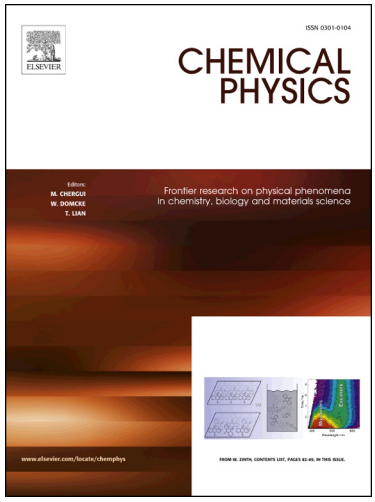

Theoretical prediction of two-dimensional CrOF sheet as a ferromagnetic semiconductor or a half-metal

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Theoretical prediction of two-dimensional CrOF sheet as a ferromagnetic semiconductor or a half-metal

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ABSTRACT Two-dimensional chromium oxide fluoride CrOF sheet was studied based on density functional theory. The investigation indicates that the CrOF sheet is an intrinsic ferromagnetic semiconductor. The corresponding Curie temperature is 150 K. In particular, the Curie temperature increases up to 410 K under hole doping and the CrOF sheet becomes a half-metal. The versatile electronic and magnetic properties indicate that the two-dimensional CrOF sheet can be a promising candidate for next-generation spintronic devices.

Keywords: Two-dimensional CrOF sheet; Ferromagnetic semiconductor; Half-metal; Curie temperature; Density functional theory

1. Introduction

Spintronics is one of the most promising next generation information technologies in the 21st century, which uses the spins of electrons as information carriers. Being different from conventional electronics, spintronics possesses potential advantages of high speed, high circuit integration density, and low power consumption [1]. Spintronic materials, such as magnetic metal and magnetic semiconductors, can serve as electrodes and the central region of spintronic devices [2]. In order to minimize the size of spintronic devices, low-dimensional ferromagnetic (FM) materials are eagerly needed. However, most of the available low-dimensional materials in the pristine form are intrinsically nonmagnetic or antiferromagnetic (AFM). Although defect, composition engineering or the proximity effect can introduce magnetic responses locally or extrinsically, intrinsic magnetism is necessary [3]. In the last year, two-dimensional $Cr_2Ge_2Te_6$ and CrI_3 sheets with long-range FM ordering were fabricated [3,4]. Nevertheless, low Curie temperatures limit their applications.

Hence, from the theoretical aspect, it is important to design and find intrinsic FM