# LDA+DCA calculations of cuprate superconductors

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Despite the still unsolved nature of the mechanism and materials dependence of high-temperature superconductivity in the cuprates, considerable insight into the materials has resulted from theoretical investigations. Zero temperature density functional (DFT) calculations within the local density approximation (LDA) have determined the atomic structure of the materials and yielded useful information on the band structure, despite obtaining a metallic ground state for the undoped cuprate materials. In contrast, quantum cluster approaches applied to the much simpler 2-dimensional Hubbard model have been able to determine the finite temperature electronic phase diagram in qualitative agreement with experiment, but lacking any materials specificity.

Here, we present calculations of the transition temperature of models of single-layer cuprate superconductors using parameters determined from LDA-DFT, combined with the Dynamic Cluster Approximation (DCA) and Quantum Monte Carlo for solving the resultant Hubbard Hamiltonian.

Contrary to expectation, the calculated superconducting transition temperature is quite sensitive to the underlying single-particle band structure. The U obtained from DFT has surprisingly little influence on transition temperatures. Unfortunately, calculations using a 3-band Hubbard model and LDA-DFT derived parameters appear to yield either very low or non-existent transition temperatures. Relatively small changes to the parameters restore the transition. We discuss approaches to obtain improved parameters while retaining a non-empirical systematic approach.

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