Topological flat bands in two-dimensional Cr doped AsH monolayers

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Discovery of two-dimensional (2D) topological insulators in such as group-V films initiates the enthusiasm to explore the exotic quantum states in low dimensions. Here, we perform first-principles calculations and tight-binding (TB) model to study the electronic properties in Cr dopped AsH monolayers(Cr@AsH). The Cr@AsH monolayer is found being a Chern metal (CM) with a nontrivial quasi-flat band appeared near the Fermi level (E_F). Interestingly, a clear band gap emerges near the E_F with a nonzero Chern number (C = -1). Under a small tensile strain （1.4% < ε < 2.05%）, the monolayer changes to a Chern insulator (CI). Under a large strain (ε > 2.05%), the quasi-flat band interacts with the conduction Dirac band, leading to a phase transition and then the system become ferrovalley insulator(FVI) with zero Chern number(C = 0). The phase transition mechanism is comprehended by a tight-binding model built. The mechanism of phase transition is from different behaviors of band inversion in spin-up and spin-down subspace. Our results provide one type of candidate materials showing fractional Chern phenomena.

Geometry structures

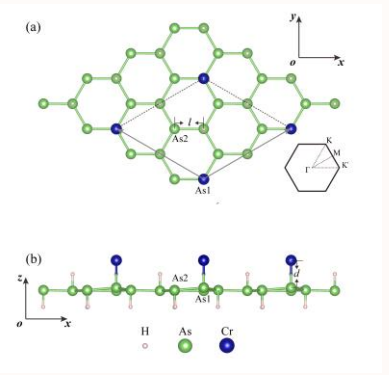

Fig 1. Top(a) and side(b) views of monolayer Cr@AsH.

Band evolution and phase diagram

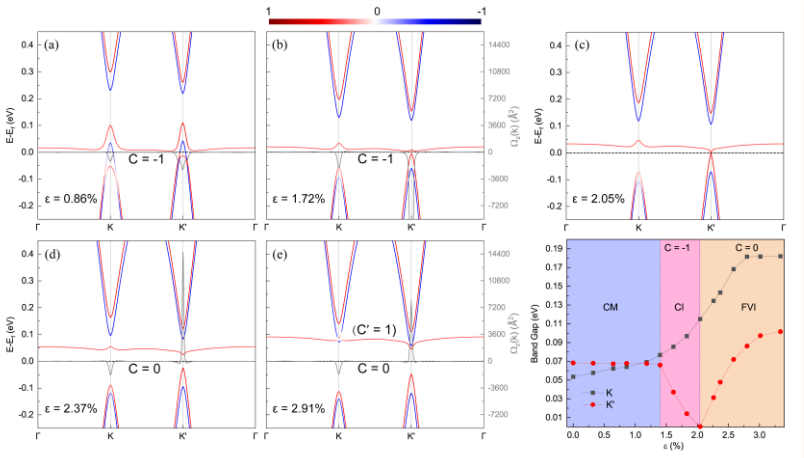

Fig 3. (a-e) Band evolution under the tensile strain. The corresponding Berry curvatures (grey curves) are also shown. (f) Phase diagram of the monolayer under the strain.

Electronic properties

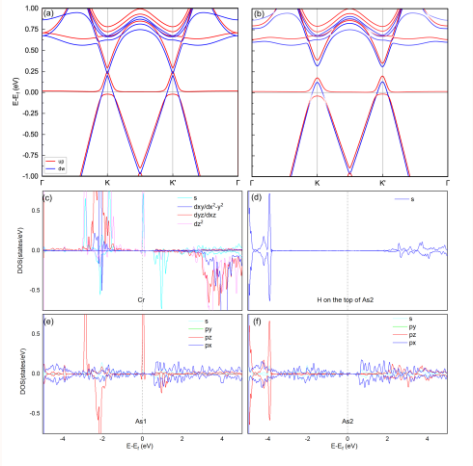

Fig 2. Band structures with (a) and without (b) spin-orbit coupling(SOC). (c-f) Atomic resolved density of states(DOS).

TB model and Schematic diagram

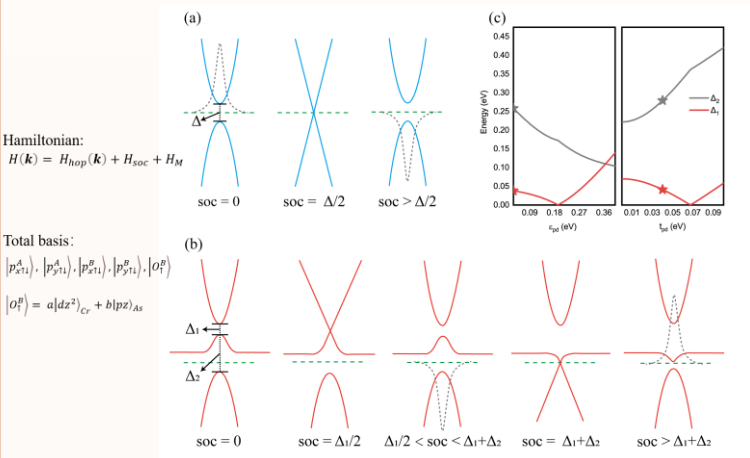

Fig 4. (a-b) Band inversion diagrams in different spin subspaces. (c) gives the influence of TB parameters.

Conclusions

- Cr@AsH is a Chern metal with a quasi-flat band appeared near the Fermi level in the ground state.
- Tensile strain can induce phase transitions in the materials from a Chern metal to a Chern insulator, half-valley metal, and ferrovalley insulator.
- The Cr@AsH monolayer is expected to show fractional Chern effects under tensile strain at the range of 1.4% < ε < 2.05%.

Reference: 1. Tong Zhou, Jiayong Zhang, et al. Nano Lett. 15, 5149−5155(2015)
2. Hao Huan, Yang Xue, et al. Phys. Rev. B 104, 165427 (2021)