Correlation-driven topological phase transition from in-plane magnetized quantum anomalous Hall to Mott insulating phase in monolayer transition metal trichlorides

XIAN-LEI SHENG, Department of Applied Physics, Beihang University, Beijing 100191, China, BRANISLAV K. NIKOLIC, Department of Physics and Astronomy, University of Delaware, Newark, DE 19716-2570, USA — Based on density functional theory (DFT) calculations, we predict that a monolayer of OsCl$_3$ (a layered material whose interlayer coupling is weaker than in graphite) possesses a quantum anomalous Hall (QAH) insulating phase generated by the combination of honeycomb lattice of osmium atoms, their strong spin-orbit coupling (SOC) and ferromagnetic ground state with in-plane easy-axis. The band gap opened by SOC is $E_g \simeq 67$ meV (or $\simeq 191$ meV if the easy-axis can be tilted out of the plane by an external electric field), and the estimated Curie temperature of such anisotropic planar rotator ferromagnet is $T_{C350}$ K. The Chern number $C=-1$ signifies the presence of a single chiral edge state in nanoribbons of finite width, where we further show that edge states are spatially narrower for zigzag than armchair edges and investigate edge-state transport in the presence of vacancies at Os sites. Since 5$d$ electrons of Os exhibit both strong SOC and moderate correlation effects, we employ DFT+$U$ calculations to show how increasing on-site Coulomb repulsion $U$ closes the gap of QAH insulator phase at $U_c$, and then reopens the gap of topologically trivial Mott insulator phase.

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