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First-principles study of large spin-orbit coupling transition-metal compounds: Electronic structure and new possibilities

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Recently Sr_2IrO_4 has attracted considerable attention due to the intriguing interplay between spin and orbital degrees of freedom, and its manifestation in the material characteristics. Along this line I will present our recent progress on the iridium oxide and other related compounds based on 4d-/5d- transition metals. The first example is Rh-doped iridate, $\text{Sr}_2\text{Ir}_{1-x}\text{Rh}_x\text{O}_4$, for which the doping dependent metal-insulator transition (MIT) has been reported experimentally and the controversial discussion developed regarding the origin of this transition. We tried to suggest a new picture for understanding the MIT. The second is the artificially-structured iridate superlattice, $\text{SrIrO}_3/\text{SrTiO}_3$. The electronic structure change caused by the interface and the strain was examined in detail and compared with the optical spectra. Finally, I will introduce a fairly different family of compounds, GaT_4X_8 (T=Nb, Mo, Ta, and X=Se,Te). Interesting similarities with Sr_2IrO_4 suggests a new possibility for the novel ground states in this series of compounds.

Biography

Myung Joon Han received BS and PhD degree from Seoul National University in 2001 and 2007, respectively. Before coming back to Korea in 2012, he spent his Postdoc period in UC Davis, Columbia University, and Argonne National Lab. He is now an Assistant Professor in Department of Physics, KAIST.

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