Topologically non-trivial electronic and magnetic states in doped copper Kagome lattices

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Abstract:

We present a theoretical investigation of doped copper kagome materials based on natural minerals Herbertsmithite [ZnCu$_3$(OH)$_6$Cl$_2$] and Barlowite [Cu$_4$(OH)$_6$FBr]. Using ab-initio density functional theory calculations we estimate the stability of the hypothetical compounds against structural distortions and analyze their electronic and magnetic properties. We find that materials based on Herbertsmithite present an ideal playground for investigating the interplay of non-trivial band-topology and strong electronic correlation effects. In particular, we propose candidates for the Quantum Spin Hall effect at filling 4/3 and the Quantum Anomalous Hall effect at filling 2/3. For the Barlowite system we point out a route to realize a Quantum Spin Liquid.