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Quantum anomalous Hall and antiferroelectric topological insulators

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In this talk I will briefly review two predictions of novel topological states. First I will present the results of a computational study of heavy adatoms chemisorbed on ferromagnetic $CrSiTe_3$ and $CrGeTe_3$ surfaces as part of a search for quantum anomalous Hall (QAH) insulators. Surprisingly, we find QAH states that emerge for La and Lu adatoms on single $CrSi(Ge)Te_3$ layers in which time-reversal symmetry is broken directly in the orbital sector [1]. These "flux states" are observed only when using hybrid functionals, suggesting that intersite Coulomb interactions may be responsible. Second, I will discuss our recent work in which we identify a class of potential "antiferroelectric topological insulators" [2], defined as materials in which either the zero-field nonpolar or high-field polar states are topological. By investigating orthorhombic members of an *ABC* family of compounds, we predict several representative examples including ones for which only one of these two states is topological, so that an electric field can potentially be used to switch between trivial and topological phases. We also investigate the ability of epitaxial strain and hydrostatic pressure to tune the topological order and the band gap of these *ABC* compounds.

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[1] J. Liu, S.Y. Park, K.F. Garrity, and D. Vanderbilt, "Flux states and topological phases from spontaneous time-reversal symmetry breaking in $CrSi(Ge)Te_3$-based systems," Phys. Rev. Lett. **117**, 257201 (2016).

[2] B. Monserrat, J.W. Bennett, K.M. Rabe, and D. Vanderbilt, "Antiferroelectric topological insulators in ABC compounds," https://arxiv.org/abs/1702.06958.