

LDA+DCA Calculations of Cuprate Superconductors

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

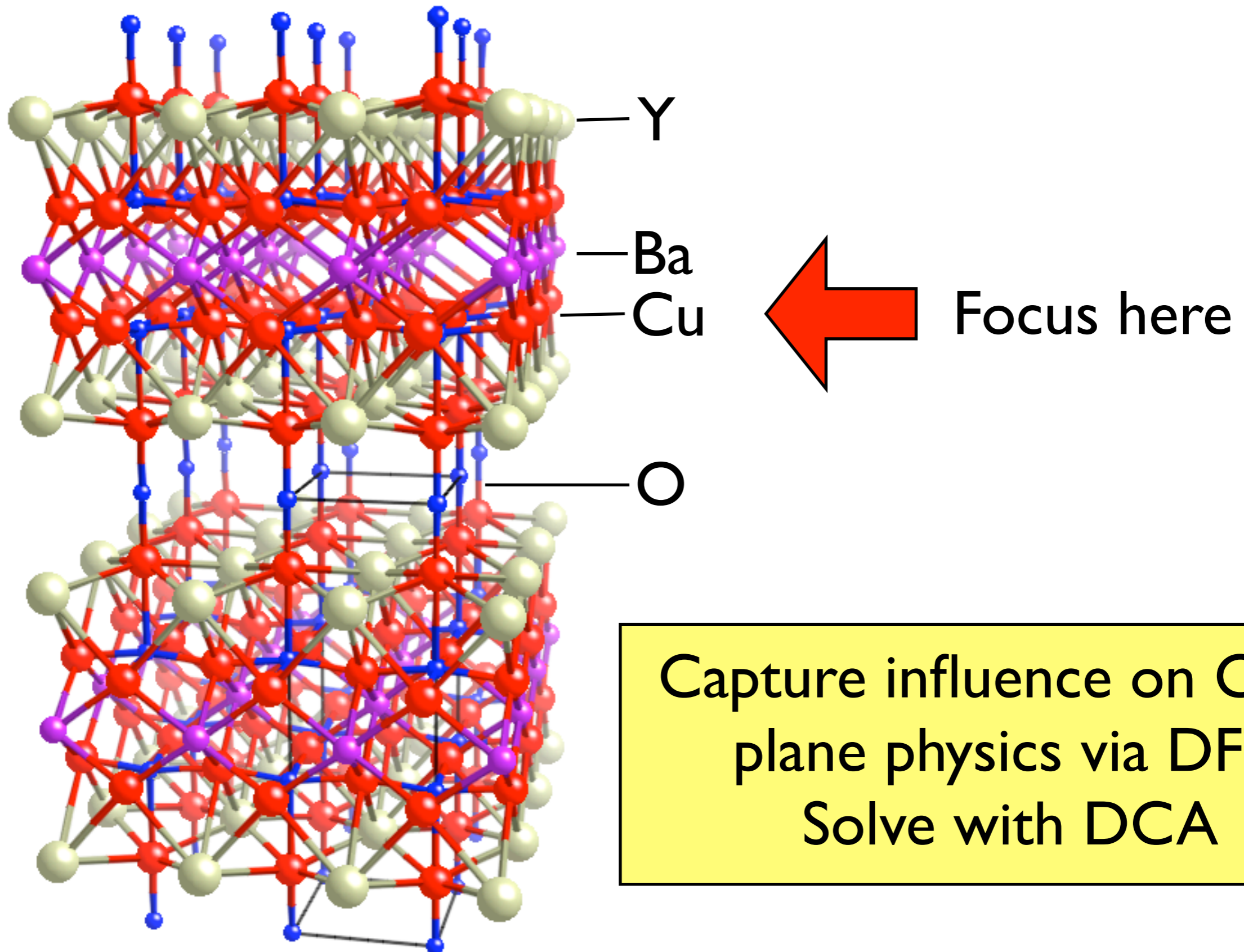
Funding:

NSF & DOE

Computer time:

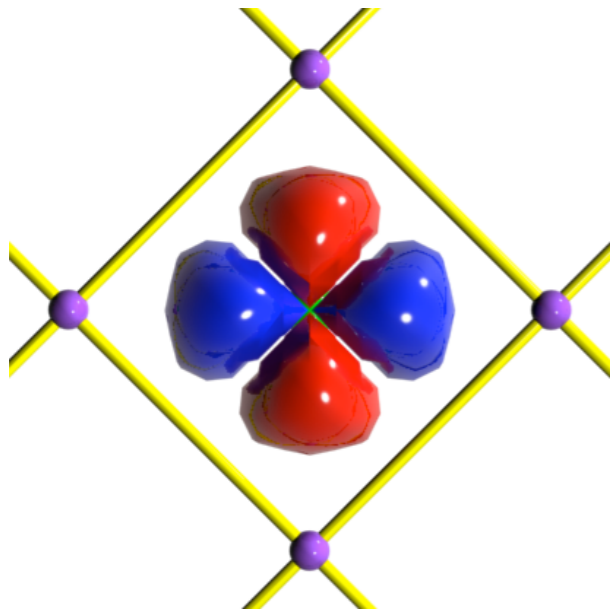
ORNL, OSC, SDSC

Aim: Capture Materials Dependence

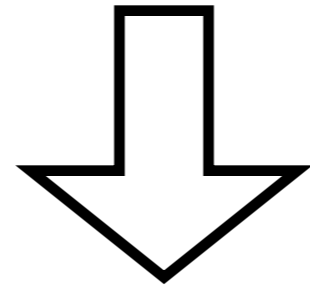


LDA+DCA Method

$n(\mathbf{r})$

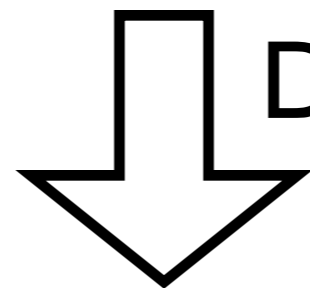


1. DFT LDA ground state



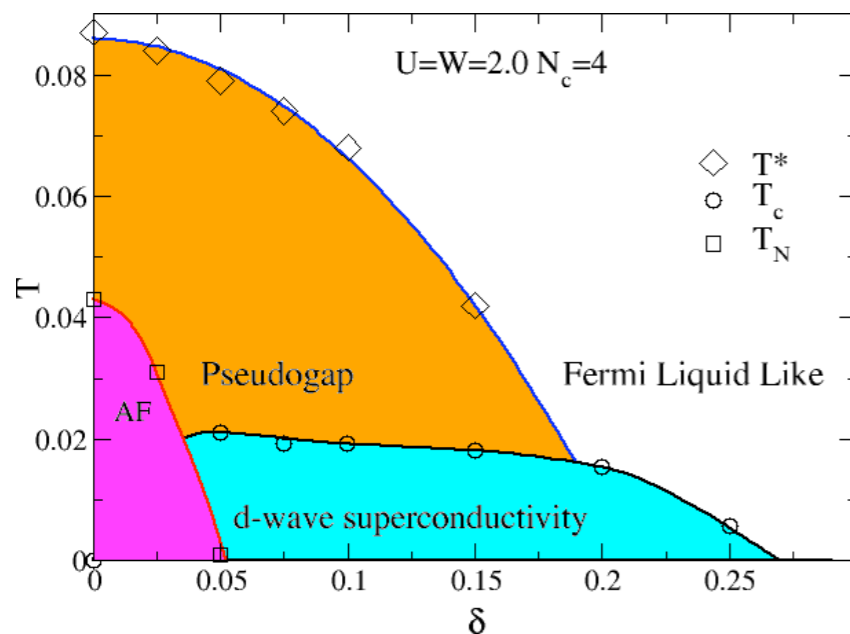
Wannier-Function
downfolding

2. Three-band Hubbard Hamiltonian
All parameters calculated, NOT fit



DCA

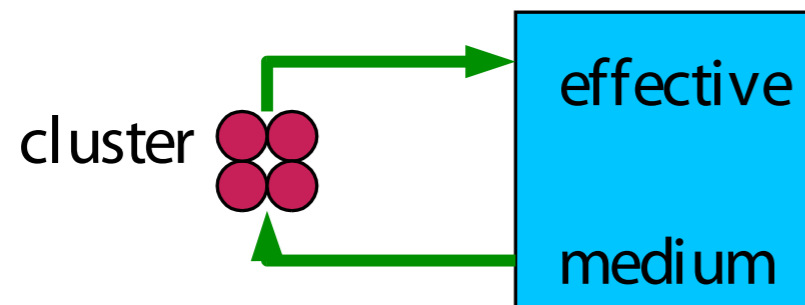
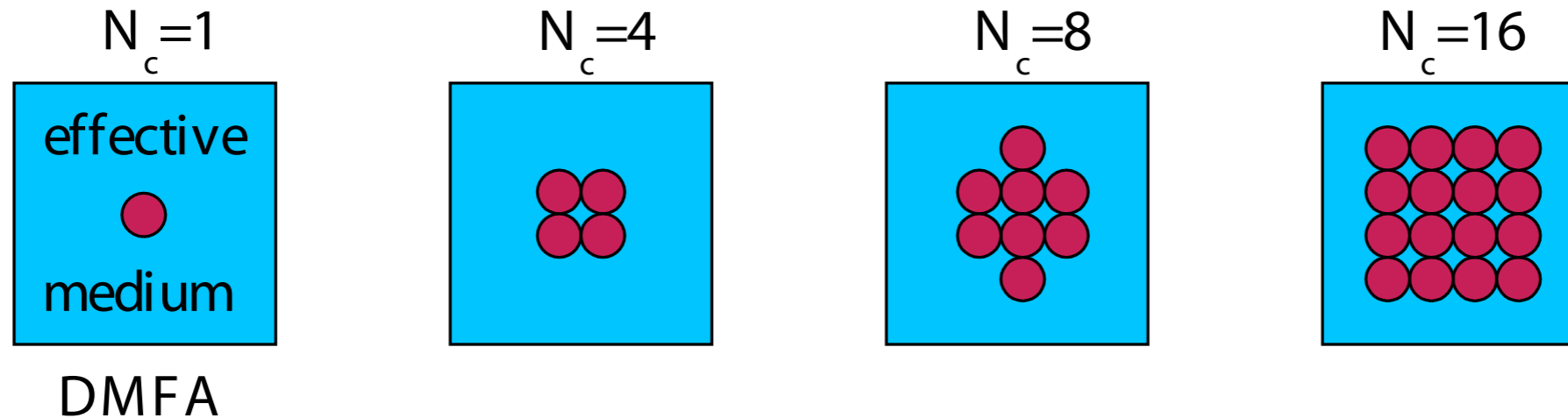
3. Phase Diagram



Similar to LDA+DMFT of Kotliar, Savrasov, others
Systematically Extensible; Self consistent schemes possible

Cluster Approximations

Dynamical Cluster Approximation: Expansion around the DMF/CPA Solutions



$$\sum_{\text{lattice}} \approx \sum_{\text{cluster}}$$

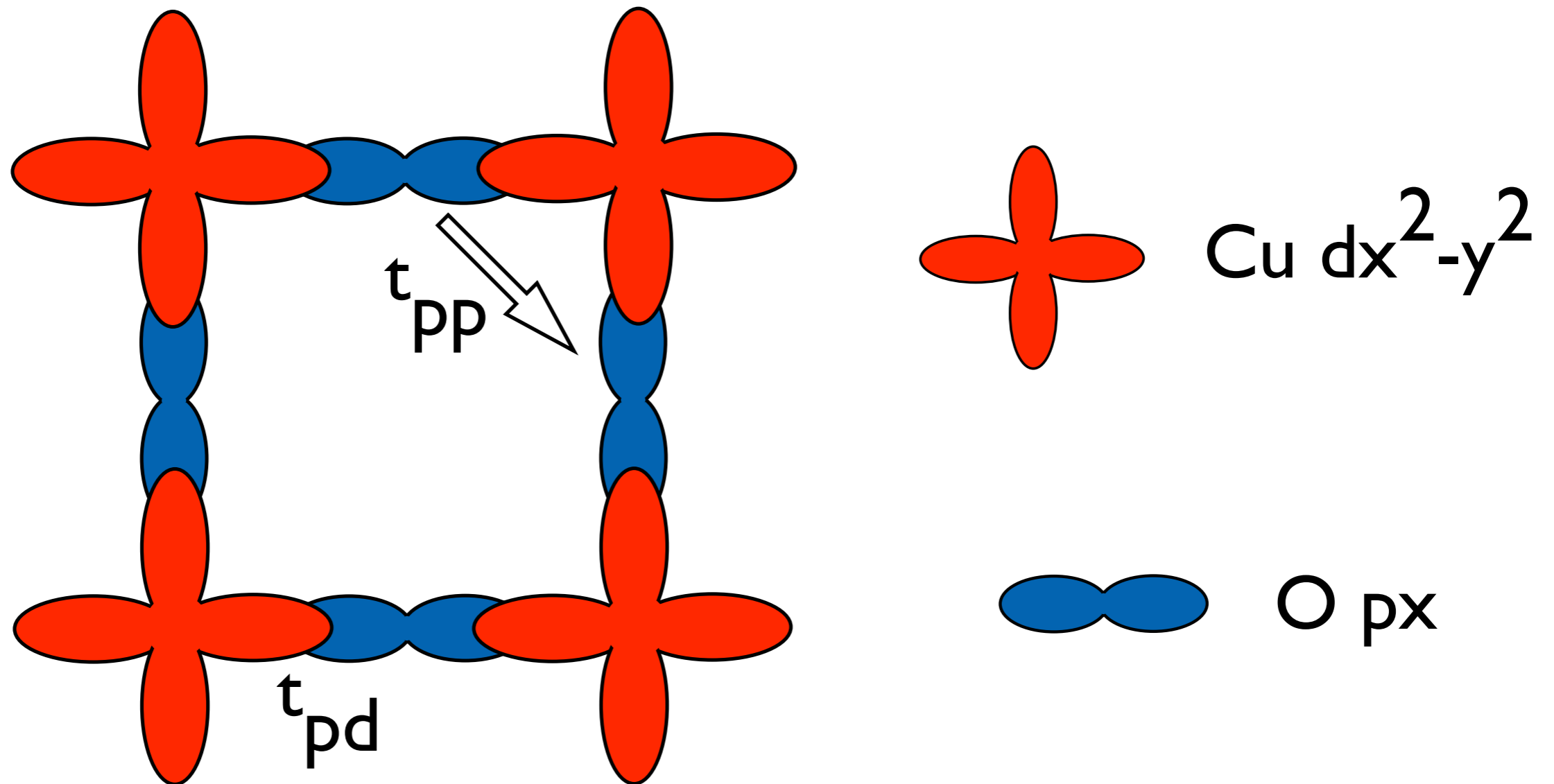
Becomes exact in large cluster size limit

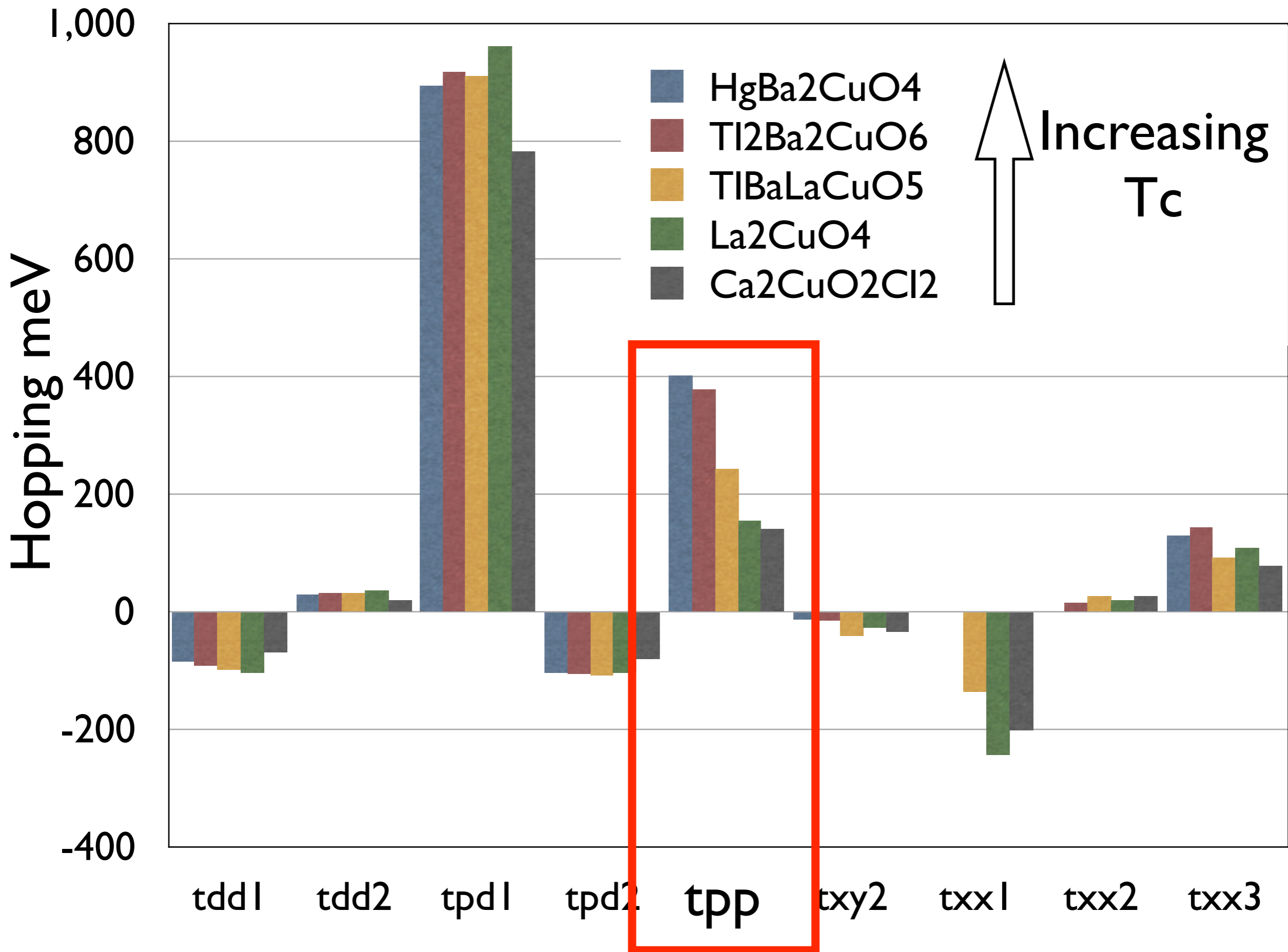
Cluster problem solved with QMC

Review: Maier et al. cond-mat/0404055

Parameter Interpretation

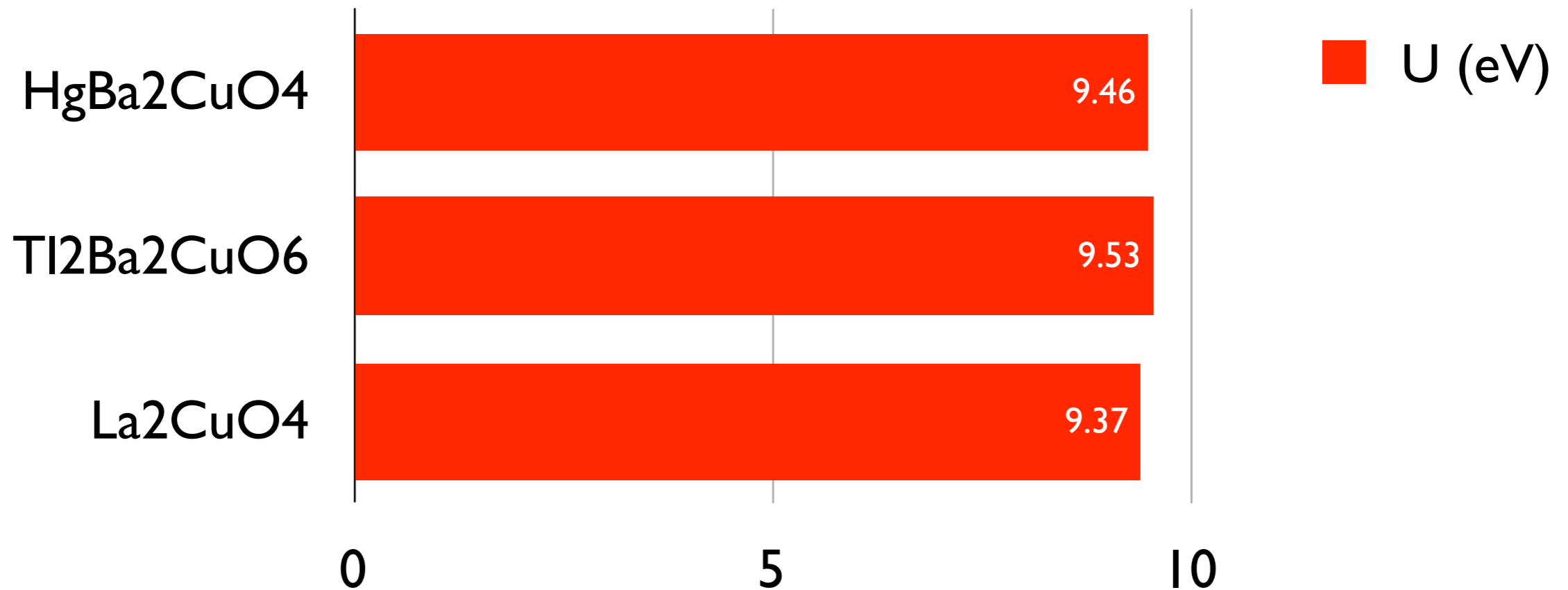
Calculated Hamiltonian parameters can be related to traditionally fit model parameters; Downfolding finds many more.





Calculated U

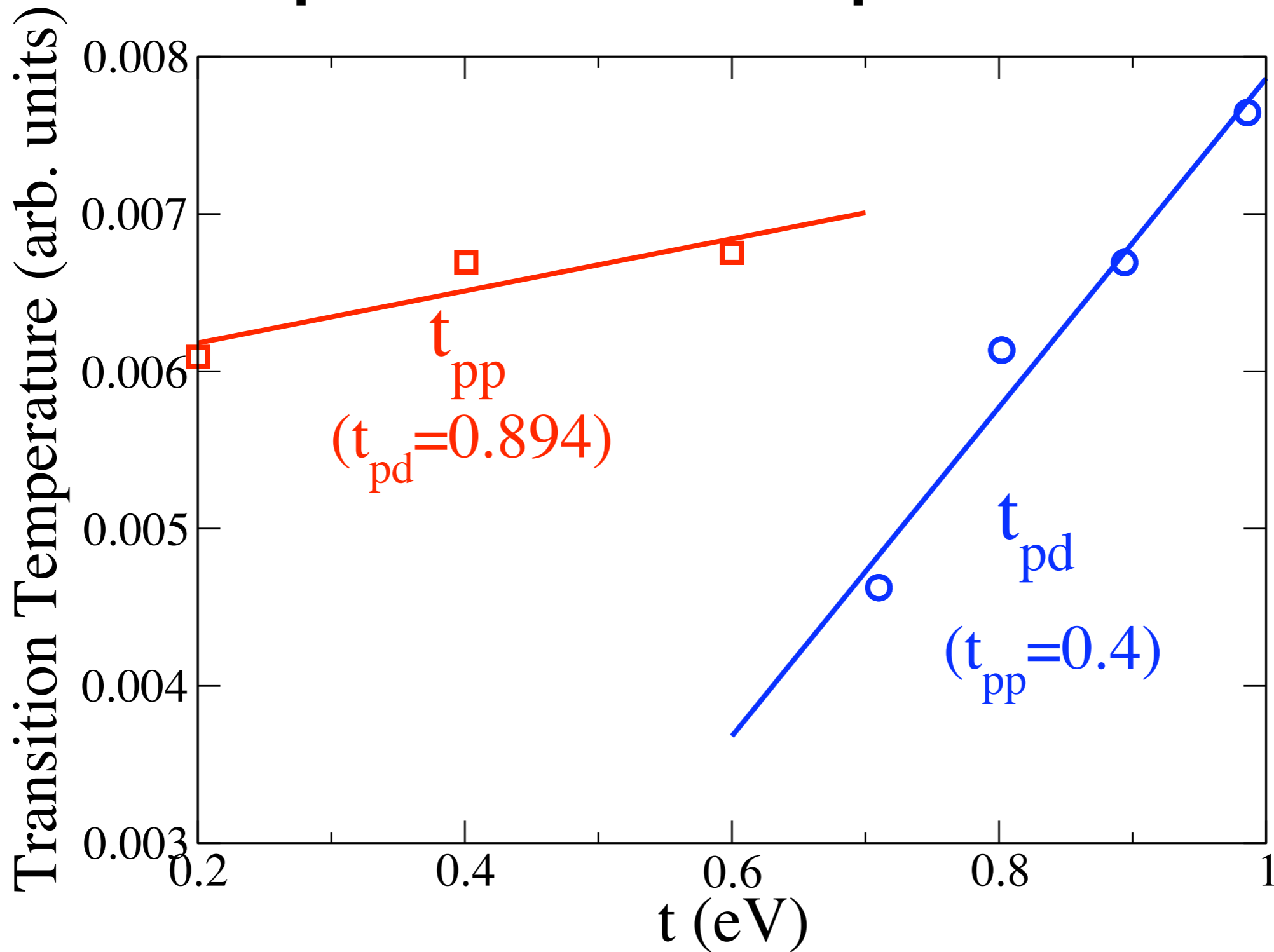
Constrained density functional calculations



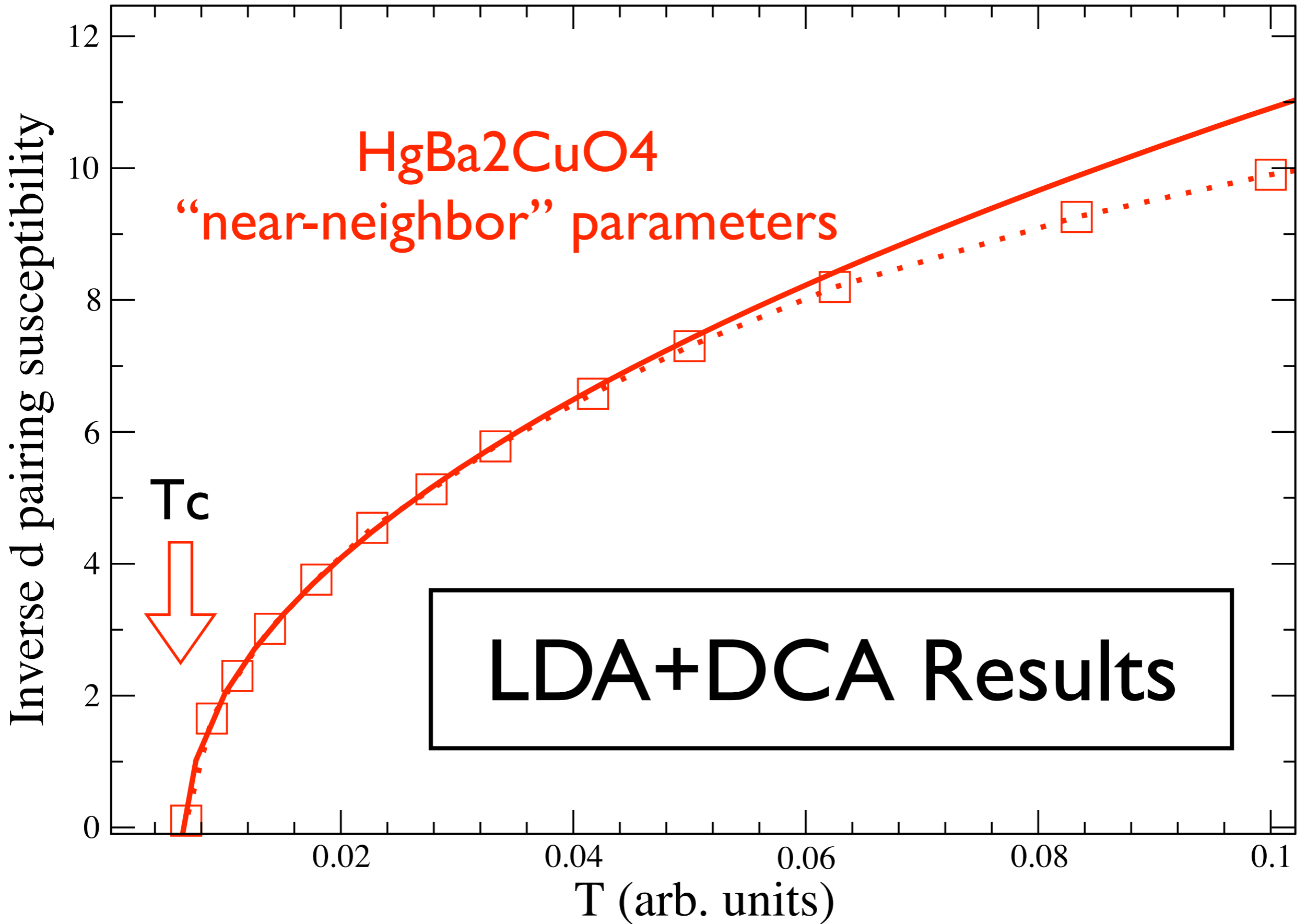
Few % variation in U; similar in all materials

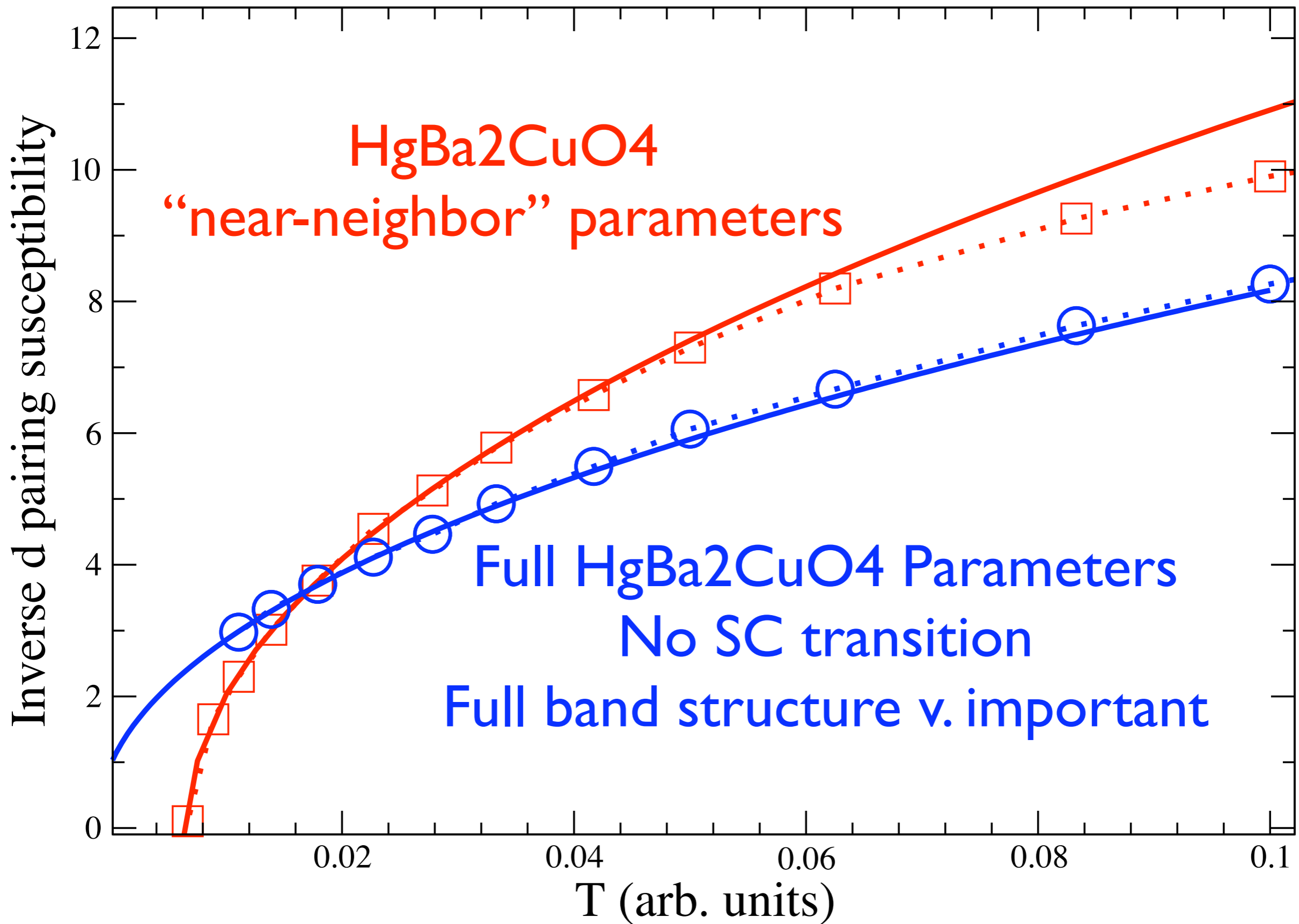
T_c essentially independent of U over this range

Tc parameter dependence

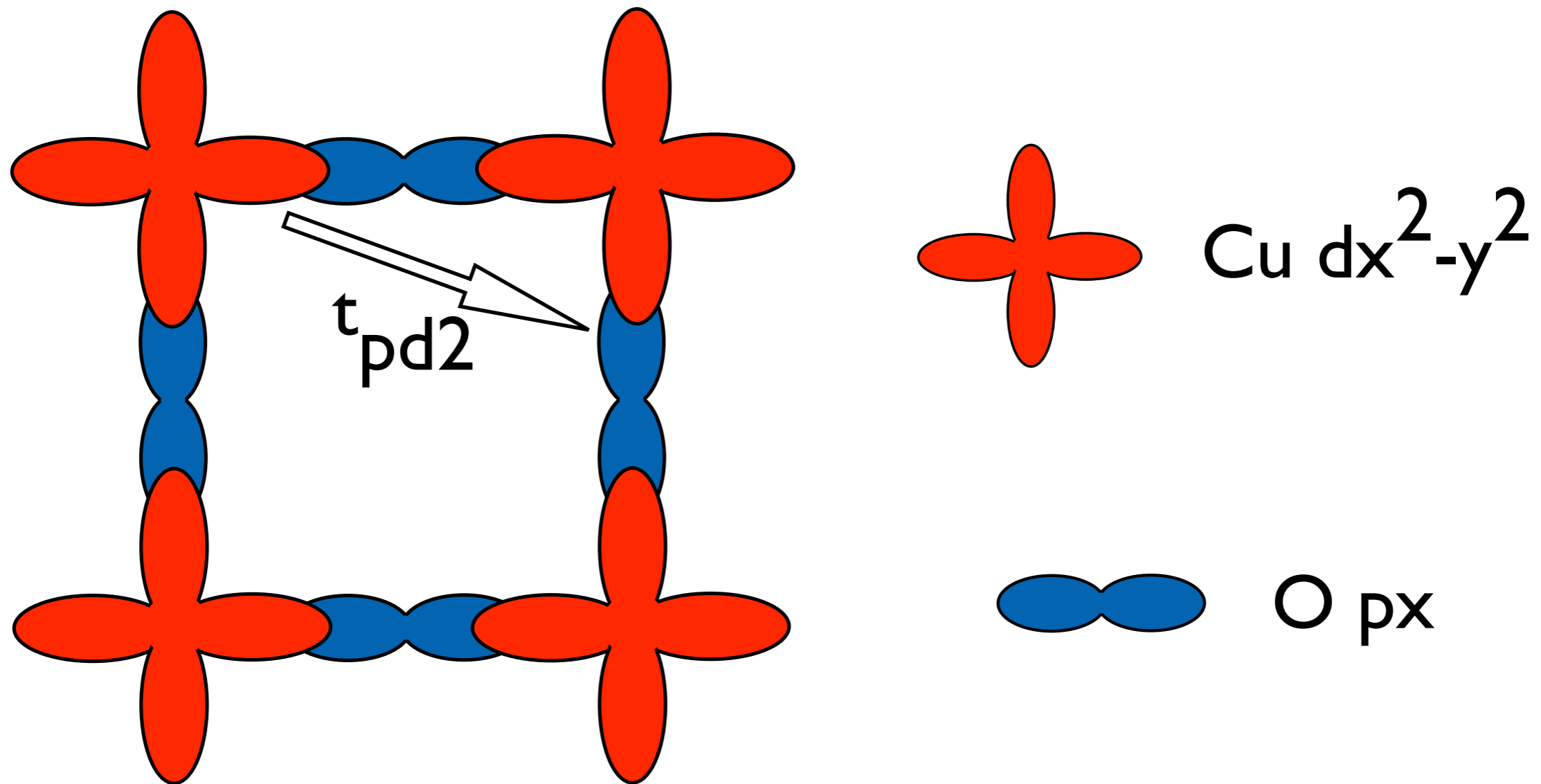


Transition temperature modestly influenced by nearest neighbor parameters





Beyond nearest-neighbor parameters are significant



Second NN p-d hybridization strongly influences T_c .
Other parameters also have strong influence.

Summary

1. Superconducting T_c strongly depends on underlying band structure parameters (e.g. 30% variation with nearest neighbour)
2. Beyond 1st nearest neighbour parameters significantly influence T_c
3. More accurate calculations are underway

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