Theoretical study of $J_{\rm eff} = 1/2$ Mott insulator in Ir oxides: cooperation of a strong spin-orbit coupling and local electron correlations

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Recent experiments on Sr_2IrO_4[1] have revealed a novel Kramer's doublet $J_{\rm eff} = S - L = 1/2$ Mott insulator induced by a strong spin-orbit coupling (SOC) and local Coulomb interactions (U). To clarify the nature of electronic and magnetic properties of this system, we have studied a two-dimensional three-band Hubbard model consisting of the t_{2g} manifold of $5d$ electrons with SOC.[2] The exact diagonalization and variational cluster approximation[3] based on the self-energy functional theory[4] are used to calculate various physical quantities including the single-particle spectra. Our results of the projected single-particle spectra onto $J_{\rm eff} = 1/2$ and $J_{\rm eff} = 3/2$ states have revealed a physical picture of the $J_{\rm eff} = 1/2$ Mott insulator. We also examine the roles of SOC and U to stabilize this novel $J_{\rm eff} = 1/2$ Mott insulator.

[1]B. J. Kim, *et.al.*, Science **323**, 1329 (2009)
[2]H. Watanabe, T. Shirakawa, and S. Yunoki, Phys. Rev. Lett. **102**, 216410 (2010)
[3]M. Potthoff, M. Aichhorn, and C. Dahnken, Phys. Rev. Lett. **91**, 206402 (2003)
[4]M. Potthoff, Eur. Phys. J. B **32**, 429 (2003)