Can Xenes be excitonic, topological and quantum spin Hall insulators?

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Abstract

Trivial insulators are characterized by a fundamental gap E_g between conduction and valence bands, while an excitonic insulator (EI) fulfills the additional condition $E_b > E_g$ with E_b as the binding energy of the lowest exciton below the absorption edge. A topological insulator (TI) appears for band inversion, e.g. the exchange of s- and p-derived bands. It is mathematically defined by the topological invariant $Z_2=1$. A quantum spin Hall (QSH) insulator may show a quantized SH conductivity equal to the conductivity quantum e^2/h. Apart from measurements all these characteristic quantities can be investigated by means of modern electronic structure methods. Excellent examples for discussion of the four insulator types are freestanding Xenes silicene, germanene, stanene and plumbene, i.e. hexagonal graphene-like, but buckled 2D crystals of group-IV elements with honeycomb structure and resulting linear bands. Spin-orbit coupling (SOC) increasing along the group IV of the periodic table opens a fundamental gap and, therefore, produces heavy Dirac particles.
In this talk important consequences of the linear Dirac band structure, the small SOC-induced gap E_g, the low screening on two-particle electron-hole excitations and a vertical electric field on band topology, exciton binding, and optical and spin Hall conductivities are discussed. The description of screening, not the band dispersion, rules the exciton binding and, consequently, the occurrence of the EI phase, while fully ab-initio many-body perturbation theory calculations suggest its absence. A vertical electric bias significantly varies the gap, the screening and finally defines a transition from the topological and QSH into a trivial insulator. Thereby, the SH conductivity will be significantly but continuously reduced.

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