Electronic structure of the harmonic-honeycomb iridates $\alpha, \beta, \gamma$-Li$_2$IrO$_3$\textsuperscript{1} ROSER VALENTI, YING LI, HARALD O. JESCHKE, Institut f"{u}r Theoretische Physik, Goethe-Universit"{a}t 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 $\alpha, \beta, \gamma$-Li$_2$IrO$_3$ 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.

\textsuperscript{1}This work is supported by the Deutsche Forschungsgemeinschaft under Grant No. FG 1346