**First principle Study on Surface States of Rocksalt SnSe**

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The rocksalt SnSe compound is known as the topological crystalline insulator in which the gapless surface state is protected by the non-trivial mirror Chern number of (110) mirror plane. In the absence of the spin-orbit coupling, however, it becomes a topological nodal line semimetal. The nodal line is a line of degenerate points in the k-space between the conduction and the valence bands. In this study, we explore the nodal line structure in rocksalt SnSe. We calculate the Zak phase of SnSe and verify that the Zak phase is quantized and jumps by π at the nodal line, which is consistent with Ref. [2]. Zak phase is a Berry phase integrated along the straight line in Brillouin zone. Recently, the bulk boundary correspondence for nodal-line semi-metal using Zak phase was suggested that there is drum-head like flat surface band in the region of π-Zak phase. However, some exceptions was also reported. In that context, we calculate the surface states of SnSe with and without spin-orbit coupling and check the bulk-boundary correspondence. Further, we explore the condition such as passivation and relaxation that reproduces the experimentally observed Dirac cone at gamma-bar point of SnSe (111) surface. There is no surface state at gamma-bar point in the calculation of pristine SnSe.

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