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Towards material-specific simulations of high-temperature superconducting cuprates[1]

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Simulations of high-temperature superconducting (HTSC) cuprates have typically fallen into two categories: (1) studies of generic models such as the two-dimensional (2D) Hubbard model, that are believed to capture the essential physics necessary to describe the superconducting state, and, (2) first principles electronic structure calculations that are based on the local density approximation (LDA) to density functional theory (DFT) and lead to materials specific models. With advent of massibely parallel vector supercomputers, such as the Cray X1E at ORNL, and cluster algorithms such as the Dynamical Cluster Approximation (DCA), it is now possible to systematically solve the 2D Hubbard model with Quantum Monte Carol (QMC) simulations and to establish that the model indeed describes d-wave superconductivity [1]. Furthermore, studies of a multi-band model with input parameters generated from LDA calculations demonstrate that the existence of a superconducting transition is very sensitive to the underlying band structure [2]. Application of the LDA to transition metal oxides is, however, hampered by spurious self-interactions that particularly affects localized orbitals. Here we apply the self-interaction corrected local spin-density method (SIC-LSD) to describe the electronic structure of the cuprates. It was recently applied with success to generate input parameters for simple models of Mn doped III-V semiconductors [3] and is known to properly describe the antiferromagnetic insulating ground state of the parent compounds of the HTSC cuprates. We will discus the models for HTSC cuprates derived from the SIC-LSD study and how the differences to the well-known LDA results impact the QMC-DCA simulations of the magnetic and superconducting properties.

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