ABSTRACT

This thesis investigates electronic structure, transport properties, and chiral magnetism in quantum materials using first-principles methods. In bulk semiconductor systems, the electronic structure and phase stability of Cu- and Ag-based chalcopyrites are studied using advanced exchange-correlation functionals within density functional theory (DFT). The rMGGAC meta-GGA functional yields band gaps in close agreement with experiment, while r^{2}SCAN provides reliable thermodynamic phase stability, together establishing an accurate computational framework for chalcopyrite materials. Their thermoelectric performance is evaluated using the dielectric-dependent hybrid (DDH) functional combined with Boltzmann transport theory, showing that band dispersion, effective mass, and carrier scattering collectively govern the Seebeck coefficient and power factor. Among the systems studied, the quaternary compound Ag_2ZnGeS_4 achieves the highest figure of merit $ZT = 2.57$ at 800 K, identifying Ag-based quaternary chalcopyrites as promising candidates for high-temperature thermoelectric applications. In two-dimensional systems, reduced dimensionality, inversion symmetry breaking, and spin–orbit coupling (SOC) strongly influence magnetic behavior. In the non-centrosymmetric H-phase $FeTe_2$ monolayer, biaxial strain and electronic correlations enable continuous tuning of the magnetic anisotropy energy (MAE) and Dzyaloshinskii-Moriya interaction (DMI), with the micromagnetic DMI constant reaching 3.06 mJ/m^2. In T-$FeTe_2$/Pt van der Waals heterostructures, interfacial SOC from the heavy-metal substrate activates a large DMI of 1.33 meV, and micromagnetic simulations confirm the stabilization of Néel-type skyrmions under an applied magnetic field. In the centrosymmetric Ti_2Si monolayer, Co and Pt co-doping simultaneously breaks inversion symmetry and enhances SOC, generating finite DMI and enabling chiral spin textures in an otherwise magnetically trivial system. These results establish a direct link between electronic structure and emergent magnetic phenomena, providing a predictive pathway for designing quantum materials with tunable transport and spintronic functionalities across different dimensional regimes.