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# Bulk, surfaces, and interface investigations of electronic and magnetic properties: A case of the half-Heusler alloy MgCaB

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ABSTRACT

For Heusler alloys to be used in spintronic applications, the half-metallic property must be maintained on surfaces. MgCaB is a half-metal with a magnetic moment of $1\mu_B$. Considerable magnetic moment arises from the B atoms, and the hybridization between the p orbitals of B with the s orbitals of Mg and Ca gives rise to half-metallic characteristic. Herein, the electronic and magnetic properties of the (001) and (111) surfaces and the interface are examined. Results show that the half-metal is retained only in the bulk and on the Ca-terminated (111) surface and the spin polarization is equal to 100%. However, it is destroyed in all surface ends and the interface due to the relaxation effect obtained on the atoms at these ends and at the interface. The excellent bulk and Ca (111) surface half-metal properties of this new material indicate its potential applications in low-power electronics.



## 1. Introduction

Spintronics, a new branch of electronics, is simply the use of the degree of rotation freedom and the degree of electron charge in several functions, the most important of which are lower energy consumption, higher storage density, and faster data processing than traditional electronics [1–6]. To produce spintronic devices for special functions, we need to search for particulate matter including only one type of spin conveyors (either spin ↑ or spin ↓). In 1903, a new alloy was discovered and named Heusler alloy according to its discoverer. During that time, studies on the alloy crystal structure were not possible because of the unavailability of the necessary measuring tools. After this discovery in 1934, Bradley and Rodgers [7] discovered that the Heusler alloy $Cu_2MnAl$ was an ordered structure with an $L_{21}$ phase comprising four lattices of overlapping face centered cubic (FCC). Then, in 1969, Webster announced the structural and magnetic properties of Heusler alloys [8]. After a period of nearly two to three decades, research into the various properties of Heusler alloys was accelerated in 1983 with the discovery of half-metallic ferromagnetism (HMF) in NiMnSb alloy [9]. To date, numerous half-Heusler alloys have been found. Heusler alloys are classified into three basic groups, namely, half Heusler, full Heusler [10] (divided into normal and inverse) [11,12], and quaternary Heusler [13]. In recent studies, several new Heusler alloys have been found in half-metallic materials with a high Curie temperature ($T_C$) and magnetic moment. The electronic and magnetic properties of new Heusler alloys are fundamentally important for spintronic devices. Semi-metallic materials can be used as thin films or multilayers, so the study of the surface properties of Heusler alloys is necessary for the development of electronic devices based on this type of material. In recent years, a new type of HMF material known as $d^0$ or sp compounds has been studied. This type does not contain a transition metal [14,15]. Among Heusler materials, $d^0$ Heusler alloys exhibit very suitable properties, such as large HM band gap ($G_{HM}$), relatively high $T_C$, and particularly low magnetic moment to prevent stray flux and power loss for spintronic devices [15,16].

Verifying the electronic and magnetic properties of surfaces is important as they often differ from those of their bulk structures. The same is true for the HM property, which may disappear on the material surface [17,18]. Therefore, for an HM to be used as a spin valve in spintronics, the surface must also have a HM property. Little research has been conducted on the surface and interface properties of some half-Heusler alloys, most of which do not preserve HM properties on surfaces [10,17]. For example, HM is destroyed in all surfaces (001) at Fe terminated and in (111) both Fe and Cr terminated of FeCrSe and the CrSe-terminated (001) and Se-terminated (111) surfaces keep the HM property [10]. In the present study, we investigate the properties of bulk, (111) and

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