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Self-consistent implementation of the multi-band Gutzwiller variational method: Formalism and combination with DFT NICOLA LANATA', HUGO STRAND, University of Gothenburg, SE-412 96 Gothenburg, Sweden, XI DAI, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, BO HELLSING, University of Gothenburg, SE-412 96 Gothenburg, Sweden — We have generalized the approach for solving the multi-band Gutzwiller variational problem with density-density interaction to an arbitrary local interaction. The main advantage of our formulation is that it allows for a self-consistent numerical implementation which doesn't require any additional computational effort as compared to the simpler case of density-density interaction. Combined with DFT and the Local Density Approximation (LDA+Gutzwiller) our method allows for ab-initio study of multi-band correlated materials with full (rotationally invariant) Hund's rule coupling. We briefly introduce the method and present applications to several systems of correlated electrons.

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