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Ab Initio Simulations of the Structure and Energetics of Harmonic Honeycomb Iridates[1] TESS SMIDT, QIMIN YAN, JEFFREY NEATON, Univ of California - Berkeley — Edge-sharing iridates present an exciting opportunity to study the competition of Mott insulator physics and strong spin-orbit coupling. Harmonic honeycomb iridates are a recently discovered homologous series of stoichometrically identical structures that host anisotropic magnetism and exotic spin ordering. We use density functional theory and lattice kinetic Monte Carlo to investigate structural, energetic, and entropic trends in determining the equilibrium ground states of harmonic honeycomb iridates. We predict the formation energies and geometry of as-yet unsynthesized series members and propose why some structures are more prevalent than others.

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