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ORIGINAL RESEARCH ARTICLE

The Structural, Electronic, Magnetic, and Optical Properties of CsTe Monolayer: Effects of the Biaxial Strain and Electrical Field

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Abstract

Herein we report intrinsic ferromagnetism in a two-dimensional layer for the hexagonal monolayer of CsTe based on first-principles calculations. The aim of this work is to explore the structural, electronic, magnetic, and optical properties of the monolayer of CsTe. To achieve this goal, we systematically investigate the effect of biaxial strain and electric field on the electronic and magnetic properties of the CsTe. Monolayer CsTe has a half metallic (HM) property, and the magnitude of the magnetic moment is equal to 1 μ_B for each unit cell. Under the influence of biaxial strain, the size of the energy gap in the spin-up channel decreases under tensile strain and increases under compressive strain. The magnetic moment values show no change, and therefore, the HM behavior can be maintained for larger strains. The electric field has a clear effect on the energy gap when the electric field increases to $E = -0.6$ V/nm, which destroys the HM characteristic since the magnetic moment of the Cs is increased far more than the Te moment, and the Te has a large effect on achieving the HM property. The calculated optical properties indicate that the investigated material is a good candidate for applications related to micro-electronic and optoelectronic devices.

Keywords First-principles study · CsTe monolayer · optical properties · biaxial strain · electric field

Introduction

Spintronics is a promising technology for the development of the next generation of information technology due to its impressive characteristics in transmitting information and energy consumption. The materials used in the manufacturing of these devices require high spin polarization (SP) for the sake of improving their efficiency and utility. Among the most important applications are the spin valve, the spin filter, and the spin diode.[1–3] Half-metallic (HM) materials are most desirable in the manufacturing of spintronic devices, as they carry high spin polarization equal to 100% for the spin of the electrons at the Fermi level and have two different spin channels, i.e., ↑ and ↓. One is conductive, and the other is either semiconducting or insulating depending on the width of the energy gap.[4] So far, HM materials have been employed in a three-dimensional (3D) compound form, such as Heusler alloys,[5] transition-metal pnictides and chalcogenides,[6] double perovskites,[7] and transition-metal oxides.[8–10] The HM property in the practical measurements of compounds is usually verified using spin-resolved photoelectron spectroscopy,[9] spin-polarized electron tunneling,[11] and Andreev reflection.[10,12] In recent years, researchers have increased their interest theoretically and practically to describe and prepare two-dimensional (2D) materials, especially since the discovery of graphene,[13] borophene,[14] hexagonal boron nitride *h*-BN,[15] and transition metal dichalcogenides.[16] Despite the rapid expansion of the family of 2D materials, a ferromagnetic HM nanosheet is still missing. The existence of 2D HM materials remains controversial from an experimental point of view, despite the existence of several theoretical studies that describe the properties of the HM materials representing a 2D compound.

In the bulk structure, the metal monochalcogenides (such as GaS, GaSe, InSe, and GaTe) are layered materials consisting of metal and chalcogen atoms linked by a covalent bond with nanometer-thick layers coupled by weak ionic bonds and van der Waal forces.[17] Like graphene, these materials can be diluted to form 2D crystals. This state can be

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