Two-Dimensional Quartic Dispersion Materials: Strong singularity, Magnetic Instability and Thermoelectric Efficiency

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The critical points and the corresponding singularities in the density of states of crystals were first classified by Van Hove with respect to their dimensionality and energy-momentum dispersions. Different from saddle-point Van Hove singularities, the occurrence of a continuum of critical points, which give rise to strong singularities in two-dimensional elemental hexagonal lattices, is shown using a minimal tight-binding formalism. The model predicts quartic energy-momentum dispersions despite quadratic or linear ones, which is also the origin of the strong singularity. Using density functional theory calculations, families of such two-dimensional materials are identified. The first family consists of hexagonal lattices of group-VA elements, namely nitrogene, phosphorene, arsenene, antimonene and bismuthine [1]. A new family of quartic dispersion materials include A₂B₂ type hexagonal crystals of groups IV (C, Si, Ge, Sn, Pb) and V (N, P, As, Sb, Bi) elements with P6m2 and P3m1 symmetries. The structures are shown to be dynamically stable and display “mexican hat” or purely quartic dispersions (E ~ k⁴) at their valence bands. The extraordinary features of quartic dispersion materials are investigated. The strong singularity gives rise to ferromagnetic instability with an inverse-square-root temperature dependence and the quartic dispersion is responsible for a step-like transmission spectrum, which is a characteristic feature of one-dimensional systems. Because of the abrupt change in transmission at the band edge, these materials have temperature-independent thermopower and enhanced thermoelectric efficiencies.

Figures

Figure 1: Linear, quadratic and quartic energy bands in one- and two dimensions with corresponding densities of states (DOS) and transmission spectra. Quartic dispersion gives rise to a strong singularity in the DOS and a step-like transmission behaviour in two-dimensions.

References