Magnetization reversal in Sr$_3$Ir$_2$O$_7$ : 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$_2$IrO$_4$ was shown to be a consequence of a novel quantum ground state of $j_{\text{eff}}=1/2$. Another compound in its series Sr$_3$Ir$_2$O$_7$ 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$_3$Ir$_2$O$_7$. Similarly to the case of Sr$_2$IrO$_4$, 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 non-zero 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$_3$Ir$_2$O$_7$.