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Anisotropic magnetic interactions in 5d iridium oxides by many-body quantum chemistry calculations VAMSHI M. KATUKURI, SATOSHI NISHIMOTO, Institute for Theoretical Solid State Physics, IFW Dresden, Germany, VIKTOR YUSHANKHAI, Joint Institute for Nuclear Research, Dubna, Russia, IOANNIS ROUSOCHATZAKIS, LIVIU HOZOI, JEROEN VAN DEN BRINK, Institute for Theoretical Solid State Physics, IFW Dresden, Germany — Ir $5d^5$ oxides are being actively studied due to the realization of novel spin-orbit coupled $j_{eff} \approx 1/2$ ground states. One remarkable feature in these compounds is the highly anisotropic magnetic interactions, orders of magnitude stronger than in 3d oxides. We address the nature of the anisotropic exchange in the 2D honeycomb $(Na/Li)_2IrO_3$ ((Na/Li)213) and square-lattice $(Sr/Ba)_2IrO_4$ ((Sr/Ba)213) iridates, by ab initio multireference configuration-interaction calculations on large embedded clusters. For Na213 we find that the Kitaev term is ferromagnetic and defines the dominant energy scale while the nearest-neighbor Heisenberg contribution is antiferromagnetic. Although Li213 is structurally similar, we predict quite different set of interaction parameters in Li213. We further analyze the magnetic order and the essential differences between these two materials by exact diagonalization and density-matrix renormalization-group calculations that additionally include 2nd and 3rd neighbor couplings. Sizable symmetric anisotropic interactions are also computed for Ba214. From the ab initio data, the relevant in-plane spin model for Ba214 turns out to be a Heisenberg-compass effective model. We finally discuss the Dzyaloshinskii-Moriya exchange in Sr214.

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