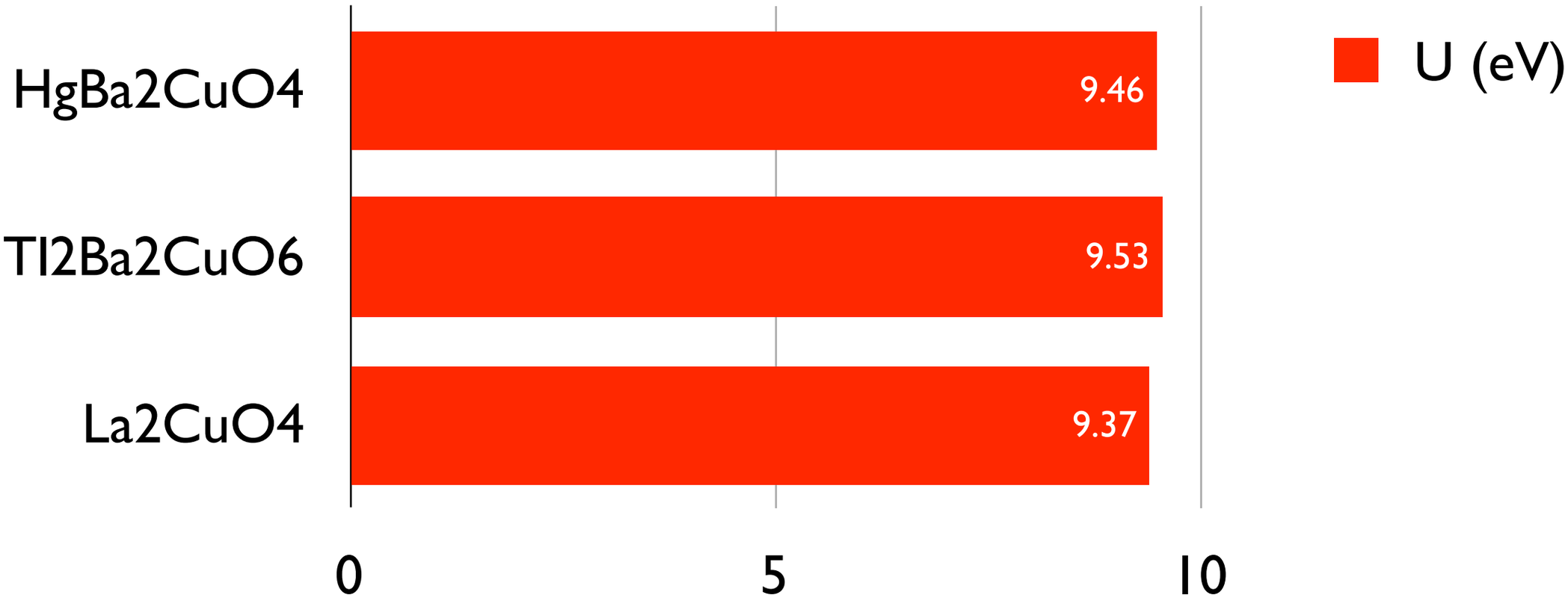
  Parametric studies are possible

  - Parameters are close to empirical parameters used in model calculations
  - Some trends apparent e.g. txy1 (=tpp) increases with increasing Tc. Similar to single band observations, but inconclusive.


1,000
800
600
400
200
0
-200
-400
Hopping meV
HgBa2CuO4
Tl2Ba2CuO6
TlBaLaCuO5
La2CuO4
Ca2CuO2Cl2
Increasing
Tc
tdd1
tdd2
tpd1
tpd2
txy1
txy2
txx1
txx2
txx3

LDA+DCA results

Calculated U



Few % variation in U; similar in all materials

Any Tc dependence must reside in orbitals or additional interactions (e.g. phonons)

HgBa2CuO4
"near-neighbor" parameters

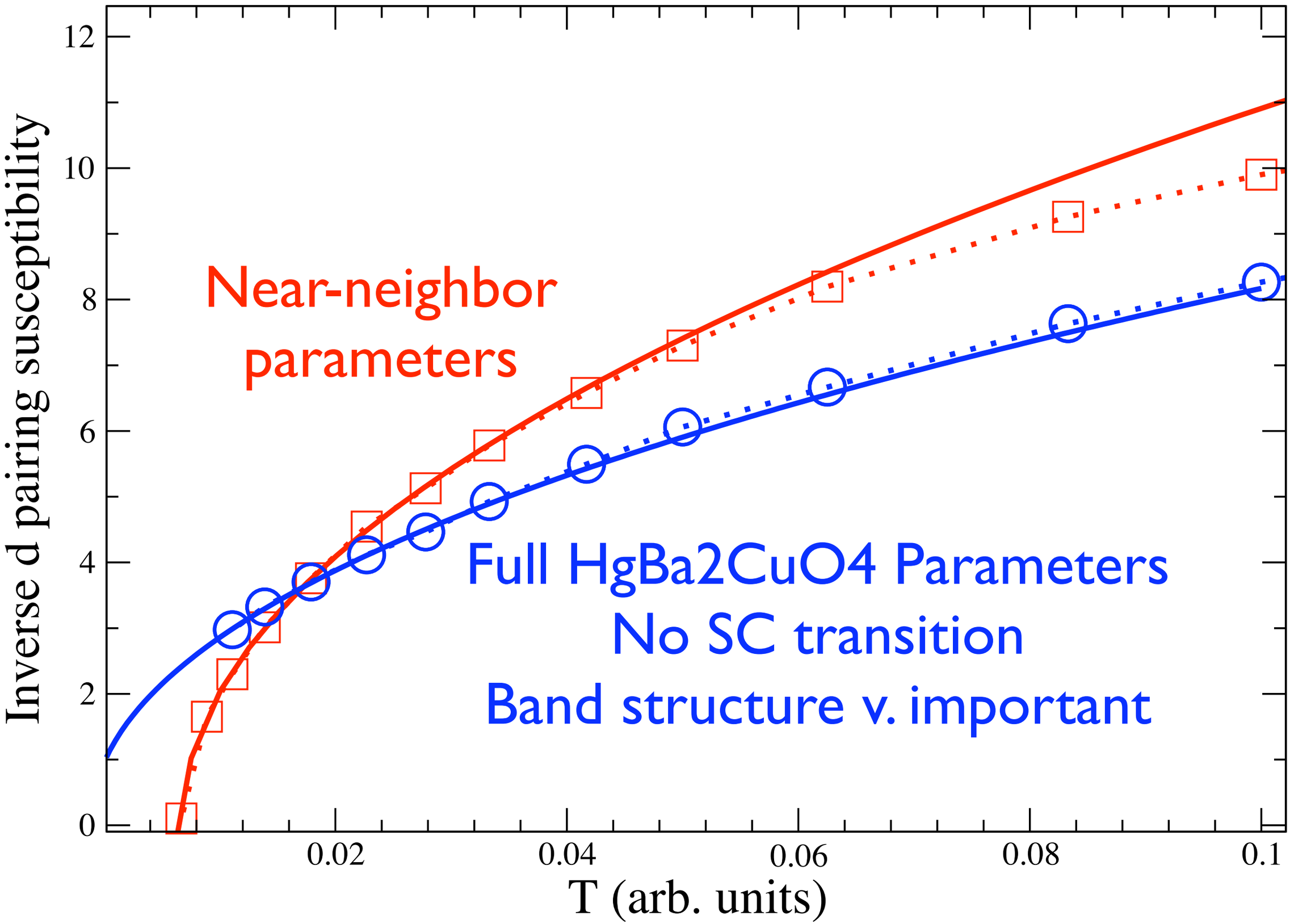
Tc

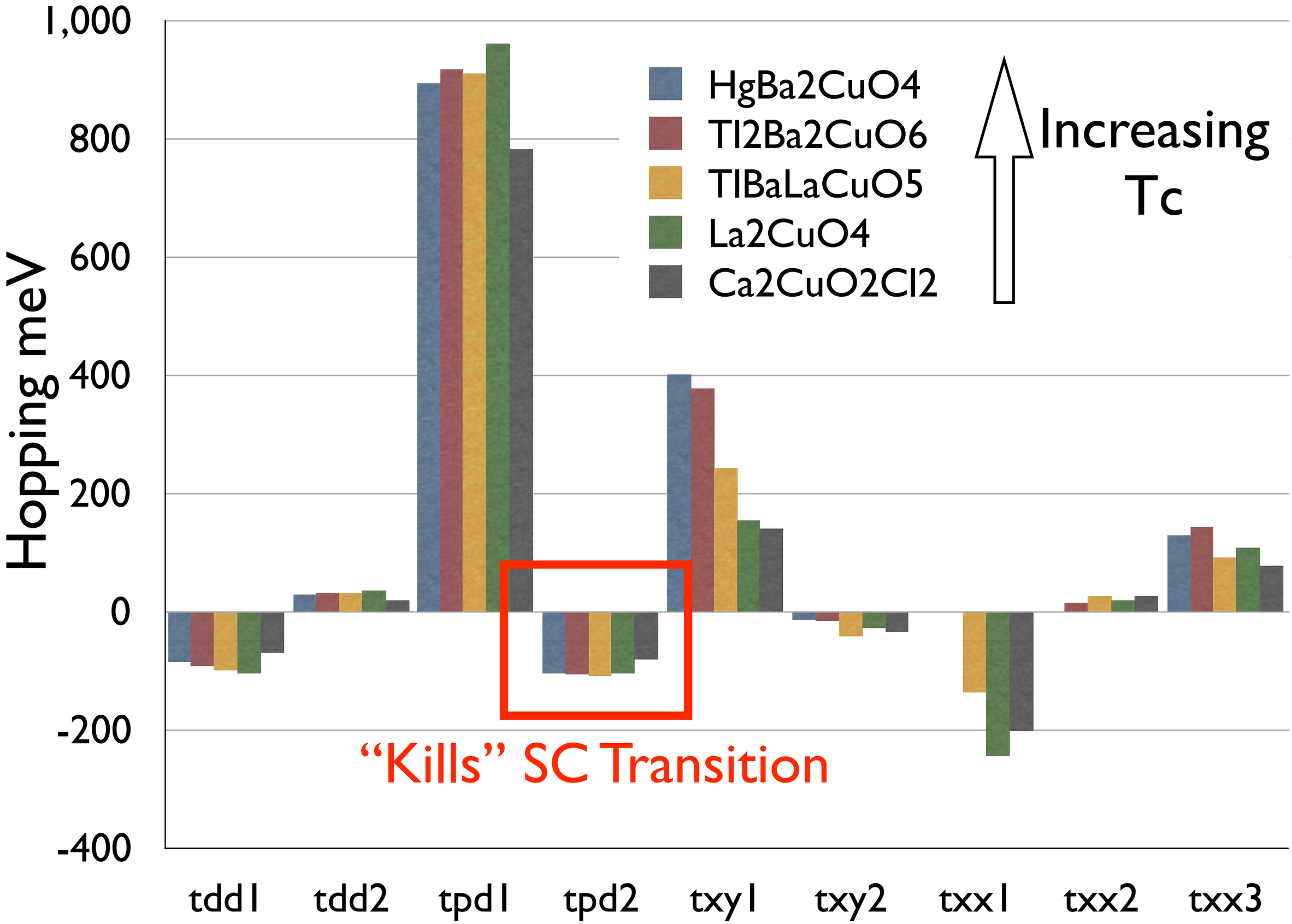
Inverse d pairing susceptibility

T (arb. units)

0
2
4
6
8
10
12

0.02
0.04
0.06
0.08
0.1


Inverse d pairing susceptibility
T (arb. units)
0
2
4
6
8
10
12
0.02
0.04
0.06
0.08
0.1
Near-neighbor parameters
Full HgBa2CuO4 Parameters
No SC transition
Band structure v. important


1,000
800
600
400
200
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-200
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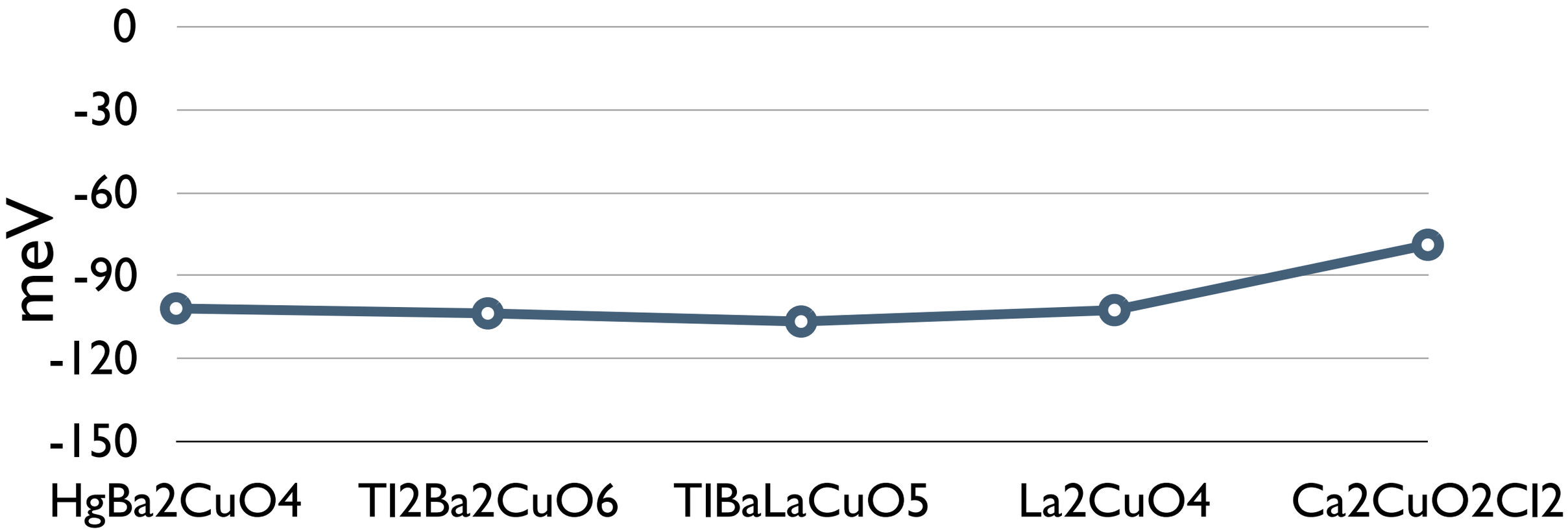
Hopping meV
HgBa2CuO4
Tl2Ba2CuO6
TlBaLaCuO5
La2CuO4
Ca2CuO2Cl2
Increasing Tc
"Kills" SC Transition
tdd1
tdd2
tpd1
tpd2
txy1
txy2
txx1
txx2
txx3

Parametric Results



2nd NN Cu-O hybridization strongly governs Tc

Toy model: +ve sign, *Tc increased ~60% from reference*

Outline

1. Superconductivity Background
2. Model theories
3. Materials specific simulation
4. Next Steps and Summary

Next Steps

Investigating influence of DFT ground state

More accurate calculations underway

If we fail, we will have shown "something extra" is needed to describe HTSC in real materials.

If we succeed, we expect to obtain "materials trends" in real HTSC materials.

Oxygen Superstructures Throughout the Phase Diagram of $(Y, Ca)Ba_2Cu_3O_{6+x}$

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[2]*Hamburger Synchrotronstrahlungslabor HASYLAB at Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, D-22603 Hamburg, Germany*

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(Received 12 November 2003; published 7 October 2004)

The doping dependence of short-range lattice superstructures in $(Y, Ca)Ba_2Cu_3O_{6+x}$ has been studied with high-energy x-ray scattering. We observe diffuse features with a well defined periodicity which depend on the oxygen concentration but not on the charge carrier concentration. In addition, we find that diffuse scattering is absent in underdoped $YBa_2Cu_4O_8$, which does not sustain oxygen defects. Our combined data highlight that the diffuse scattering arises from short-range oxygen ordering and associated lattice distortions. Signatures of stripe ordering or fluctuations are not seen and therefore must be much weaker.

DOI: 10.1103/PhysRevLett.93.157007 PACS numbers: 74.72.Bk, 61.10.Eq, 74.25.–q

Four-Unit-Cell Superstructure in the Optimally Doped $YBa_2Cu_3O_{6.92}$ Superconductor

Zahirul Islam,[1,*] X. Liu,[2] S. K. Sinha,[2] J. C. Lang,[1] S. C. Moss,[3] D. Haskel,[1] G. Srajer,[1] P. Wochner,[4] D. R. Lee,[1] D. R. Haeffner,[1] and U. Welp[5]

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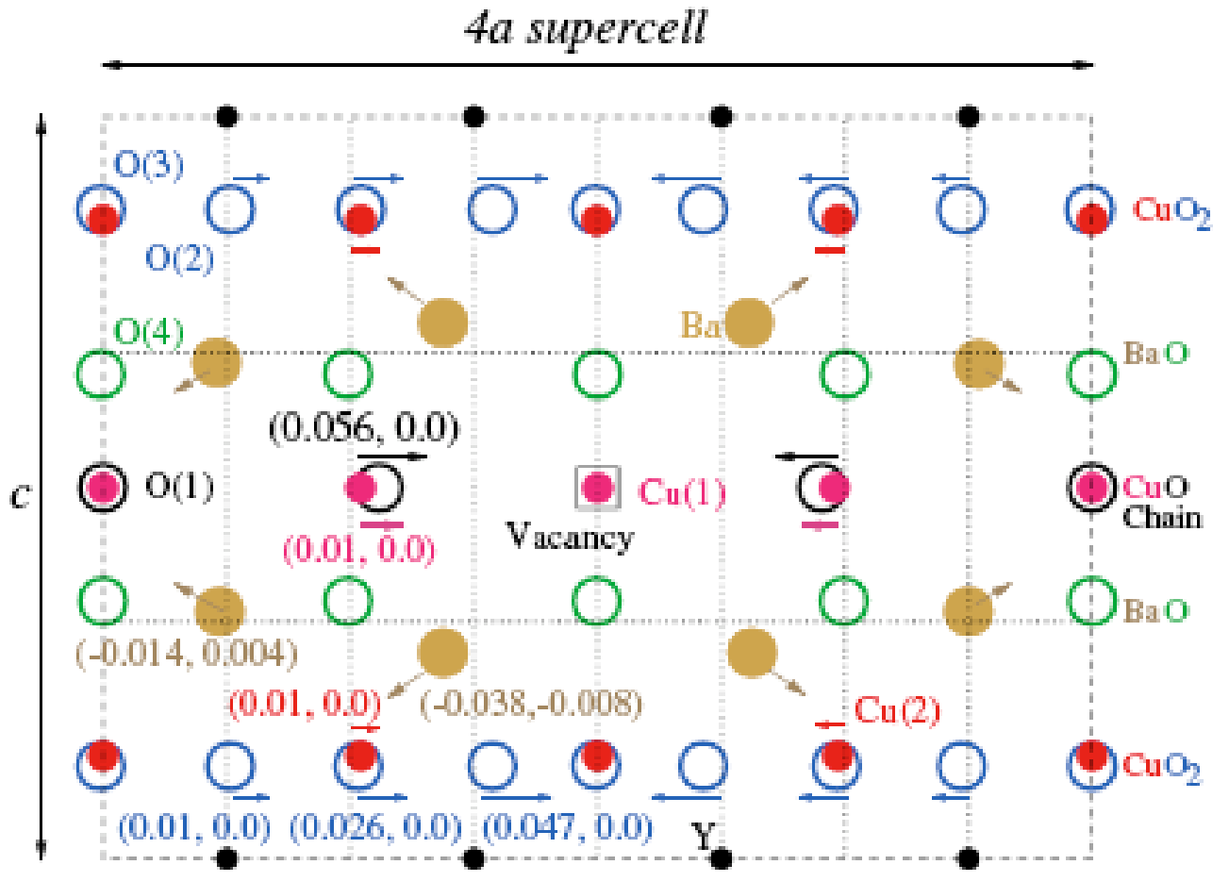
(Received 23 December 2003; published 7 October 2004)

Diffuse x-ray scattering measurements reveal that the optimally doped $YBa_2Cu_3O_{6.92}$ superconductor is intrinsically modulated due to the formation of a kinetically limited 4-unit-cell superlattice, $\mathbf{q}_0 = (\frac{1}{4}, 0, 0)$, along the shorter Cu-Cu bonds. The superlattice consists of large anisotropic displacements of Cu, Ba, and O atoms, respectively, which are correlated over ~3–6 unit cells in the *ab* plane, and appears to be consistent with the presence of an O-ordered "ortho-IV" phase. Long-range strains emanating from these modulated regions generate an inhomogeneous lattice which may play a fundamentally important role in the electronic properties of yttrium-barium-copper-oxides.



Summary

Small cluster DCA Hubbard calculations display key features of cuprate phase diagram.

LDA+DCA calculations are feasible. We are testing fundamental assumptions of many cuprate theories.

http://www.physics.uc.edu/~pkent