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Magnetization reversal in $Sr_3Ir_2O_7$: DM interactions vs. magnetic single-ion anisotropy HOSUB JIN, JAEJUN YU, Department of Physics and Astronomy, Seoul National University — Recently the unusual insulating ground state of Sr_2IrO_4 was shown to be a consequence of a novel quantum ground state of $j_{\rm eff}$=1/2. Another compound in its series $Sr_3Ir_2O_7$ with double layers of the IrO_2 planes exhibits anomalous magnetic responses such as magnetization reversal during field-cooling processes. We performed density-functional theory calculations to investigate the electronic and magnetic properties of $Sr_3Ir_2O_7$. Similarly to the case of Sr_2IrO_4, both spin-orbit (SO) and on-site Coulomb interactions are found to be responsible for the insulating ground state. Based on the analysis of our first-principle calculations for the various spin and lattice configurations, we found that the nonzero angular momentum state originating from large SO interactions with lattice distortions plays a crucial role in determination of both single-ion anisotropy and Dzyaloshinski-Moriya interactions, which explains anomalous magnetic responses in $Sr_3Ir_2O_7$.

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