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Quasimolecular electronic structure of Na_2IrO_3 IGOR MAZIN, Naval Research, HARALD JESCHKE, FOYEVTSEVA KATERYNA, ROSER VALENTI, University of Frankfurt, DANIEL KHOMSKII, University of Cologne — Spin-orbit (SO) coupling can lead to many nontrivial effects such as Rashba effect, topological insulators, or topologically protected states in systems described the Heisenberg-Kitaev model, recently proposed for Na_2IrO_3. This proposal is based on the fact the SO coupling for iridium is very strong, and cannot be quenched by the small trigonal crystal field. We show, however, that Na_2IrO_3 represents a highly unusual case, in which the electronic structure is dominated by the formation of quasi-molecular composite orbitals (QMOs). The QMOs consist of six atomic orbitals on an Ir hexagon, and the orbital moment of each QMO is quenched, so that spin-orbit effects only affect the inter-QMO interaction. The concept of such composite orbitals in solids is completely new, and invokes very different physics compared to the models considered previously. For instance, one has to account for Hubbard correlations among the QMOs, and not individual atomic orbitals. Both the insulating behavior and the experimentally observed zigzag antiferromagnetism in Na_2IrO_3 naturally follow from the QMO model.

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