UNIVERSITI TEKNOLOGI MARA

FIRST PRINCIPLES STUDY ON STRUCTURAL, ELECTRONIC AND MAGNETIC PROPERTIES OF HEUSLER-TYPE FERROMAGNET USING DENSITY FUNCTIONAL THEORY

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ABSTRACT

Heusler compound is one of the potential half-metallic materials for applications including shape memory alloy (SMA), spintronic devices and magnetic sensor. Effort to develop more efficient half-metallic materials provide new opportunities and challenges in this field. Existing half-metallic materials were modified to enhance their existing properties. One of the known half-metallic materials is Co_2FeSi (CFS) which has a great potential to exhibit half-metallic property at room temperature. In this work, the investigation focused on the variety functional and physical properties of ternary and quaternary Heusler alloy. The calculations were performed using first principles study based on Density Functional Theory (DFT) that has been implemented in CASTEP computer code. The atomic arrangement was demonstrated by using Material Studio Visualizer and convergence test were calculated before optimization and further energy calculation were made. The geometry optimizations of these Heusler alloys were calculated using Local Density Approximation (LDA-CAPZ) and Generalized Gradient Approximation (GGA). The structural, electronic and magnetic properties of CFS were preliminary determined. The results of structural, electronic and magnetic properties are in good agreement with other available calculations and experimental data. CFS shows direct energy band gap at G-point. The origin of the energy gap comes from the hybridization of Co-Co and Fe bonding. The structural, electronic and magnetic properties of Co_2VSi (CVS) was then studied via first principles calculation. The calculation revealed that the possibility of gap disappearing at the Fermi level of Heusler alloy. Weak hybridization between Co-Co and V bonding have been identified as the reason for disappearance of the gap. Further calculations include the structural, electronic and magnetic properties of disordered CFS II and CFS III. It has been found that CFS I and CFS II have almost identical in their properties. The elastic properties values confirms that CFS and CVS as well as CFS II and CFS III are mechanically stable. Additionally, the modified CFS was investigated by substituting one of the Co with Ag and Pt. The novel quaternary Heusler alloy CAFS and CPFS were successfully designed in this work first principles calculation method. These novel compounds have been found to exhibit metallic properties. It is noted that CAFS has lower magnetic moment compared to CFS while CPFS has higher magnetic moment than CFS and may be possible to exhibit half-metallic properties by substituting partially. Thus, the partial substitution technique or virtual composition atom (VCA) is suggested as a potential method to further study these materials. These findings show that interruption of the non-magnetic material or magnetic material can affect the magnetic moment of Heusler compounds.

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CHAPTER ONE
INTRODUCTION

1.1 Research Background

Half-metallic ferromagnets (HMF) represent a relatively new class of materials which have attracted a lot of interest recently, due to their possible applications in semiconductor spintronic [1] and magneto electronics [2]. This class of materials was initially proposed by de Groot et al. [3] in the early 1980s. In conventional ferromagnets, the spin polarization arises from an imbalance in the density of states for majority (spin-up) and minority (spin-down) spin electrons. These materials show a completely different behaviour between their energy bands. While one of the band usually the majority-spin band or spin-up band shows a typical metallic behaviour with a non-zero density of states at the Fermi level, E_F, the minority-spin band or spin-down band exhibits a semiconducting behaviour with an energy gap at E_F [4]. Therefore, such half-metals can be considered as a hybrid between metals and semiconductor. A schematic representation of the density of states of a normal metal, a semiconductor and a half-metal is shown in Figure 1.1. This half-metals exhibit, ideally, a 100% spin polarization at the Fermi level and therefore these compounds should have a fully spin-polarized current and be ideal spin injectors into a semiconductor, thus maximizing the efficiency of spintronic devices [5], [6].

Heusler compounds have attracted intense interest during the last century due to the possibility to study in the same family of alloys, a series of interesting diverse magnetic phenomena like itinerant and localized magnetism [7], [8], helimagnetism [9], antiferromagnetism [10], [11], Pauli magnetism [12] or heavy-fermionic behaviour [13]. Nowadays, their application as a shape-memory alloy has been discussed vigorously. The first Heusler alloys studied were of the form X_2YZ and crystallize in the $L2_1$ structure which consists of four face-centred cubic (FCC) sublattices, two of which are occupied by the same type of X-atoms as shown in Figure 1.2. Afterwards, the XYZ Heusler alloys of $C1_b$ structure were discovered, where one sublattices remains unoccupied. This $C1_b$ compounds are often called half- or semi-Heusler alloys, while the $L2_1$ compounds are referred to as full-Heusler alloys.