

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Electronic structure of the harmonic-honeycomb iridates α , β , γ -Li₂IrO₃¹ ROSER VALENTI, YING LI, HARALD O. JESCHKE, Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany — Using ab-initio density functional theory we investigate the electronic and magnetic properties of the harmonic-honeycomb iridates α , β , γ -Li₂IrO₃ with honeycomb, hyperhoneycomb and stripyhoneycomb crystal structures, respectively. We discuss the distinct features of each class of systems in terms of possible Ir-based molecular-orbitals and the implications on the magnetism in these materials. We further relate the electronic structure to proposals of generalized Kitaev-Heisenberg models.

¹This work is supported by the Deutsche Forschungsgemeinschaft under Grant No. FG 1346

Roser Valenti
Institut für Theoretische Physik, Goethe-Universität Frankfurt,
Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany

Date submitted: 14 Nov 2014

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