Materials Science & Engineering Doctoral Defense

Computational Design of Compositionally Complex 3D and 2D Semiconductors

School for Engineering of Matter, Transport and Energy

Duo Wang

Advisor: Houlong Zhuang

Abstract

The structural and electronic properties of compositionally complex semiconductors have long been of both theoretical interest and engineering importance. As a new class of materials with an intrinsic compositional complexity, medium entropy alloys (MEAs) are immensely studied for their excellent mechanical properties. The electronic properties of MEAs, however, are less well investigated. In this thesis, the electronic, spin, along with thermal properties of two three-dimensional (3D) and two two-dimensional (2D) compositionally complex semiconductors are demonstrated for various applications in photovoltaic, thermoelectric, and spin quantum bits (qubits).This thesis introduces the semiconducting 3D Si-Ge-Sn and C3BN alloys. Density functional theory (DFT) calculations and Monte Carlo simulation results show that the Si1/3Ge1/3Sn1/3 MEA exhibits large local distortion effect yet no chemical short-range order. The single vacancies in MEA can be stabilized by bond reformations while the alloy retains semiconducting. DFT and molecular dynamics calculations predict that increasing the compositional disorder in SiyGeySnx MEAs enhances their electrical conductivity while weakens the thermal conductivity at room temperature, making the SiyGeySnx MEAs promising functional materials for thermoelectric devices. Furthermore, the nitrogen-vacancy (NV) center analog in C3BN (NV-C3BN) is discussed for the applications in quantum computing. The NV-C3BN possesses similar properties to the NV center in diamond such as a highly localized spin density and strong hyperfine interactions, making the C3BN suitable for spin qubits. The NV-C3BN also displayed two zero-phonon-line energies corresponding to wavelengths close to the ideal telecommunication band for quantum communications. Moreover, this thesis presents the semiconducting 2D transition metal chalcogenides (TMCs) and PtPN. The quaternary compositionally complex TMCs reveal tunable properties such as in-plane lattice constants, band gaps, and band alignment, using a high throughput workflow from DFT calculations. Besides, the novel 2D semiconducting PtPN based on pentagonal tessellation structure is predicted. The structurally stable semiconducting 2D PtPN maintains a direct band gap. The tunable band gaps are achieved by obtaining PtPN nanotubes, which opens up various applications of electronic and optoelectronic devices. The works in the thesis offer guidance to the experimental realization of these materials. They are also valuable for future discovery of compositionally complex systems from other elements.

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