O 55: Poster Topology and Symmetry-protected Materials

Time: Tuesday 18:00–20:00 Location: P2

O 55.1 Tue 18:00 P2

Native Bi_2Se_3 bulk and surface defects calculated from first principles — •Juntao Kong[1], Timur Biktagirov[2], Uwe Gerstmann[3], and Wolf Gero Schmidt[4] — [1]Warburger Str. 100,33098 Paderborn,Germany — [2]Warburger Str. 100,33098 Paderborn,Germany — [3]Warburger Str. 100,33098 Paderborn,Germany — [4]Warburger Str. 100,33098 Paderborn,Germany

Bi_2Se_3 attracts great attention presently because it is a strong topological insulator with its surface state consisting of a single Dirac cone at Γ which is protected by timereversal symmetry. Defects in the bulk, such as selenium vacancies, may introduce charge carriers that interfere with these surface states and reduce the ability to isolate surface conduction, which is critical for applications in quantum computing and spintronic devices. Surface defects, on the other hand, may act as active sites for adsorbing gas molecules, enabling changes in electronic properties that can be used for gas sensing. Here, we present a first principles study of native point defects in Bi_2Se_3. In particular, the formation energies of vacancies, antisites and interstitials [1,2] are investigated in dependence on Fermi level position and preparation conditions.

O 55.2 Tue 18:00 P2

Exploring magnetism, topology, and magnetoresistance in rare-earth based compound GdAuSn: Ab initio study — •Sumit Mondal[1], Japsreet Singh[2], and Kanachana Venkatakrishnan[2] — [1]Central University of Haryana — [2]Indian Institute of Technology, Hyderabad

Among rare-earth intermetallics, Gd-based compounds have garnered particular interest due to their diverse magnetic ground states and interesting non-trivial topological properties. In the present work, we investigate the magnetic, electronic, and dynamical properties of the equiatomic ternary compound GdAuSn using first-principles calculations. We explore its crystal structure and analyse various magnetic configurations to determine the ground state. Our results indicate that the C-type antiferromagnetic configuration has the lowest energy. By correlating the spin configurations with the underlying Heisenberg spin model, we determine the exchange interactions and calculate the critical tempera- ture using the mean-field approximation. Additionally, we examine the electronic band structure and find evidences of nodal surface and Dirac points, indicative of non-trivial topology. Furthermore, we analyse the longitudinal and transverse magnetoresistance behaviour of GdAuSn under varying magnetic fields, observing intriguing trends that suggest a correlation between magnetic field strength and magnetoresistance. Finally, we assess the phonon dispersion of our compound and find the topological phononic states with nodal surfaces. Our findings shed light on the magnetism, topology, and transport properties in rare-earth-based intermetallic compound.

O 55.3 Tue 18:00 P2

Graphene intercalation of the large gap quantum spin Hall insulator bismuthene — •Lukas Gehrig[1,2], Cedric Schmitt[1,2], Bing Liu[1,2], Jonas Erhardt[1,2], Simon Moser[1,2], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg, D-97074 Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, D-97074 Würzburg, Germany

Bismuthene, a honeycomb monolayer of bismuth atoms synthesized on a SiC(0001) substrate, is a topological insulator with a breakthrough bulk band gap of 800 meV due to giant spin-orbit coupling. The magnitude of this gap exposes bismuthene as a promising candidate for room temperature spintronic applications based on the quantum spin Hall effect. However, oxidation of bismuthene in air confines most experiments on this system to UHV conditions. Here we demonstrate the intercalation of bismuthene between SiC and a single sheet of graphene. This protective layer effectively prevents bismuthene from oxidation, while it fully conserves its structural and topological properties as we readily demonstrate by scanning tunneling microscopy and photoemission spectroscopy. This paves the way for ex-situ experiments and ultimately brings bismuthene closer to the fabrication of spintronic devices.