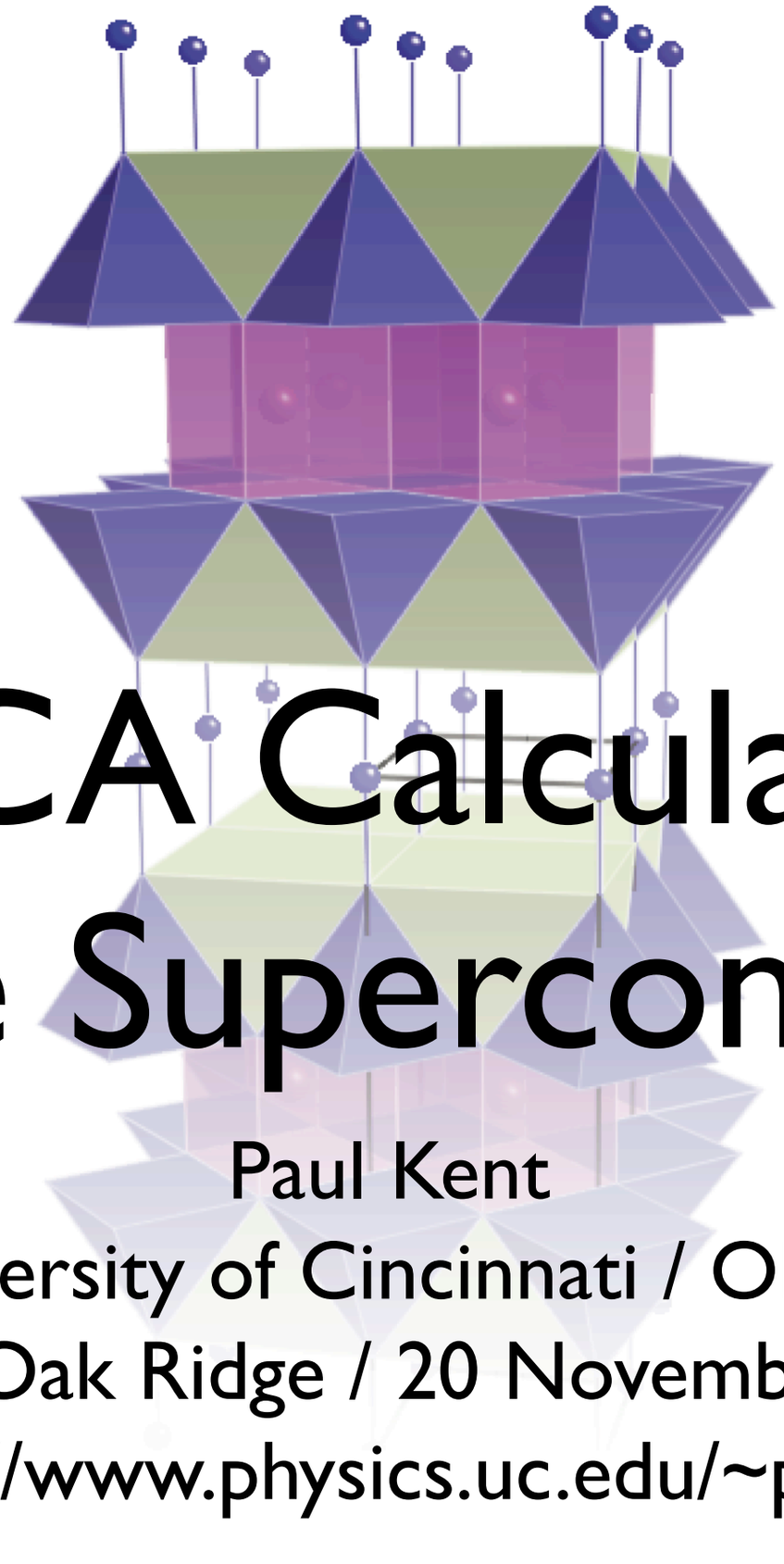
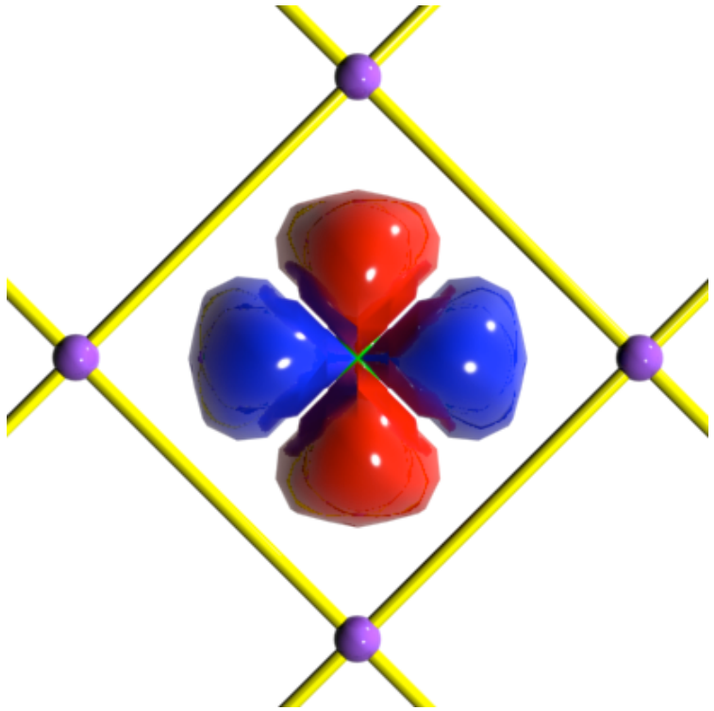


LDA-DCA Calculations of Cuprate Superconductors

Paul Kent
University of Cincinnati / ORNL
CMSN Oak Ridge / 20 November 2004
http://www.physics.uc.edu/~pkent

$n(\mathbf{r})$

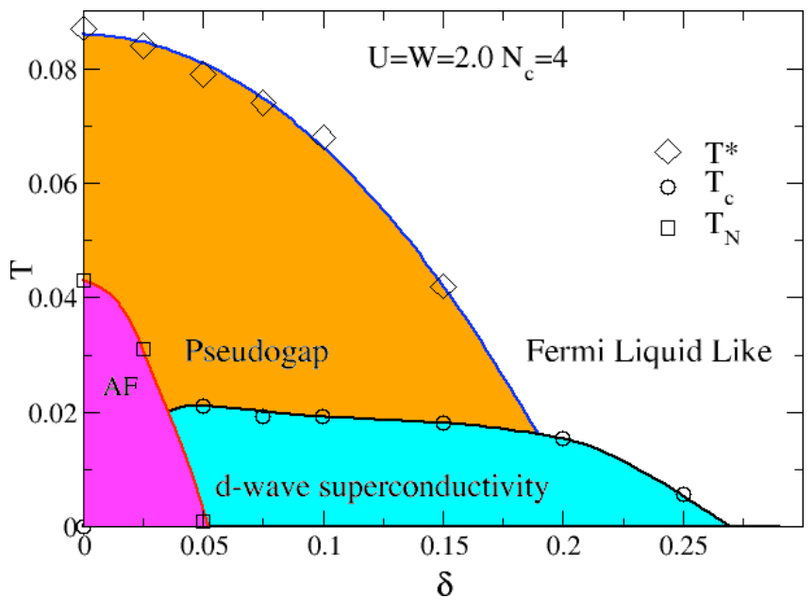


1. DFT LDA ground state

Downfold

2. Wannier Basis & Hamiltonian

DCA



3. Tc, Phase Diagram

Aims: Avoid empirical parameters

What are the materials trends in Tc?

Acknowledgements

Collaborators:

Mark Jarrell, Alexandru Macridin / UC

Thomas Maier, Thomas Schulthess / ORNL

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

Funding:

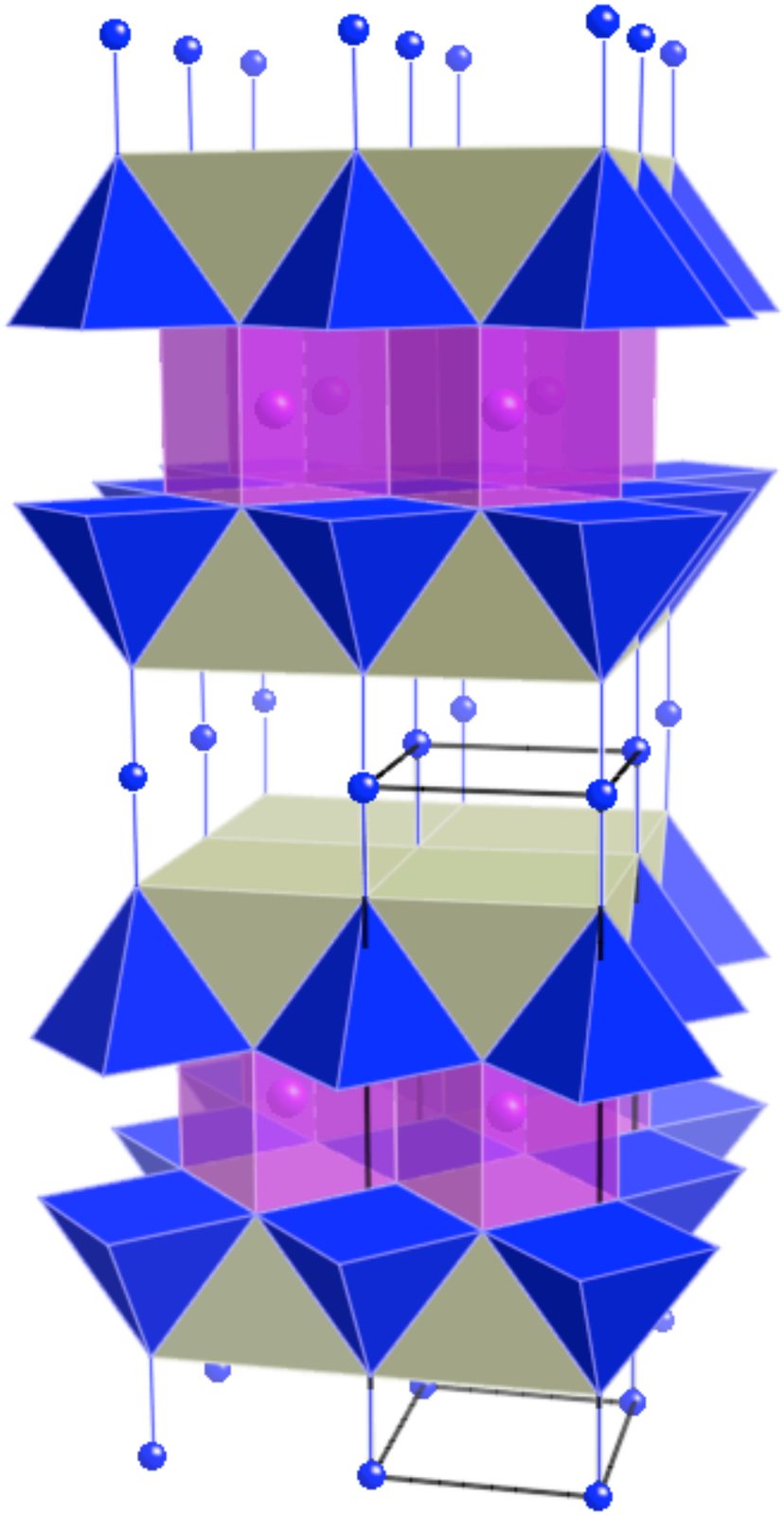
DOE / CMSN

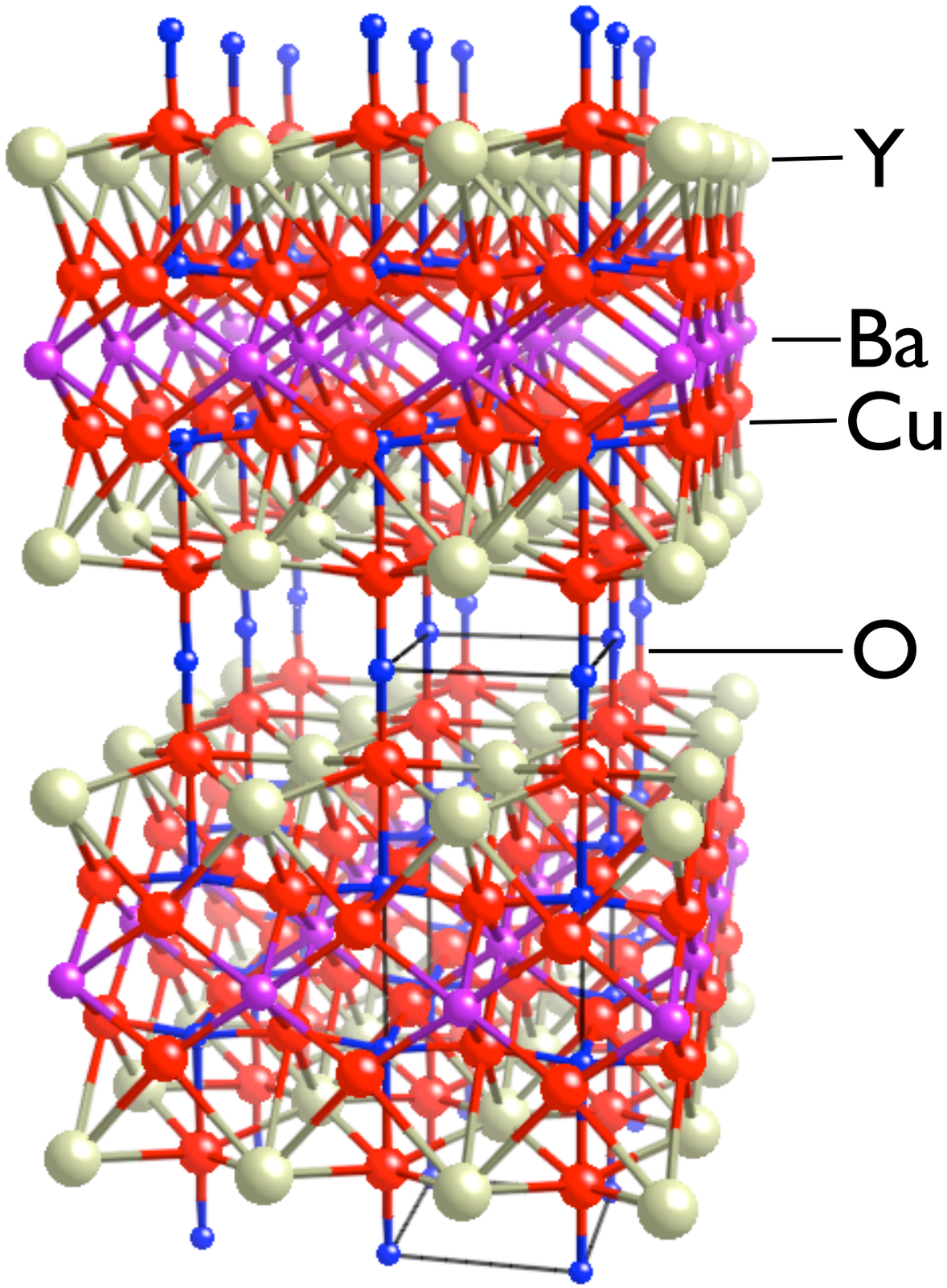
Computer time:

Cray X1 / ORNL

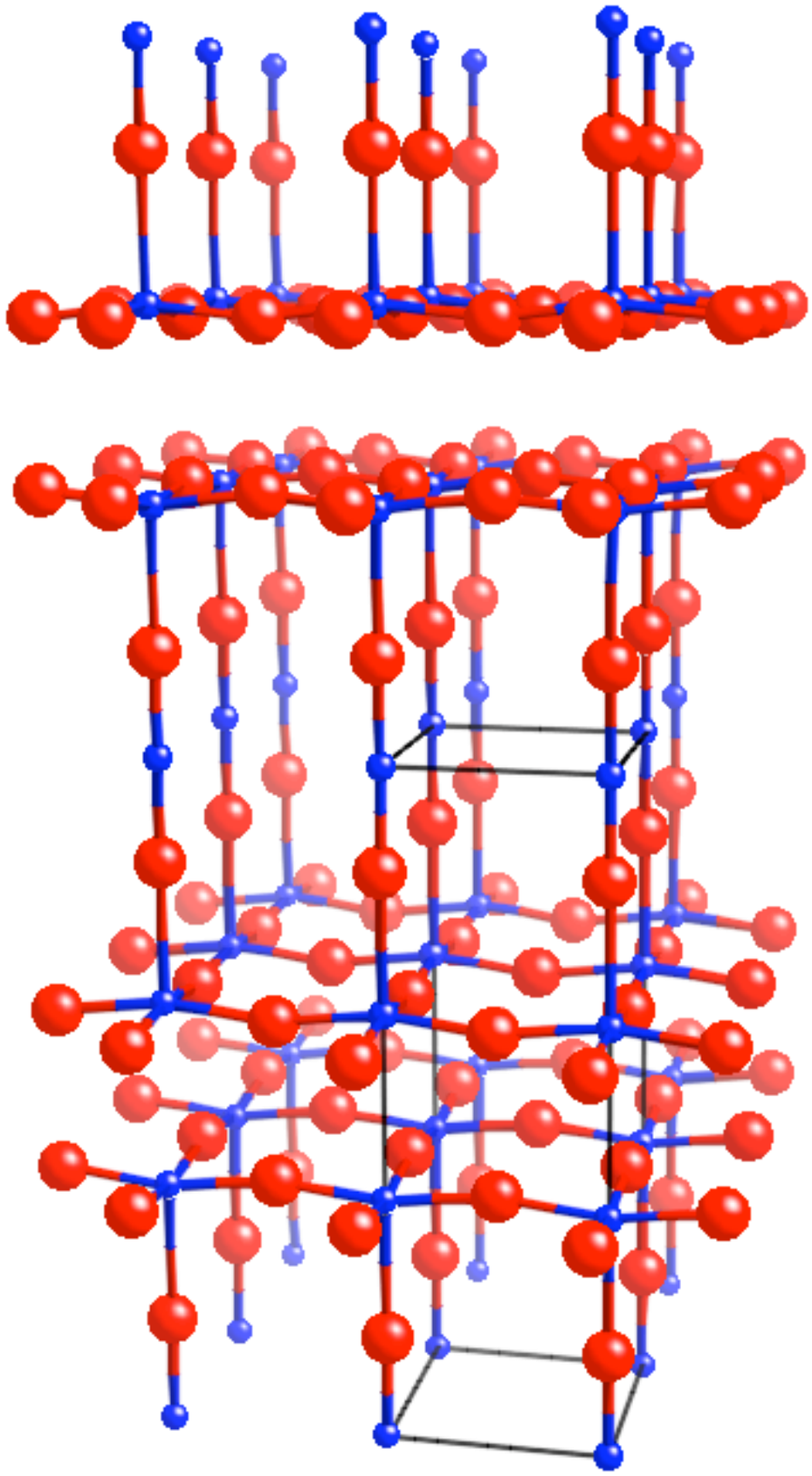
Outline

1. Background - Experiment and Theory
2. Our Approach
3. Results for single-layer materials
4. Next Steps and Summary





YBa2Cu3O6

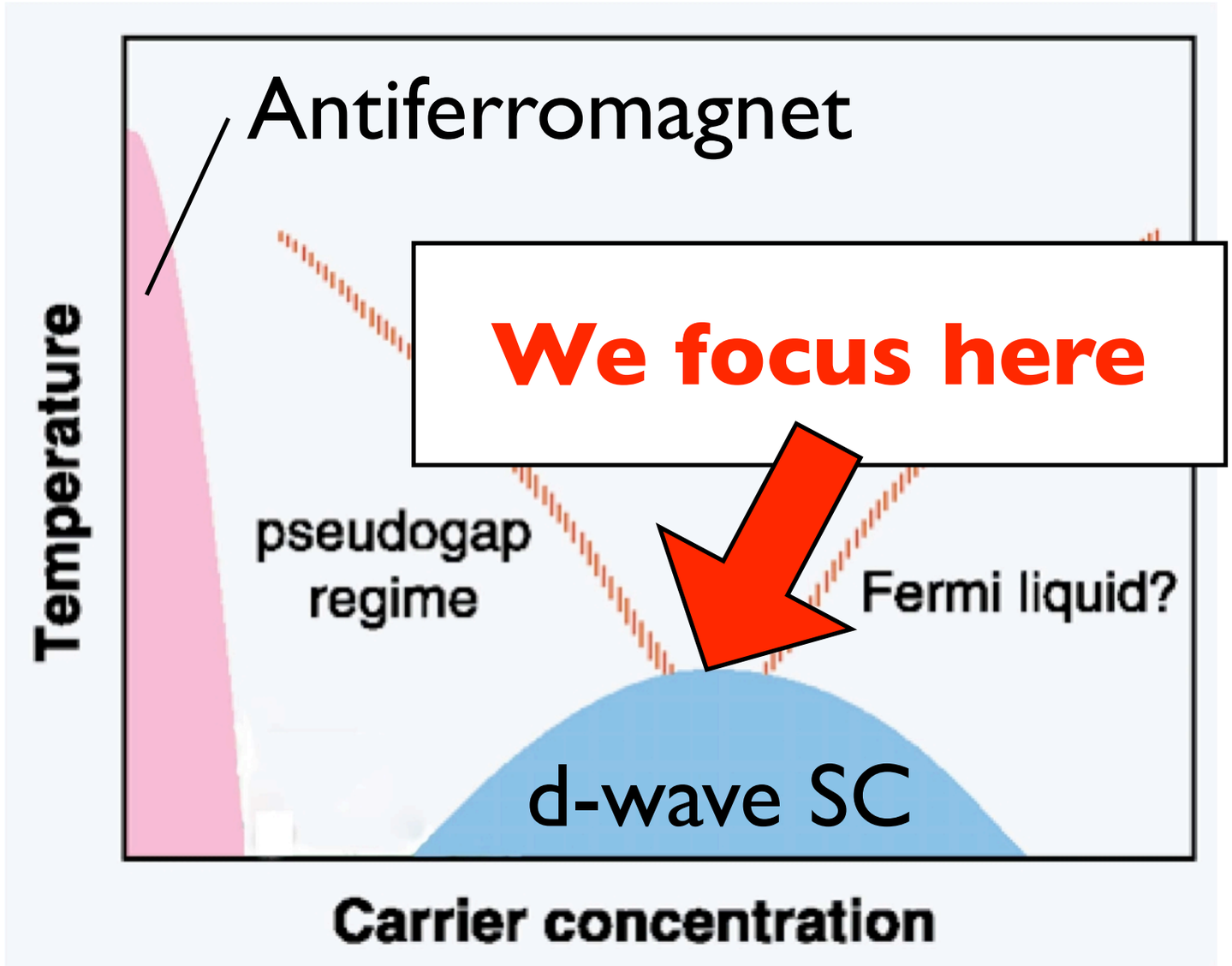


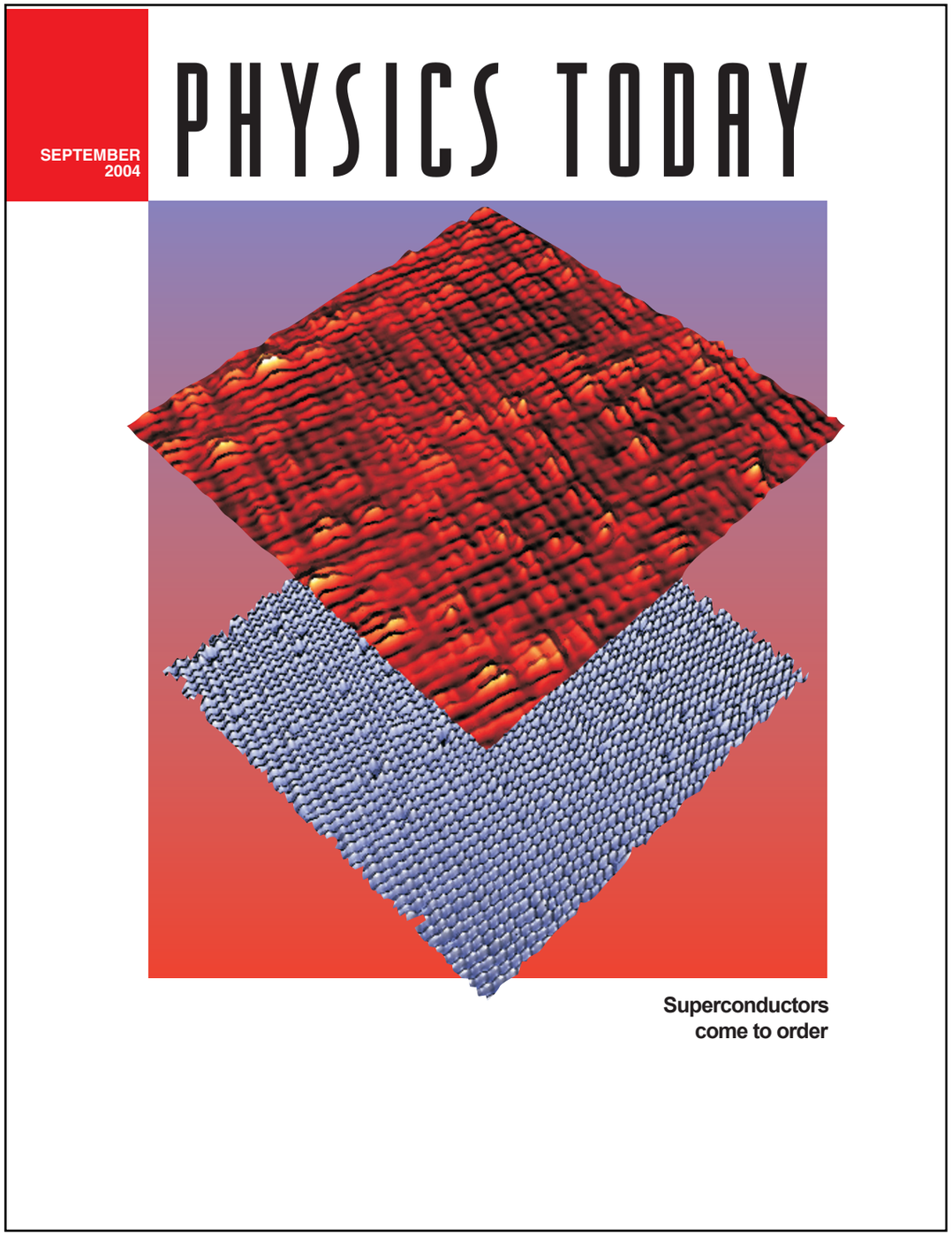
Cu-O plane common to all cuprates

How does entire structure influence Cu-O plane physics?

YBa2Cu3O6: Cu,O atoms only

Rich Phenomenology





“Key” Properties

Single layer compounds: Tc=30-80K

e.g. La2CuO4 “La214” Tc=40K

Highest Tc~130K HgBa2Ca2Cu3O8

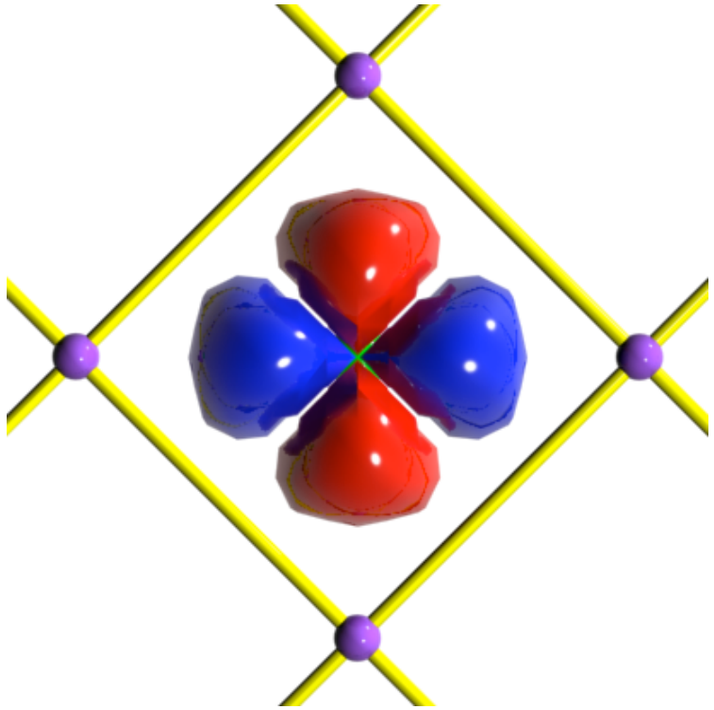
Pressure increases 1K/GPa to ~30GPa

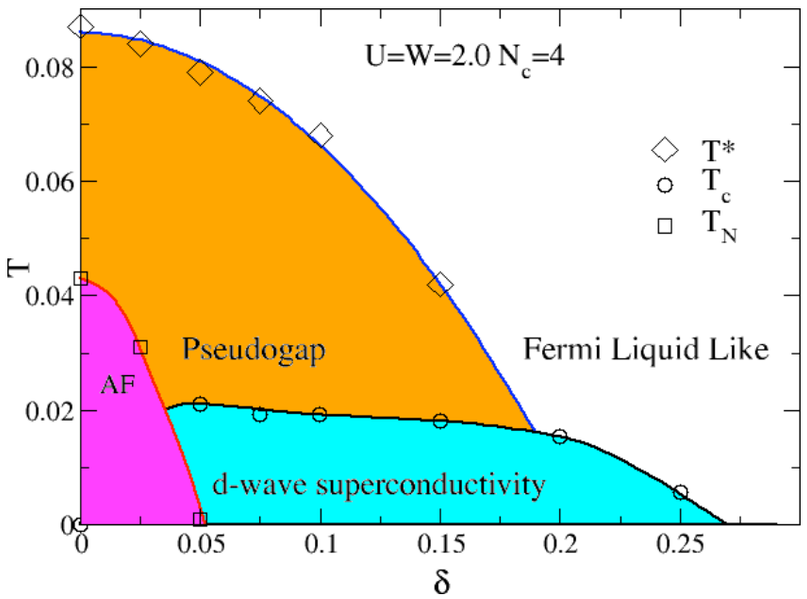
We aim to find some of these trends from first-principles calculation

Outline

1. Background - Experiment and Theory
2. **Our Approach**
3. Parametric results for single-layer materials
4. Next Steps and Summary

$n(\mathbf{r})$





1. DFT LDA ground state

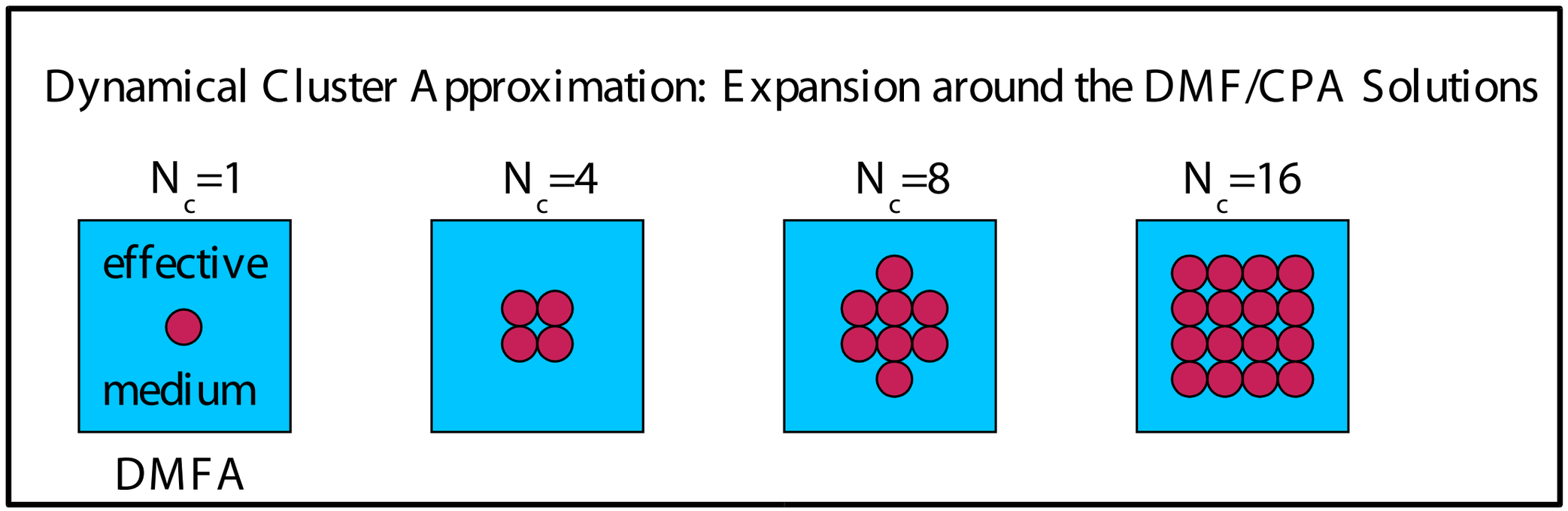
Downfold

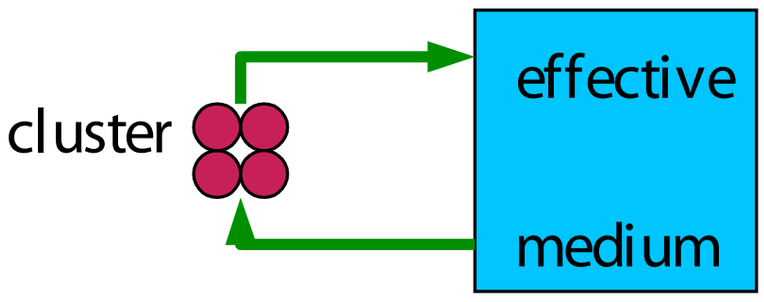
2. Wannier Basis & Hamiltonian

DCA

3. Tc, Phase Diagram

Cluster Approximations

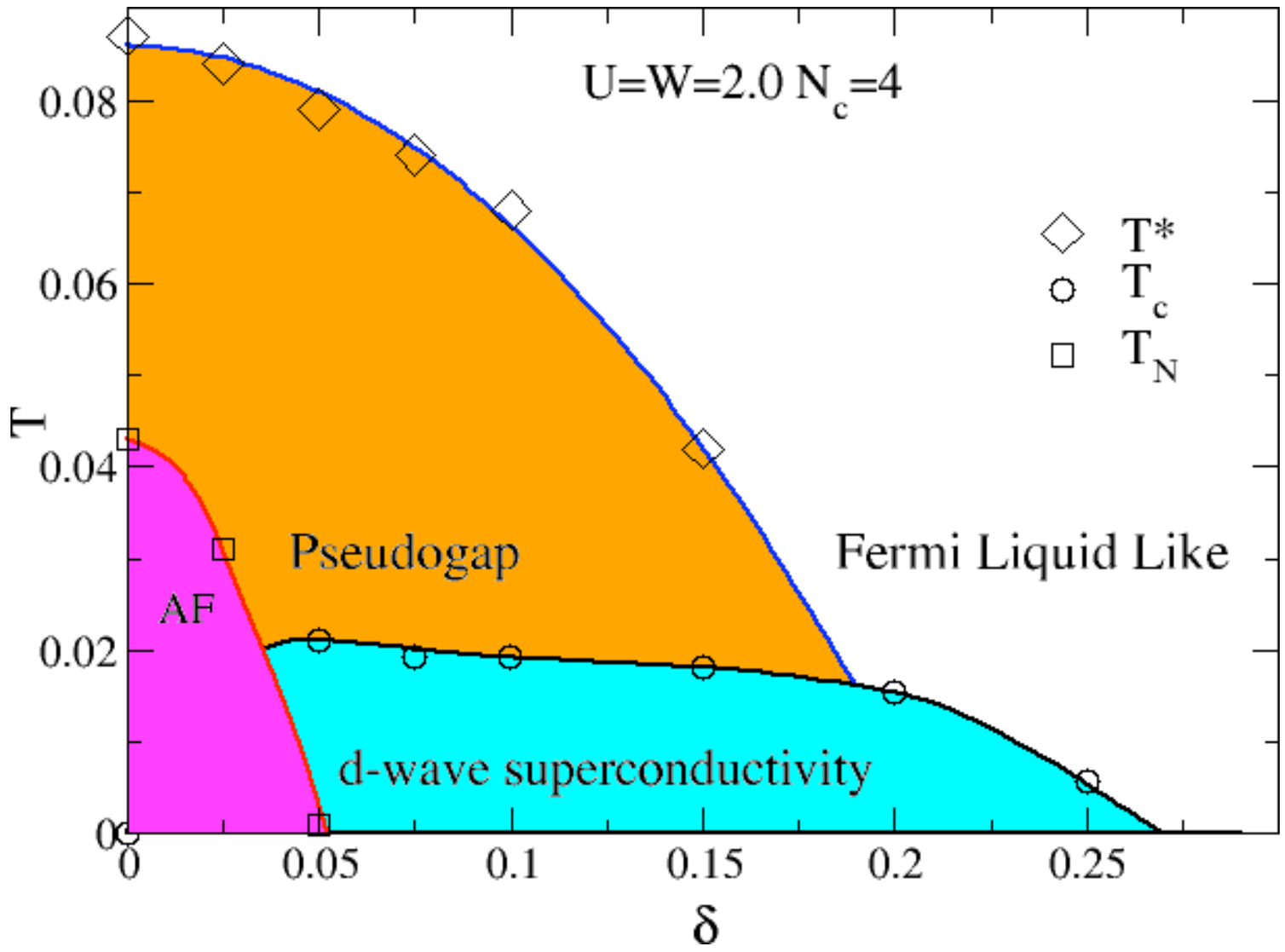




$$\Sigma_{\text{lattice}} \simeq \Sigma_{\text{cluster}}$$

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

2x2 DCA Results



Phase diagram for 2x2 single band Hubbard model

LDA Downfolding

Per Ole Andersen's talk last meeting; also Eva Pavarini's talk this evening

Andersen J. Phys.Chem. Solids ***56*** *1573 (1995)*

We obtain a 3 band Hamiltonian:

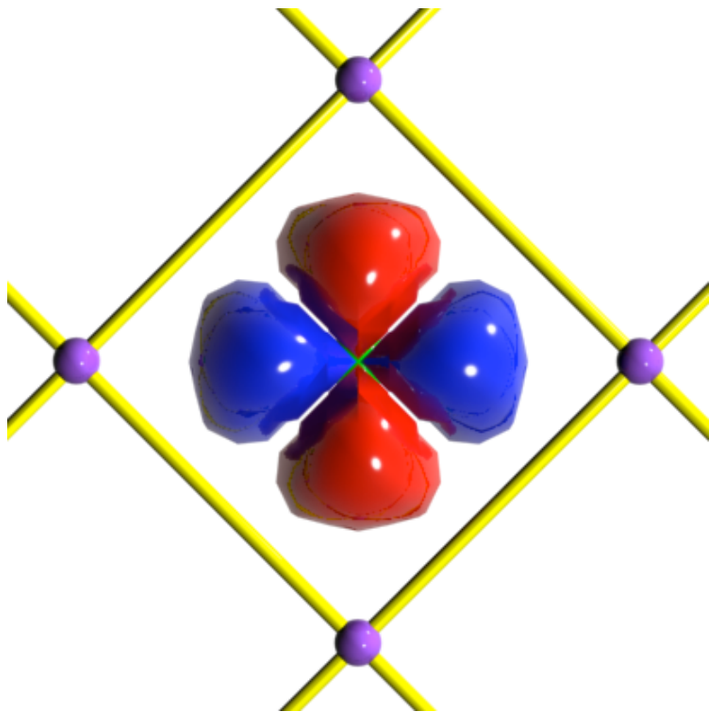
- Chemically intuitive hopping terms between orbitals
- Explicit single particle picture; not many-body (single band)

Calculate U with correct d orbital occupation

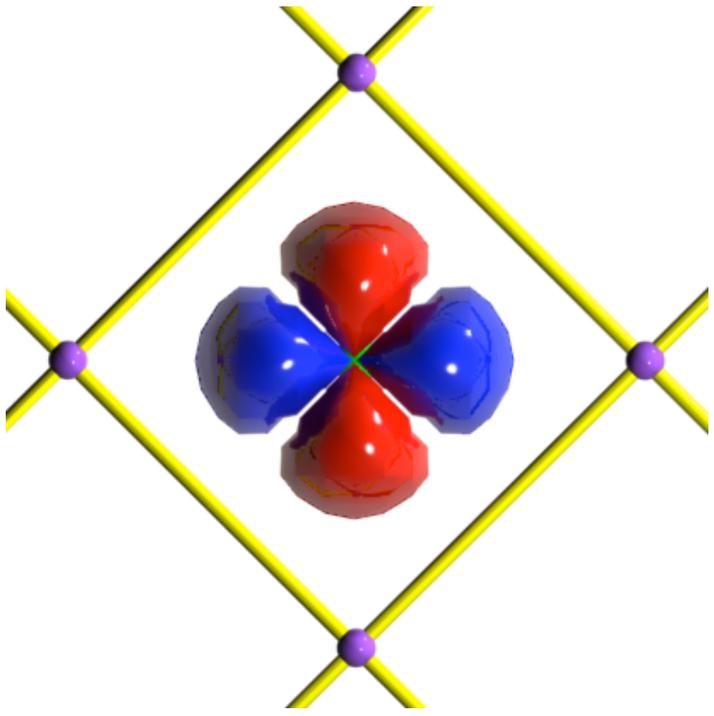
Wannier Orbitals

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

O px, py: strong hybridization.

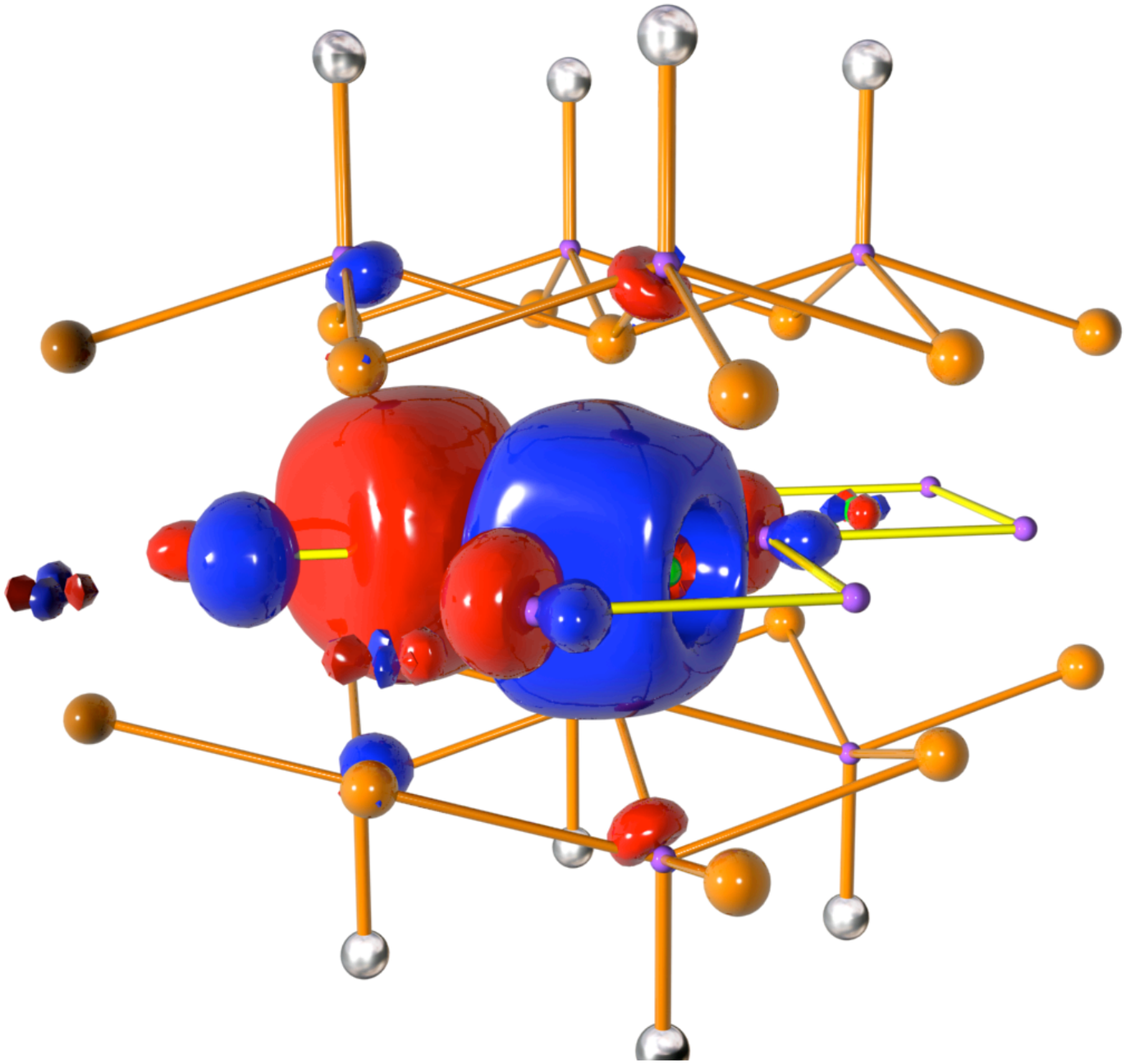


La2CuO4



HgBa2CuO4

Wannier Orbitals



LDA DCA Hamiltonian

Only the Cu d orbital is correlated

$$\mathrm{H}_t = \begin{pmatrix} E_d & V_{1d} & V_{2d} \\ & E_1 & V_{12} \\ & & E_{12} \end{pmatrix}$$

$$\mathrm{E}_d(k) = E_d + 2t_{dd1}(cos(k_x) + cos(k_y)) + ...$$
$$\mathrm{E}_1(k) = E_p + 2t_{pp1}cos(k_x) + ...$$
$$\mathrm{V}_{1d}(k) = -2t_{pd1}sin(k_x/2) - 4t_{pd2}sin(k_x/2)cos(k_y) + .$$

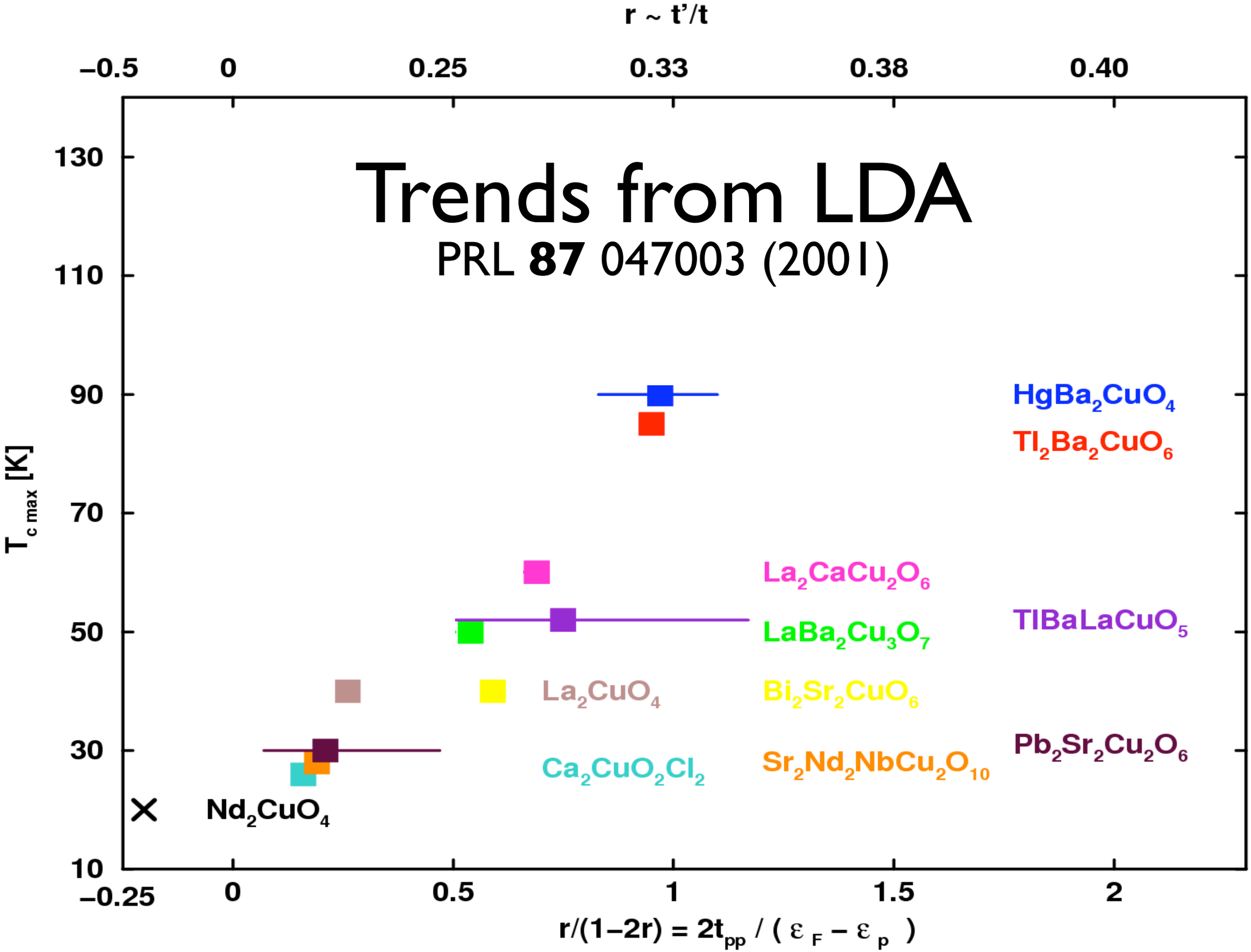
+ Hubbard terms for d orbital

Can this work?

LDA already shows interesting trends/correlations

Trends from LDA

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

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

Outline

1. Background - Experiment and Theory
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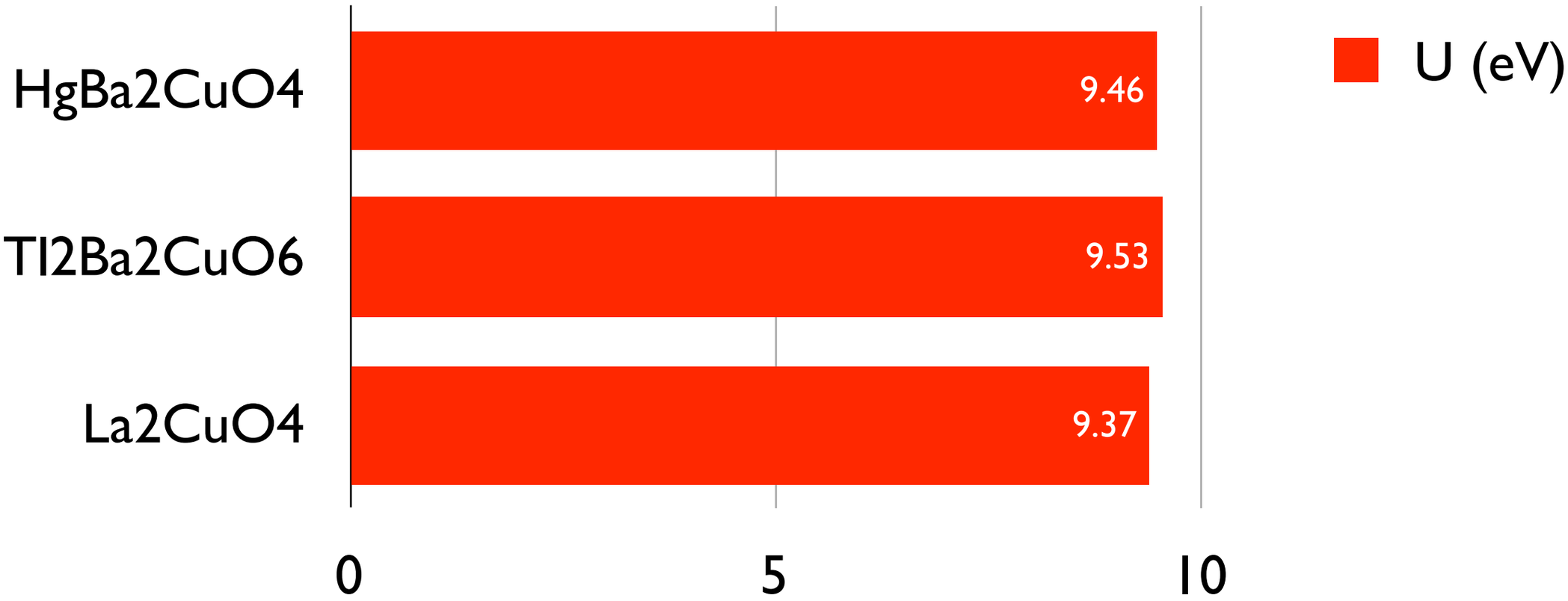
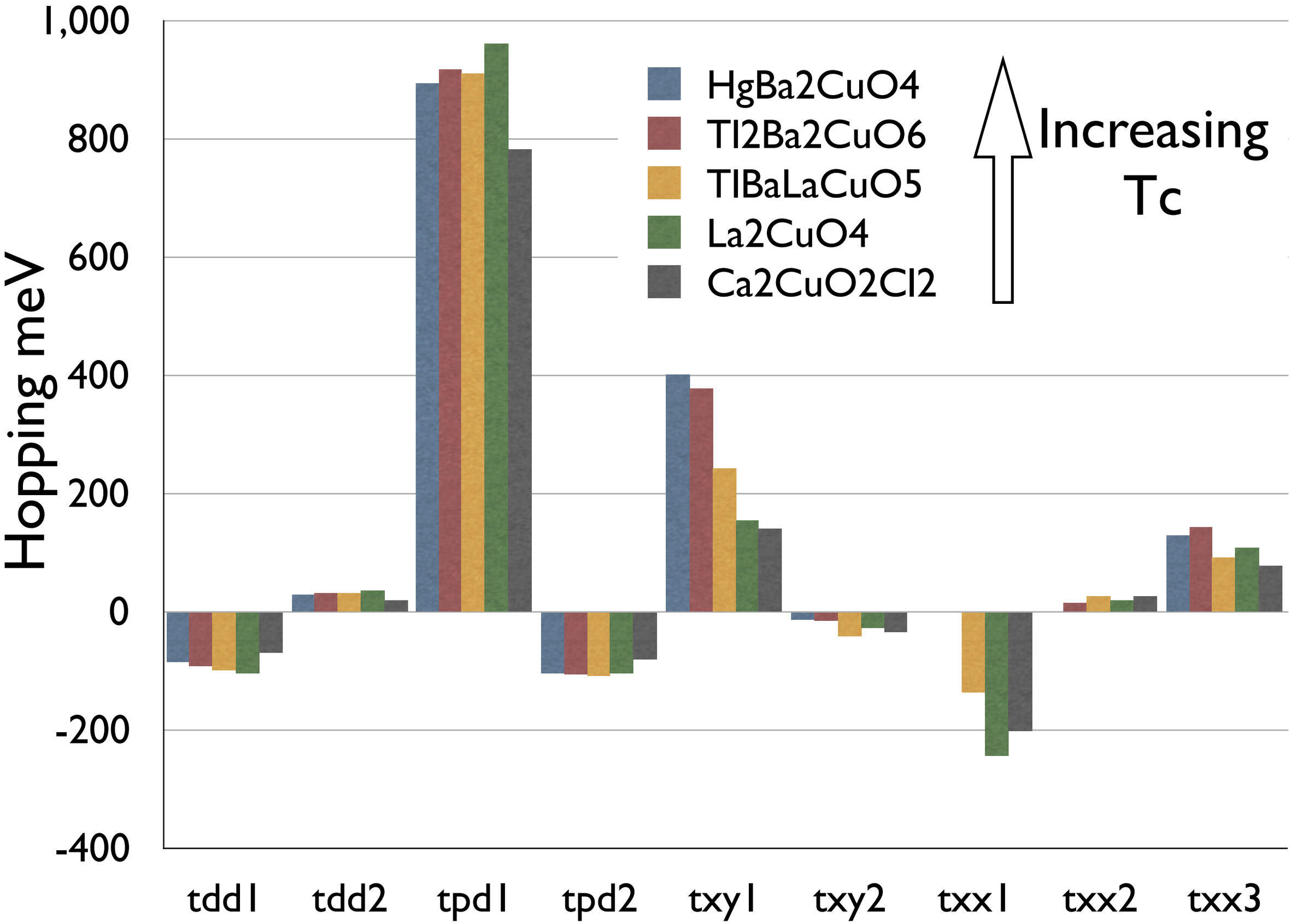
3. **Results for single-layer materials**
4. Next Steps and Summary

Calculated U



Few % variation in U; similar in all materials

Any Tc dependence must reside in Wannier orbitals

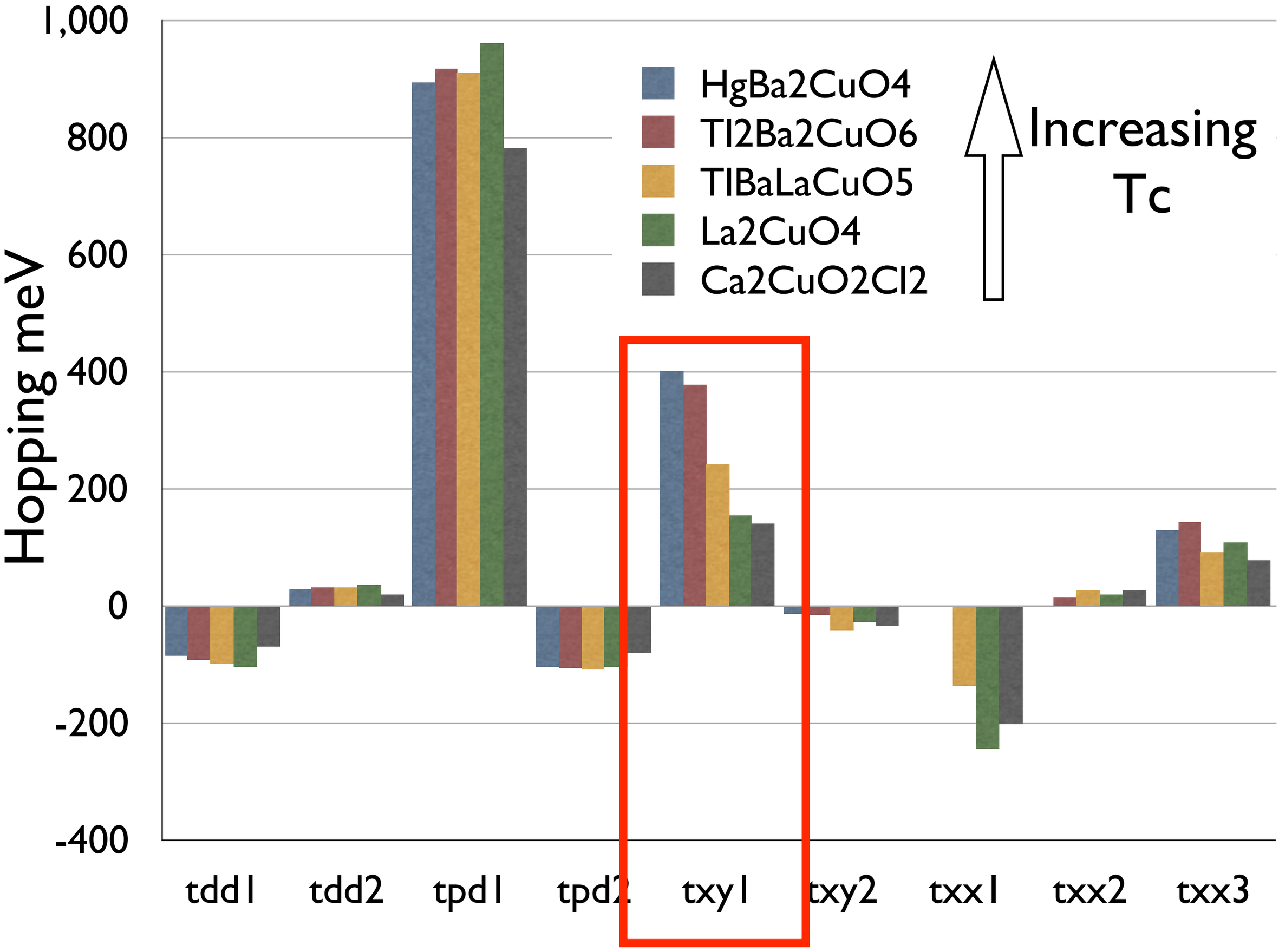

1,000
800
600
400
200
0
-200
-400
Hopping meV
HgBa2CuO4
Tl2Ba2CuO6
TlBaLaCuO5
La2CuO4
Ca2CuO2Cl2
Increasing Tc
tdd1
tdd2
tpd1
tpd2
txy1
txy2
txx1
txx2
txx3

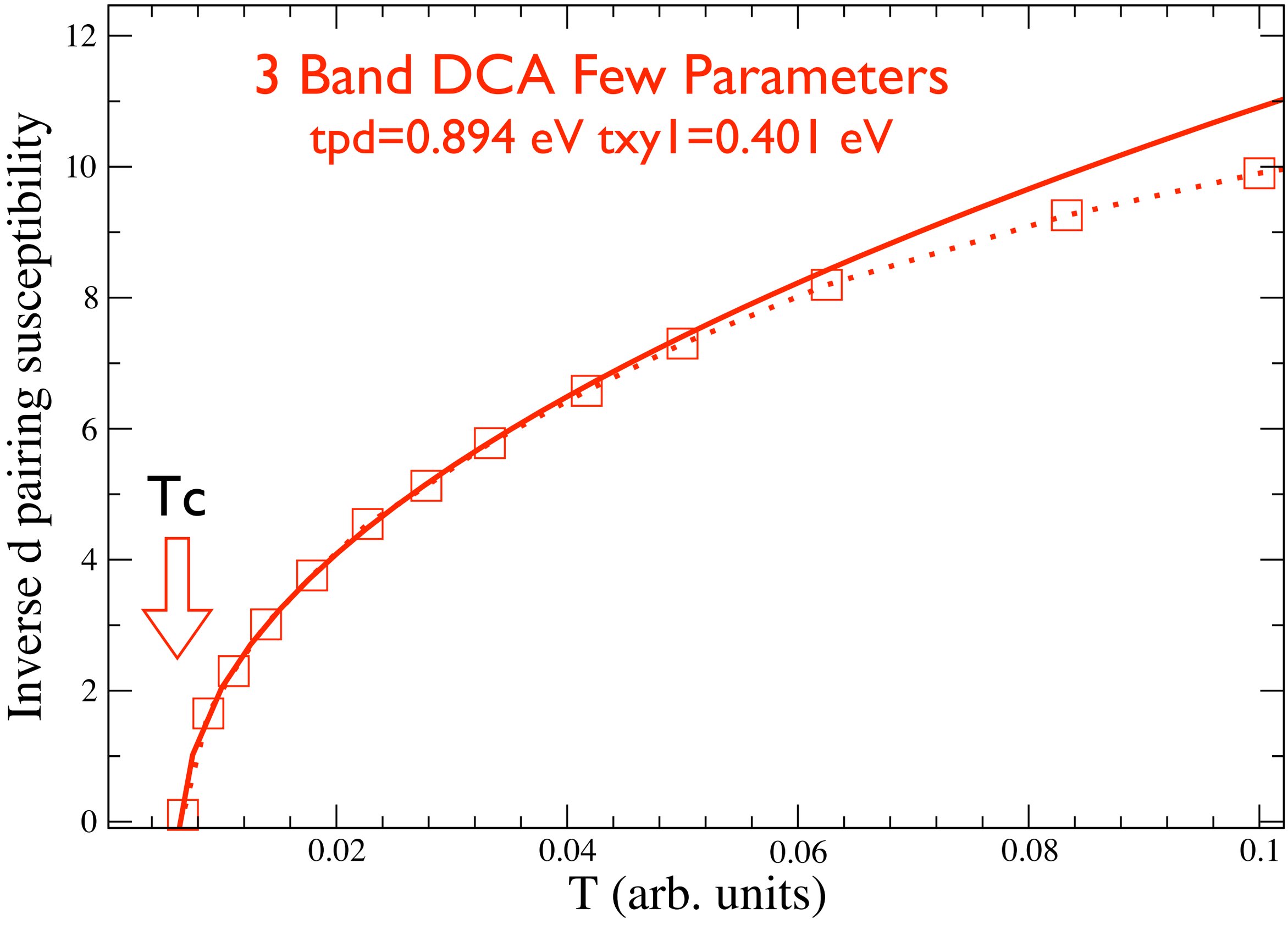
Downfolding Results

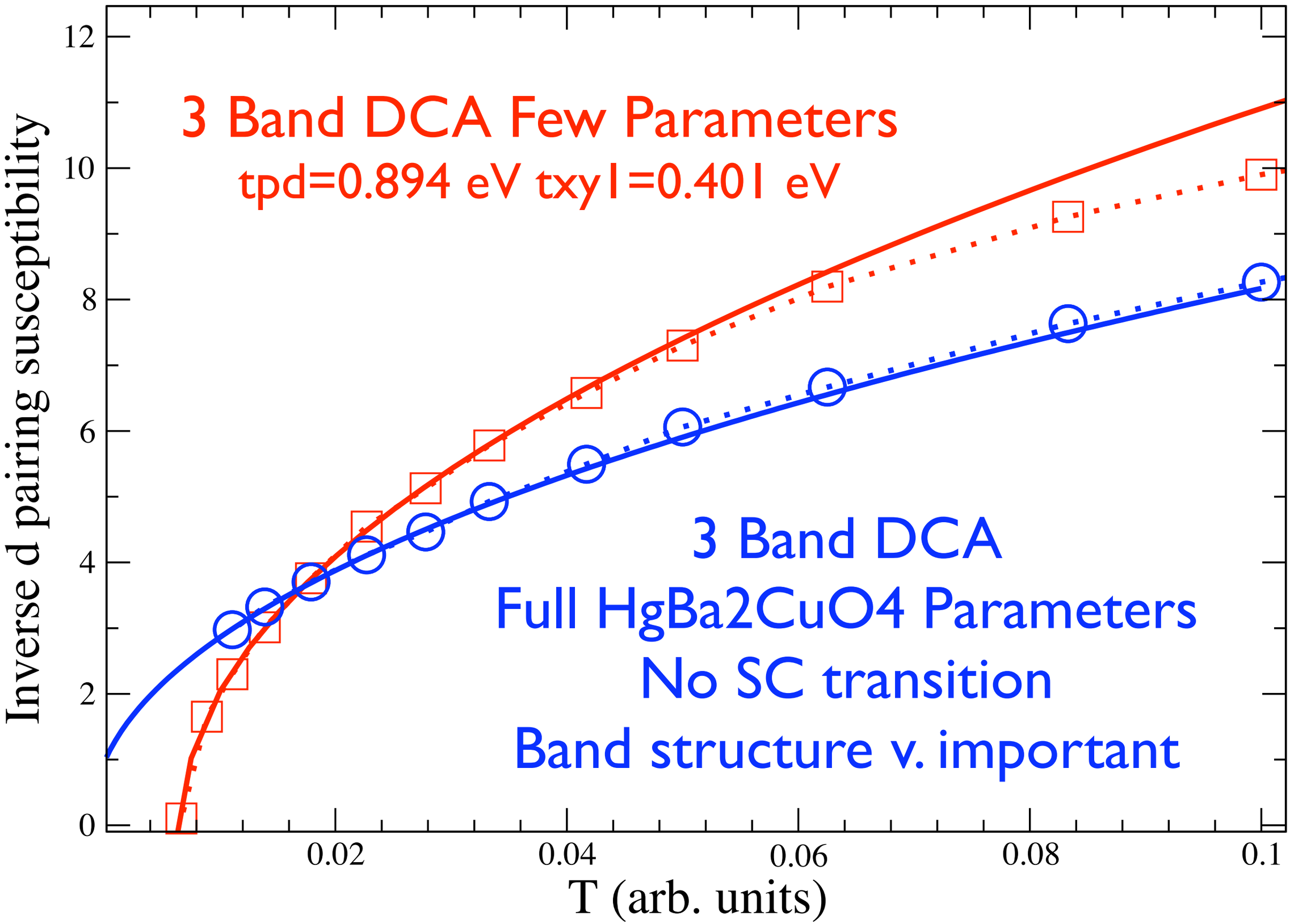
- ~6 terms appear significant, in this basis

  Parametric studies are possible

  - Some terms are ~constant e.g. tpd2
  - 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


3 Band DCA Few Parameters
tpd=0.894 eV txy1=0.401 eV
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


3 Band DCA Few Parameters
tpd=0.894 eV txy1=0.401 eV
3 Band DCA
Full HgBa2CuO4 Parameters
No SC transition
Band structure v. important
Inverse d pairing susceptibility
T (arb. units)
0
2
4
6
8
10
12
0.02
0.04
0.06
0.08
0.1

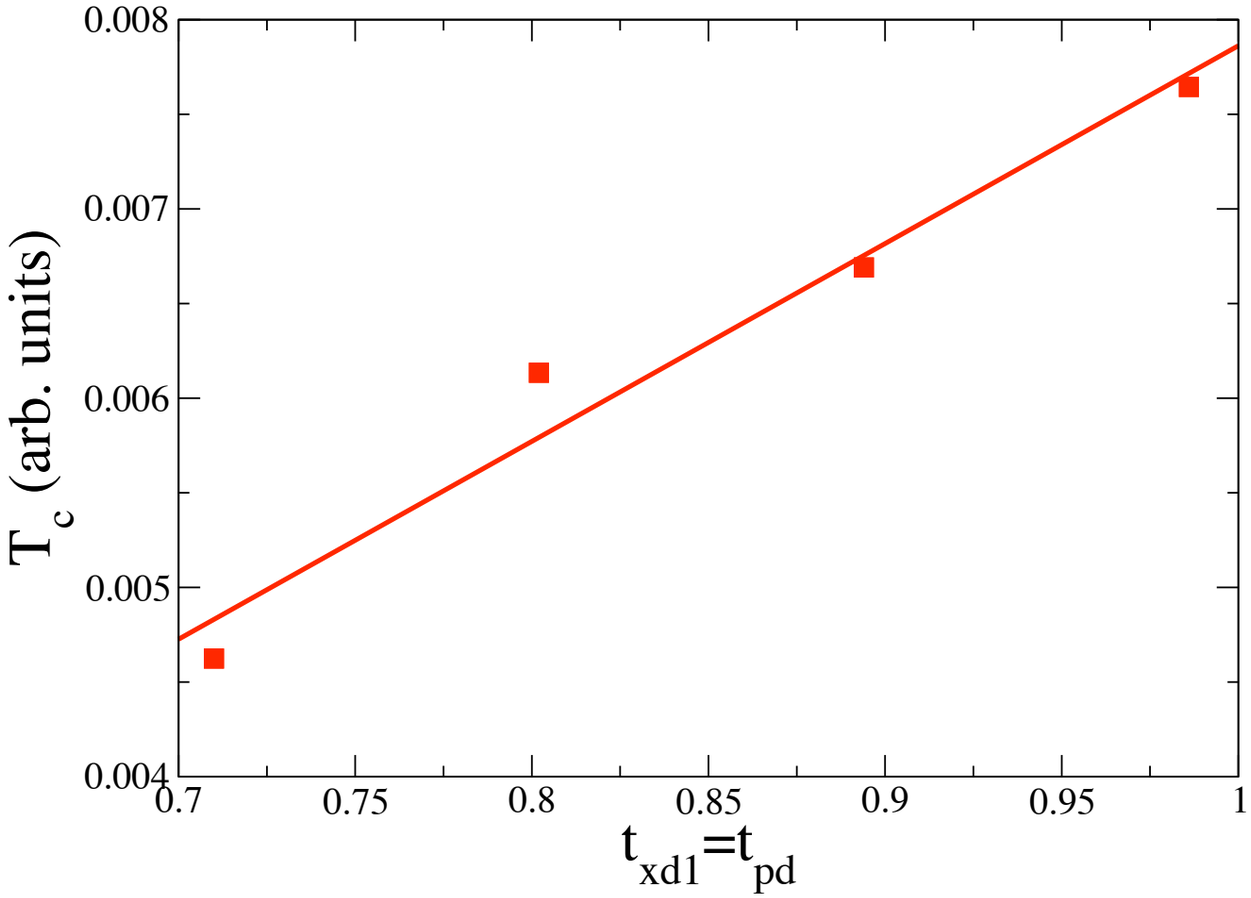
Bug or Feature?

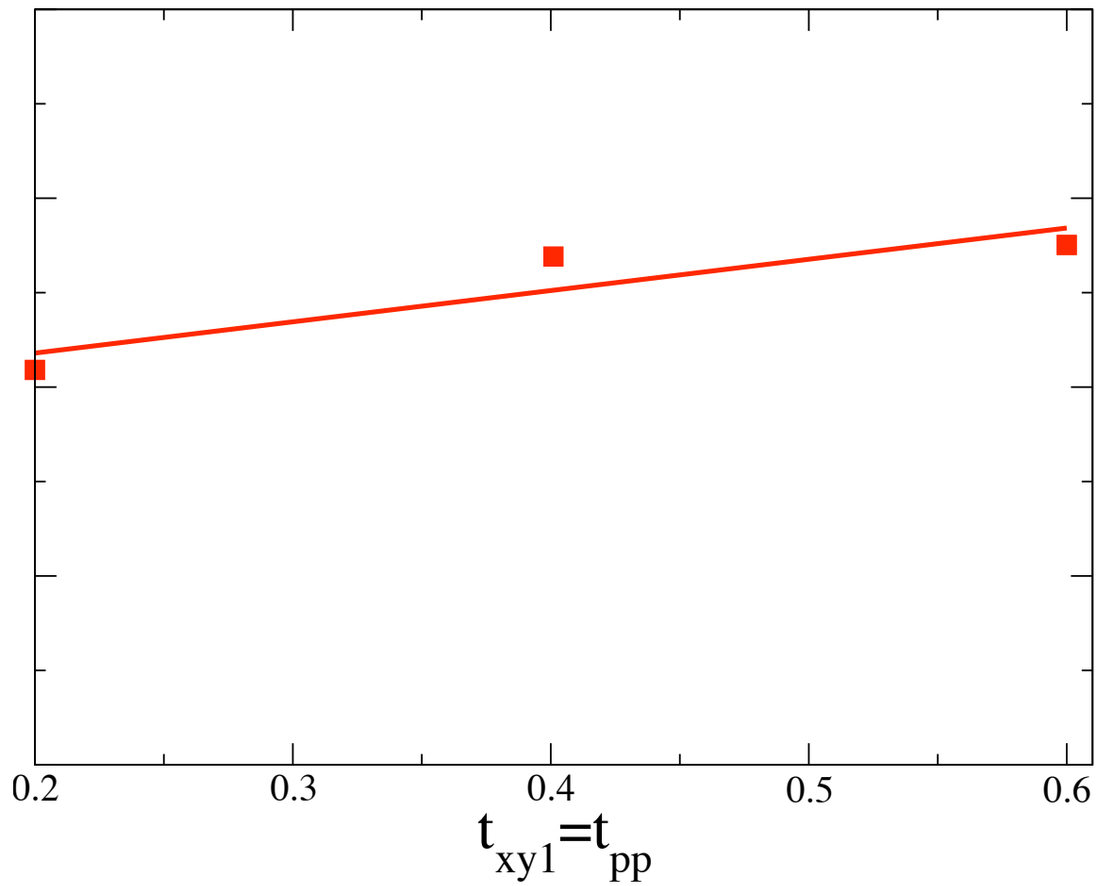
Favour “feature” - real physics - but checks continue

Unsuspected parameters strongly influence Tc

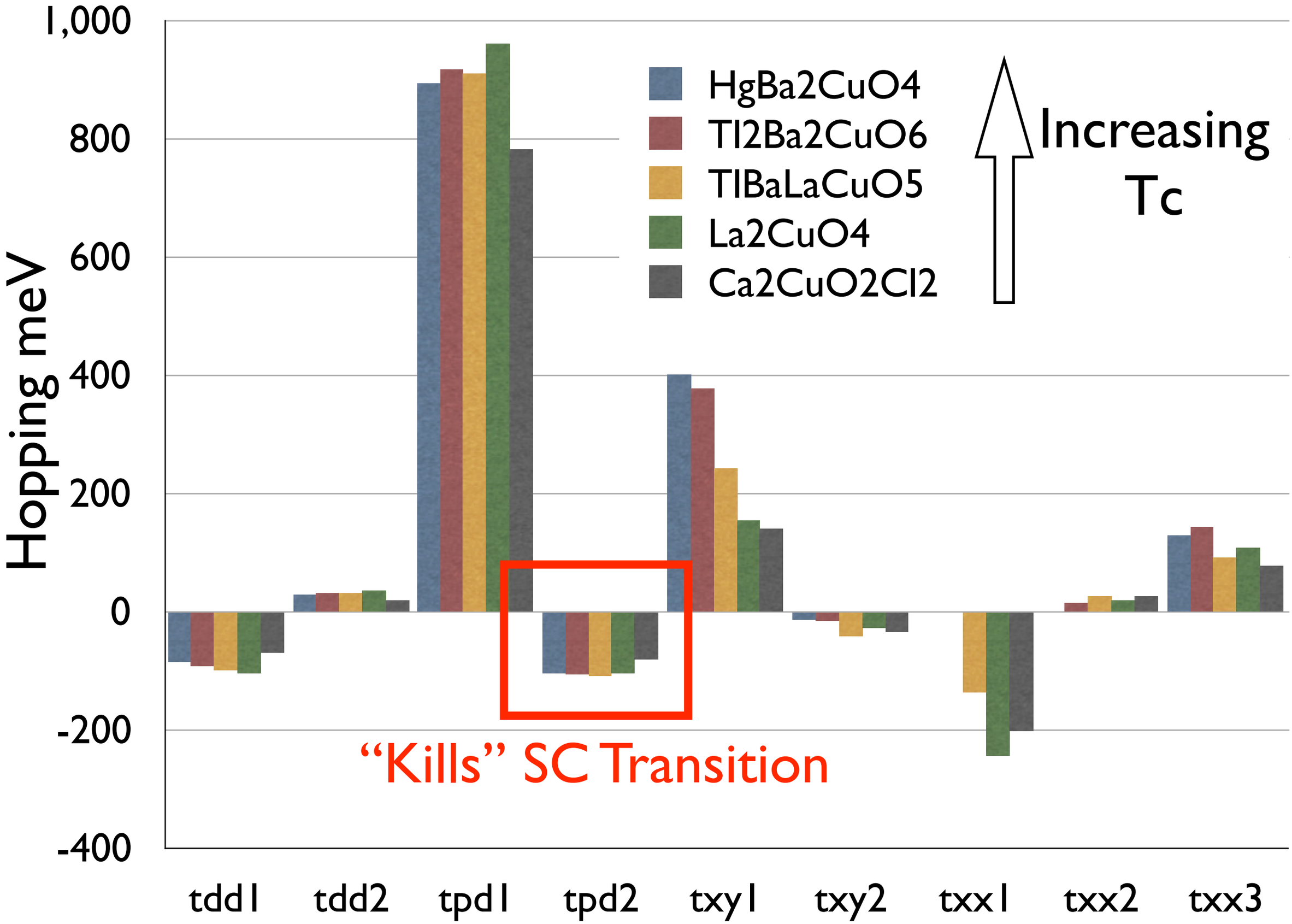
Parametric Results

We have checked ~10 dependencies in combination

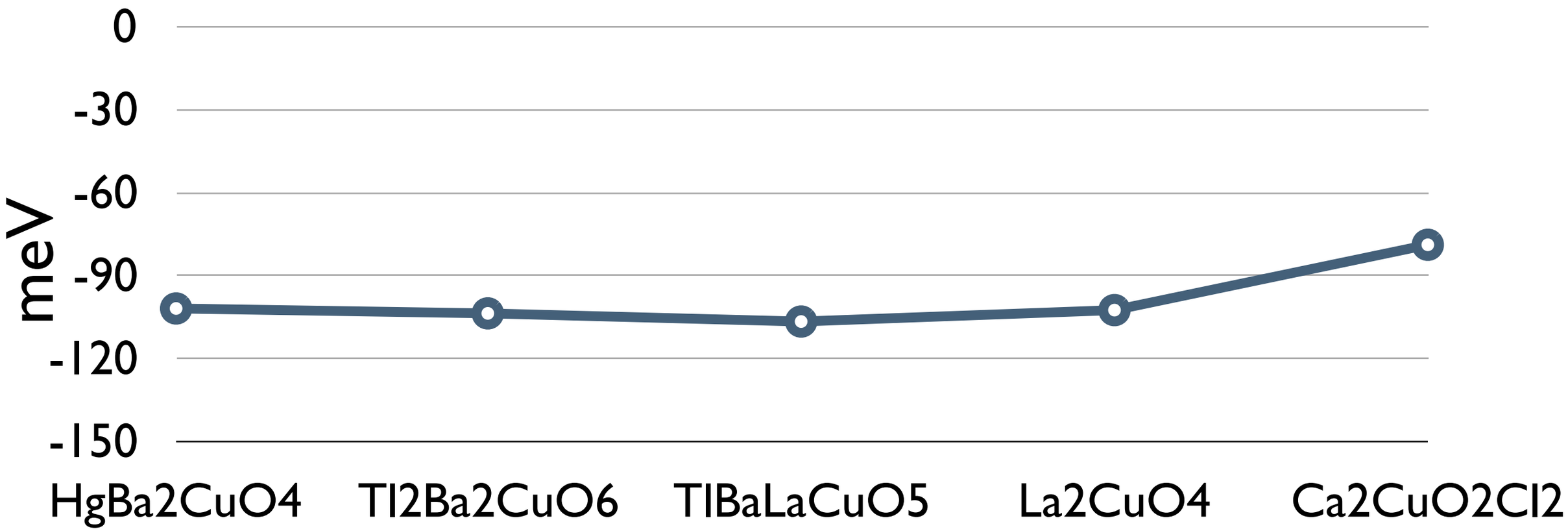




- ☑ Tc increases with increasing tpd and tpp
- ☑ Tc not critically dependent on U above theshold


1,000
800
600
400
200
0
-200
-400
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. Background - Experiment and Theory
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3. Results for single-layer materials
4. **Next Steps and Summary**

Next Steps

(a) Investigating influence of DFT ground state:

- LDA+U based calculations underway
- Expect “bad” p-d hybrizations to weaken...

...But other hybrizations will also change

(b) Different downfoldings

(c) Self-consistency?

1. DFT LDA ground state

Downfold

2. Wannier Basis & Hamiltonian

DCA

3. Tc, Phase Diagram

$n'(\mathbf{r})$

Summary

We have identified a "good set" of parameters for the 3 band Hubbard model. LDA DCA calculations find:

- Strong influence of 2nd NN p-d hybridization. Destroys SC transition with LDA parameters
- Tc scales with 1st NN parameters "correctly"
- A need to go beyond LDA for ground state?

Copies of this talk at http://www.physics.uc.edu/~pkent