Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

First principles calculations of La_2CuO_4 ANDREI PLAMADA, Institute for Theoretical Physics, ETH Zurich, ANTON KOZHEVNIKOV, Swiss National Supercomputer Centre, ETH Zurich, URS HAEHNER, MI JIANG, Institute for Theoretical Physics, ETH Zurich, PETER STAAR, IBM Research - Zurich, THOMAS MAIER, Computer Science and Mathematics Division and Center for Nanophase Materials Sciences, Oak Ridge National Laboratory , THOMAS SCHULTHESS, Institute for Theoretical Physics, ETH Zurich — We use the DFT+DCA method for a high-end study of the electronic structure properties of La_2CuO_4. The parameters of a tight-binding model are created using the first-principles electronic structure calculations. The all-electron full-potential linearised augmented plane-wave method is used to solve the non-interacting band problem. Then the set of physically relevant Wannier functions is chosen as a basis for the underlying Hubbard model. The Wannier functions and the corresponding non-interacting Hamiltonian $H^0_{nm}(\mathbf{k})$ are created using the well-established downfolding approach. The screened Coulomb interaction parameters U_{nm} of the model are computed using the constrained random-phase approximation technique. The double counting term is assumed to be a constant multiplied by the identity operator in the correlated subspace and it is determined based on first-principles considerations. The resulting *ab-initio* parameterisation of the Hubbard model is solved within dynamical cluster approximation (DCA).

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Date submitted: 06 Nov 2015 Electronic form version 1.4