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Comparative study of impurity solvers for Dynamical Mean Field Theory 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, Seoul 03722, Korea
— The dynamical mean field theory (DMFT), which maps interacting electrons in solid to a single-impurity Anderson model (SIAM) is a methodology to study correlated electron systems. To perform DMFT approach, one needs a numerical method to solve the mapped impurity problem. Among various methods, we implemented three impurity solvers. The first one is the iterative perturbation theory (IPT), which approximates the self-energy by its second order perturbation expansion. It can be conducted within very short time and gives real-frequency quantities without any post-process. Second, we considered the exact diagonalization (ED) method, which approximates infinite bath in SIAM to some finite number of states. Lastly, we implemented the hybridization-expansion continuous-time quantum Monte Carlo (CT-HYB). It is numerically exact in the imaginary frequency, and analytic continuation is needed to get real-frequency quantities like spectral functions. Using three solvers, we calculated physical properties of several systems from simple models to real materials and compared the results. This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2016-C3-0052).

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