The Existence of Liftshitz Transitions in ZrSiSe under High Pressure: The Experimental and First Principles Calculation

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The family of WHM (W=Zr, Hf, La, H = Si, Ge, Sn, Sb, M=O, S, Se, Te) with the PbFCl-type structure has attracted much attention as a large pool of topological materials, which possess the nodal-line, or Dirac Fermi surface. [1, 2] This family has shown some fantastic physical properties, for example, protected by the nonsymmorphic symmetry, a wide energy range of linearly dispersed near the Fermi level, unusual surface states hybridized with bulk band and strong Zeeman splitting — de Haas–vanAlphen (dHvA).

In this work, the band structure evolution under high pressure was obtained with the first principles calculation. The conduction bands and valance bands transverse the Fermi surface contribute to the Liftshitz Transitions in this material. In experiment, the single crystal ZrSiSe was investigated under high pressure generated by diamond anvil cell (DAC) setup. The predicted phase transitions can be clearly discerned from the Raman spectra, the resistance and magnetoresistance measurment. This finding makes ZrSiSe more interesting in a study of the relationship between topology proprty and the pressure.

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