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Effects of the potassium dosing on the electronic correlation in FeSe : DFT+DMFT study YOUNG-WOO CHOE, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University, Seoul 03722, Korea and Center for Computational Studies of Advanced Electronic Material Properties — Recently, dosing the potassium (K) on the surface of the bulk and thick-film FeSe has been proved as an effective way to induce the surface electron doping to the samples. According to the recent ARPES experiments, the phase diagram of the K-dosed FeSe shows the enhancement of the superconducting transition temperature (Tc) from 8K for the undoped case up to 46K for the optimal dosing level. Furthermore, beyond the optimal dosing, Tc decreases until an insulating phase emerges. This behavior is accompanied by increasing effective mass and diminishing spectral weight of metallic bands near the Fermi level, indicating the effects of the electronic correlations are enhanced. In this regard, we study the K-dosed FeSe systems using the first-principles density functional theory calculations combined with the dynamical mean-field theory. We analyze the evolution of the orbital-resolved effective masses and the spectral functions according to the potassium dosing levels. As a result, we illustrate the role of K-dosing in the enhancement of the electronic correlation effects in FeSe. 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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