Summary

Magnetic topological semimetals (TSMs) represent a unique class of materials where the intriguing interplay between magnetic order and unconventional electronic band structures gives rise to novel physical properties. These materials possess a remarkable feature called band crossings: Energy bands intersect either at specific points (0D) or lines (1D), or even entire surfaces (2D) within their electronic structure. This unique overlap unlocks fascinating properties in these materials. Notably, these crossings can be classified based on protected, nontrivial boundary states – special electronic states that exist at the edges of the material. Depending on the dimensionality and degeneracy of the band crossings, different types of TSMs emerge, such as nodal point semimetals (Dirac and Weyl semimetals), nodal line semimetals, and nodal surface semimetals. While they can be realized in both nonmagnetic and magnetic materials, their magnetic counterparts offer additional possibilities. By manipulating the magnetic order, one can exert greater control over the material's properties, making them particularly promising for exploring phenomena like chiral anomalies and novel transport mechanisms.

This Ph.D. thesis delves into the world of magnetic TSMs, utilizing first-principle electronic structure calculations to investigate their topological behavior and associetd transport phenomena. Part one of the thesis investigates a fascinating class of hexagonal materials (*e.g.*, Mn_3Sn) characterized by a 120° planar antiferromagnetism within a kagome plane. It displays a remarkable capability of the antiferromagnetic order on controlling the topological phases in the band structures. This work introduces the concept of *vector-chirality* as a switch for controlling topological properties. Within the kagome plane, the spins arrange themselves in a specific pattern that, while maintaining zero overall magnetization, possesses the *vector-chirality* with a magnitude of one. By switching the sign of *vector-chirality* via an unconventional *staggered rotation*, the research demonstrates a topological transition from a nodal-ring semimetal to a Weyl semimetal. Furthermore, depending on the spin arrangements keeping *vector-chirality* unaltered, the Weyl points are created on a desirable position on the boundary of a nodal-ring.

Building on the insights gained from the first part on topological phases, the second part focuses on how fine-tuning the antiferromagnetic order in this material influences its unusual transport properties, such as the anomalous Hall and Nernst effects. The study reveals that the intriguing transport properties disappear entirely in the nodal-ring semimetal phase due to an inherent symmetry within the material's magnetic structure. Interestingly, it concomitantly reveals a switchable anomalous Hall conductivity, transitioning from zero to a significant value, directly linked to the topological phase transition. Additionally, the research shows that the in-plane components of the anomalous Hall effect can be tuned depending on the location of Weyl points on an elliptic ring. Even a minor staggered rotation which breaks the rotation symmetry is found to tailor both anomalous conductivities.

Part three explores Fe_4GeTe_2 (F4GT), a two-dimensional van der Waals ferromagnet that exhibits a giant anomalous Hall effect. This effect, driven by Berry curvature, is significantly enhanced by the material's unique electronic structure, as revealed by our first-principles electronic structure calculations. Specifically, in the absence of spin-orbit coupling (SOC), the calculations predict the emergence of a topological nodal line. However, when SOC is introduced, this degeneracy is lifted, resulting in a gapped nodal line with significant Berry curvature. This finding highlights the role of SOC in manipulating the band structure near the Fermi level, ultimately leading to the exceptionally large anomalous Hall effect.

In the final part, the thesis explores the effects of chemical substitution in kagome Weyl ferromagnet $Co_3Sn_2S_2$. This involved replacing Sn with In atoms and analyzing the impact on the material's magnetic and transport properties. The analysis revealed that In doping shifts the Fermi level away from the electronic band responsible for ferromagnetism in $Co_3Sn_2S_2$, leading to a loss of its topological character and affecting its transport properties.