

First-principles calculations of topological nodal line semimetal phase induced by strain in γ -GeSe

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A recent experiment has reported the synthesis of the first hexagonal polymorph, γ - phase GeSe, from the family of group IV-VI monochalcogenides [1]. Motivated by the experiment, we study the effects of in-plane strain on the electronic structure of γ -GeSe by using first-principles calculation. Our calculations predict that the strain can drive band inversion between the conduction and valence bands near the 5% tensile strain. The band inversion leads to forming a nodal line in momentum space, thus realizing a topological nodal line semimetal phase. Furthermore, we provide symmetry and topological analysis that explain the stability of the nodal lines. Our findings suggest the advent of novel topological material with strain-tunability.

[1] Nano Lett. 2021, 21, 10, 4305–4313