ABSTRACT

The subject of topological materials has gained significant attention in the scientific community because of its distinctive and captivating features. In this thesis, we focus our attention on the two most interesting classes of topological semimetals: Dirac semimetal (DSM) and Weyl semimetal (WSM). Thus far, the majority of research on these topological semimetals has been conducted using simplified model Hamiltonians. These approaches offer a straightforward guideline for previously unobserved properties of materials in a comprehensive manner. However, their ability to quantitatively predict material-specific outcomes is limited as they do not account for the atomic configuration of the material and the corresponding energy bands. Therefore, the accurate estimation of the topological properties of real materials necessitates a multi-band approach that accounts for the exact crystal structure of the system. Our initial investigation centered around circular dichroism (CD), an optical response proportional to the Berry curvature of the system, to probe mirror anomalies in DSMs using a low-energy model Hamiltonian. We observed that DSMs show exceptional dichroic behavior when subjected to a magnetic field in any mirror-symmetric plane of the material. In particular, for different orientations of the light field with respect to the mirror-symmetric plane, the CD in type-II DSMs can detect the presence of a mirror anomaly by showing sharply distinct patterns at the mirror-symmetric angle. Our work also showed that the CD can tell the difference between a type-II DSM (with a single Dirac point at a time-reversal invariant momentum) and a type-I DSM (with two Dirac points lined up with the crystal's rotation axis). Subsequently, employing numerical techniques in combination with density functional theory and maximally-localized Wannier functions, we found a way to calculate the properties of topological materials, considering contributions from all the bands. We apply this methodology first to investigate the anomalous thermal Hall effect, a transverse transport of heat caused by Berry curvature, in a ferromagnetic Weyl semimetal $Co_3Sn_2S_2$ with broken time-reversal symmetry. We obtained a large Hall signal that can be tuned as well as reversed by changing the chemical potential. Furthermore, we observed that applying a compressive strain along the c-axis of the crystal enhances the conductivity; a 5% strain results in a 33% gain. Following that, we focused on CeAlSi, another WSM with noncollinear magnetic order, which breaks both time-reversal and inversion symmetries. In this work, we examined the shift current that causes the bulk photovoltaic effect and the injection current that is accountable for the circular photogalvanic effect in CeAlSi. Our investigation identifies a significant injection current of 1.2 mA/V^2 over a broad range in the near-infrared region of the electromagnetic spectrum, exceeding previously reported findings. In addition, we explored several externally controllable parameters to further enhance the photocurrent. A substantial boost of 64% is observed in the injection current when applying a 5% uniaxial strain along the *c*-axis. The results we obtained using this first-principles approach suggest potential applications in electronics and photonics and can be directly tested in experiments.

Keywords: Topological material, Dirac semimetal, Weyl semimetal, Berry curvature, Anomalous transport, Nonlinear photocurrent, Density functional theory, Wannier functions.