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# CALCULATION OF ANISOTROPIC EXCHANGE COUPLING CONSTANTS IN IRIDATES

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Because of strong spin-orbit coupling within the Iridium 5d shell magnetic interaction in $Ir4^+$ oxides cannot be described by an isotropic Heisenberg-like model and anisotropic exchange interactions become important. In α-$Na_2IrO_3$ and α-$Li_2IrO_3$, in which edge sharing IrO octahedra form a honeycomb lattice, magnetic interaction was suggested to be bond-dependent and to be described by the Kitaev model. Recently, another complex Ir oxide β-$Li_2IrO_3$ has been synthesized which is expected to be close to forming a Kitaev spin liquid. Ir ions in this compound form a "hyper-honeycomb" lattice, a three-dimensional analogue of the honeycomb lattice of α-$Na_2IrO_3$. In $Sr_2IrO_4$, $Sr_3Ir_2O_7$ and in $R_2Ir_2O_7$ compounds, where *R* is a rare-earth ion, with the pyrochlore structure, on the other hand, the dominant anisotropic exchange is the anti-symmetric Dzyaloshinskii–Moriya interaction. We present results of LSDA+U band structure calculations for $Na_2IrO_3$, $Sr_2IrO_4$, and some $R_2Ir_2O_7$ iridates. The strength of the Coulomb repulsion U is adjusted by comparing the calculated optical conductivity to experimental optical spectra. Then, magnetic interactions in these compounds are estimated by mapping the total energy calculated for various non-collinear magnetic configurations constrained by magnetic symmetry onto an effective model which includes isotropic Heisenberg-like as well as bond-dependent anisotropic magnetic interactions. It is shown that the variation of the total energy cannot be described by the isotropic Heisenberg-like model and anisotropic terms may be as strong as the isotropic ones.