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LDA+DCA calculations of cuprate superconductors PAUL KENT, University of Tennessee, ALEXANDRU MACRIDIN, MARK JARRELL, University of Cincinnati, THOMAS SCHULTHESS, Oak Ridge National Laboratory, OLE KROGH ANDERSEN, TANUSRI DASGUPTA, OVE JEPSEN, Max Planck Institute for Solid State Research — We present calculations of the properties of realistic models of single-layer cuprate superconductors. A multi-band Hubbard model is obtained from downfolded material specific local density approximation (LDA) density functional theory (DFT) calculations. The on-site U is obtained from constrained DFT calculations. The resulting model is solved using the dynamic cluster approximation (DCA) and quantum Monte Carlo, for small clusters. Some of us have previously shown that DCA calculations of the single band Hubbard model, with empirical parameters, reproduce key features of the experimental phase diagram, including the d-wave superconducting region and pseudogap. In the multi-band model, we find a superconducting region, and discuss how the computed transition temperature depends on the downfolded band structure. In model calculations, we test the sensitivity of the transition temperature to changes in the individual hopping terms, including the copper-oxygen and oxygen-oxygen hybridization. Work supported by the Division of Materials Science and Engineering, U.S. Department of Energy, under Contract DE-AC05-00OR22725 with UT-Battelle LLC.

Paul Kent

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