

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

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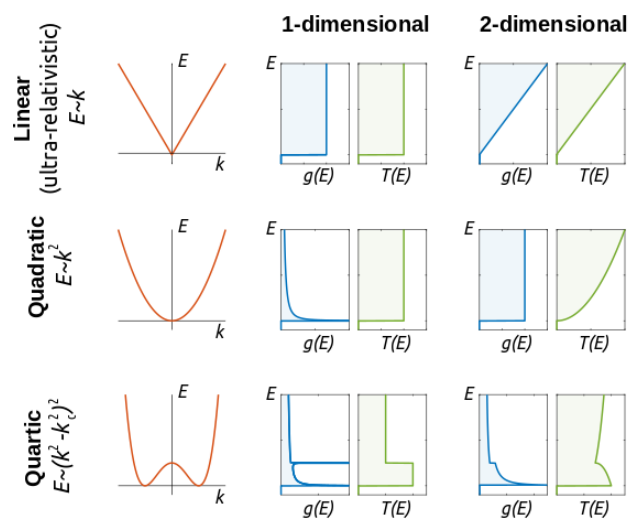
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The critical points and the corresponding singularities in the density of states of crystals were first classified by Van Hove with respect to their dimensionality and energy-momentum dispersions. Different from saddle-point Van Hove singularities, 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  $A_2B_2$  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 ( $E \sim k^4$ ) 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

- [1] H. Sevinçli, Nano Letters, 17 (2017) 2589.
- [2] B. Ozdamar, G. Ozbal, M. N. Cinar, G. Kurt, B. Kaya, H. Sevinçli, Physical Review B, 98 (2018) 045431.