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DFT+DMFT versus DFT+U description of Mott insulators: DMFT restores spin and orbital symmetry and removes metastables states BERNARD AMADON, CEA, DAM, DIF, F 91297 Arpajon, France — In the last twenty years, the developpement of methods based on the coupling of Density Functional Theory in the Local Density Approximation and Hubbard-like terms has led to a successfull description of many strongly correlated systems. These methods include DFT+U which contains a static description of interaction and the combination of DFT with Dynamical Mean Field Theory (DFT+DMFT) which adds fluctutations to the description of interactions. We present implementations of DFT+U and DFT+DMFT in the same framework, and with the same approximations. We show, in agreement with previous results in the litterature, and even in the simple Hubbard I approximation to DMFT,that DFT+DMFT is able to describe Mott insulator without any breaking of spin and orbital symmetry. We show that this improvement simply remove the appearance of metastable states, and thus solve a practical and physical problem encountered in particular in the description of actinides oxydes in DFT+U calculations.

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