Design of Mott and topological phases on buckled 3d-oxide honeycomb lattices\textsuperscript{1}

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The honeycomb lattice, as realized e.g. in graphene, has rendered a robust platform for innovative science and potential applications. A much richer generalization of this lattice arises in (111)-oriented bilayers of perovskites, adding the complexity of the strongly correlated, multiorbital nature of electrons in transition metal oxides. Based on first principles calculations with an on-site Coulomb repulsion, here we provide trends in the evolution of ground states versus band filling in (111)-oriented (LaXO\textsubscript{3})\textsubscript{2}/(LaAlO\textsubscript{3})\textsubscript{4} superlattices, with \textit{X} spanning the entire 3\textit{d} transition metal series. The competition between local quasi-cubic and global triangular symmetry triggers unanticipated broken symmetry phases, with mechanisms ranging from Jahn-Teller distortion, to charge-, spin-, and orbital-ordering. LaMnO\textsubscript{3} and LaCoO\textsubscript{3} bilayers, where spin-orbit coupling opens a sizable gap in the Dirac-point Fermi surface, emerge as much desired oxide-based Chern insulators, the latter displaying a gap capable of supporting room-temperature applications \cite{1} Further realizations of the honeycomb lattice and geometry patterns beyond the perovskite structure will be addressed. \cite{1} D. Doennig, S. Baidya, W.E. Pickett and R. Pentcheva, arXiv: 1510.09177.

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