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

Capture influence on Cu-O plane physics via DFT. Solve with DCA
LDA+DCA Method

1. DFT LDA ground state
   \( n(r) \) \rightarrow \text{Wannier-Function downfolding}

2. Three-band Hubbard Hamiltonian
   \( \text{All parameters calculated, NOT fit} \)

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

\[ \begin{align*}
N_c = 1 & & \text{effective medium} \\
N_c = 4 & & \text{effective medium} \\
N_c = 8 & & \text{effective medium} \\
N_c = 16 & & \text{effective medium}
\end{align*} \]

DMFA

\[ \sum_{\text{lattice}} \approx \sum_{\text{cluster}} \]

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.

\[
\begin{align*}
Cu \ dx^2 - y^2 \\
O \ px
\end{align*}
\]
Hopping meV

Increasing Tc

HgBa2CuO4
TI2Ba2CuO6
TIBaLaCuO5
La2CuO4
Ca2CuO2Cl2

tdp1

tpp

txy2
txx1
txx2
txx3
Calculated U

Constrained density functional calculations

- HgBa2CuO4: 9.46 eV
- Tl2Ba2CuO6: 9.53 eV
- La2CuO4: 9.37 eV

Few % variation in U; similar in all materials

Tc essentially independent of U over this range
Transition temperature modestly influenced by nearest neighbor parameters
HgBa$_2$CuO$_4$ “near-neighbor” parameters

LDA+DCA Results
HgBa₂CuO₄
“near-neighbor” parameters

Full HgBa₂CuO₄ Parameters
No SC transition
Full band structure v. important
Beyond nearest-neighbor parameters are significant

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

1. Superconducting Tc strongly depends on underlying band structure parameters (e.g. 30% variation with nearest neighbour)

2. Beyond 1st nearest neighbour parameters significantly influence Tc

3. More accurate calculations are underway

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