

Abstract Submitted
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SmS: a mixed valence semi-metal with topological band structure JIAN-ZHOU ZHAO, Institute of Physics, Chinese Academy of Science, FENG LU, Nankai University, HONGMING WENG, ZHONG FANG, XI DAI, Institute of Physics, Chinese Academy of Science — The electronic structure of typical mixed valence compound SmS has been revisited by applying the local density approximation(LDA) plus Gutzwiller method. We predict that the black phase of SmS is a narrow gap semiconductor with band structure strongly renormalized by correlation effect. While for the golden phase of SmS, which will be stabilized under pressure, the electronic structure is similar to the strong three dimensional topological insulator with non-trivial Z_2 index but zero indirect gap. The surface state for (001), (111) and (011) surfaces have been obtained by our LDA+Gutzwiller calculations, indicating its non-trivial topological nature. We have also calculated the thin film sub band structure of SmS growing along both (001) and (111) directions. Our calculations show that the double layer thin film shown along the (111) direction is a 2D topological insulator.

Jian-Zhou Zhao
Chinese Academy of Sci (CAS)

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