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Development of a DFT+DMFT method using multi-orbital impurity solver MANCHEON HAN, HYUNGJU OH, CHOONG-KI LEE, HYOUNG JOON CHOI, Department of Physics, IPAP, and Center for Computational Studies of Advanced Electronic Material Properties, Yonsei University — The density functional theory (DFT), often performed with the local density approximation or the generalized gradient approximation, is very successful for ab initio calculations of various materials. However, it has limited accuracy for strongly correlated materials. The dynamical mean field theory (DMFT), which maps a correlated lattice system to an interacting impurity site in a non-interacting bath, may describe local correlation effects. Combination of above methods, DFT+DMFT, can be an adequate approach for investigation of strongly correlated materials. We have implemented a DFT+DMFT method based on the ab-initio pseudopotential method of the SIESTA code, where electronic wavefunctions are expanded with pseudo-atomic orbitals. An exact diagonalization method is used in our DFT+DMFT method to obtain the local Green function of the impurity site with multiple orbitals. We apply our DFT+DMFT method to the electronic structure of LaFeAsO and compare the results with those from DFT and experiments. This work is supported by the NRF of Korea (Grant No.2011-0018306). Computational resources have been provided by KISTI Supercomputing Center (Project No. KSC-2013-C3-062).

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