Exploring Structural and non-trivial electronic properties of Ta_2NiSe_5 under pressure

A. R. Atique Ulla (Bhabha Atomic Research Centre, Homi Bhabha National Institute, Mumbai, India),
P. Modak(Bhabha Atomic Research Centre, Homi Bhabha National Institute, Mumbai, India)

Abstract

Ta_2NiSe_5 is a layered material that exhibits two ambient pressure crystallographic phases, orthorhombic Cmcm and monoclinic C2/c. The system undergoes structural transition from the high temperature orthorhombic phase to low temperature monoclinic phase C2/c below 300K [1]. In this work, both phases were optimized using semi-empirical DFT-D3 corrections in conjunction with the optB86b van der Waals functional to properly describe interlayer interactions. The monoclinic phase is a slight distortion of the orthorhombic structure, with $\beta \neq 90°$, while other lattice parameters remain nearly unchanged. Mechanical stability was confirmed by the Born stability criteria, and dynamical stability was verified through phonon dispersion calculations. Enthalpy pressure and volume pressure analyses indicate a pressure induced structural transition from the ambient pressure Cmcm phase to a Pmnm phase at 15 kbar within the same Bravair lattice, accompanied by a volume collapse of ~3%.

As Ta_2NiSe_5 is narrow band gap semi conductor (~100eV-300eV) [2], the calculated electronic band structure exhibits semi metallic behavior, which can be attributed to the well known underestimation of band gaps in density functional theory. The valence band is mainly composed of Ni-d orbitals and Se-p orbitals, while the conduction band is dominated by Ta-d orbitals, and multiple band inversions are observed near the Fermi level. Although the calculated band structure does not show a direct band crossing or touching, the Kane-Mele parity analysis reveals that both ambient pressure phases are topologically non-trivial, with a Z_2 index of (1;000), identifying them as strong topological insulators even in the absence of spin orbit coupling. With increasing pressure, the bands near the Fermi level move closer together, and the orthorhombic phase remains a strong topological insulator up to 15 kbar. Above this pressure, the closing of the bands drives a transition to a topological semimetal. Topological surface states were also calculated for all topologically non-trivial phases. Overall, this study provides a detailed understanding of the pressure driven structural and electronic evolution of Ta_2NiSe_5, highlighting its significance as a pressure tunable topological material.

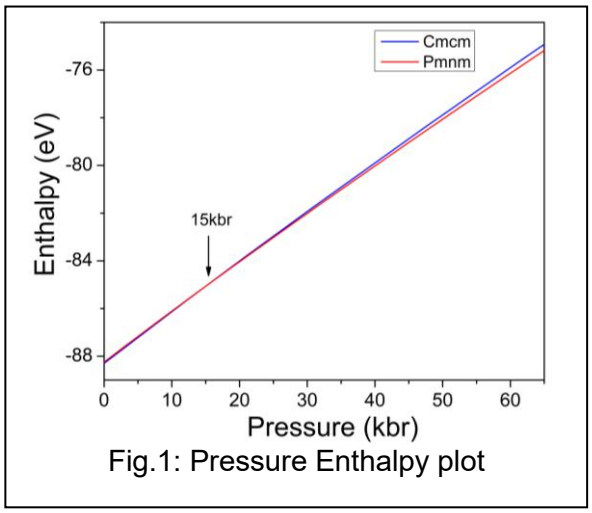

Fig.1: Pressure Enthalpy plot

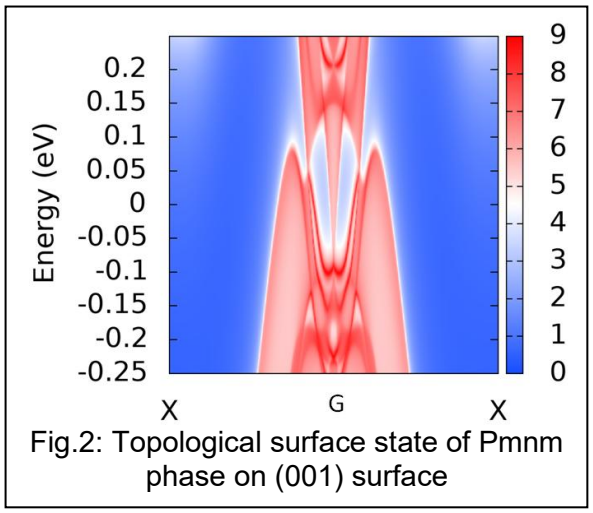

Fig.2: Topological surface state of Pmnm phase on (001) surface

Referrences:

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2. S. Pal, S. Grover, L. Harnagea, P. Telang, A. Singh, D. V. S. Muthu, U. V. Waghmare, and A. K. Sood, Phys. Rev. Research 2, 043182 (2020).