

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Correlation-driven topological phase transition from in-plane magnetized quantum anomalous Hall to Mott insulating phase in monolayer transition metal trichlorides¹ 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 OsCl₃ (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 $\mathcal{C} = -1$ 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 $5d$ 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.

¹This work was supported by NSF Grant No. ECCS 1509094. The supercomputing time was provided by XSEDE, which is supported by NSF Grant No. ACI-1053575.

Branislav Nikolic
University of Delaware

Date submitted: 10 Nov 2016

Electronic form version 1.4