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Implementation of DFT+DMFT in local-orbital pseudopotential code HYUNGJU OH, CHOONG-KI LEE, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University. Center for Computational Studies of Advanced Electronic Material Properties, Yonsei University. — Density functional theory (DFT) has been remarkably successful at describing ground-state properties of many solids from first principles. This is also the state-of-the-art method for band structure calculations, with the additional assumption that Kohn-Sham eigenvalues can be interpreted as single-particle excitations. However, DFT has limitations for strongly correlated materials. Dynamical mean-field theory (DMFT) is one of various approaches that have been developed for overcoming the shortcomings of DFT. DMFT goes beyond DFT by allowing the interaction potential of the correlated orbitals to be energy (frequency) dependent. This frequency dependent potential, or self-energy, is computed for the correlated orbitals using many-body techniques within an accurate impurity solver. We have implemented DMFT to the SIESTA code based on pseudo-atomic orbital basis set. For an impurity solver, we use exact diagonalization. We calculate electronic states of LaFeAsO using our DFT+DMFT code and confirm the band-narrowing, corresponding to an enhancement of the effective masses of quasiparticles. This work was supported by the NRF of Korea (Grant No. 2011-0018306). Computational resources have been provided by KISTI Supercomputing Center (Project No. KSC-2013-C3-008).

Hyungju Oh
Yonsei Univ

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