

Materials Science & Engineering and Metallurgical Engineering Graduate Seminar

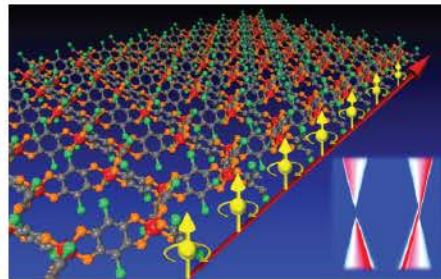
Wednesday, October 24 2018, 4:10-5:00PM, WEB 1230

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Intrinsic Quantum Anomalous Hall Effect in Two-dimensional Anilato-based Lattice

Using first-principles calculations, we predict an intrinsic quantum anomalous Hall (QAH) state in a monolayer anilato-based metal-organic framework $M_2(C_6O_4X_2)_3$ ($M = Mn$ and Tc , $X = F, Cl, Br$ and I). Spin-orbit coupling of M d orbitals opens a nontrivial band gap up to 18 meV at the Dirac point. The electron counting rule is used to explain the intrinsic nature of the QAH state. The calculated nonzero Chern number, gapless edge states and quantized Hall conductance all confirm the nontrivial topological properties in the anilato-based lattice. Our findings provide an organic materials platform for the realization of QAH effect without the need of magnetic and charge doping, which are highly desirable for the development of the low-energy-consumption spintronic devices. (Nanoscale, 2018, 10, 11901)



Xiaojuan Ni is a fourth-year PhD student working on the percolation phenomena in multi-component nanocomposites and topological properties in 2D materials. She has contributed to 7 papers and presented some of them in APS March Meeting and Gordon Research Conference of Quantum Materials. She received Cao Scholarship for graduate students last year.