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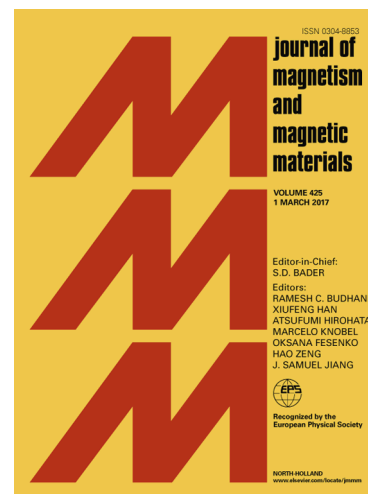
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Spin polarization in Co₂CrAl/GaAs 2D- slabs: a computational study

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Abstract: Co₂CrAl/GaAs slabs have been constructed to study the electronic structure and magnetic properties by Structeditor program implemented in WIEN2k Code. GGA and LDA parameterizations have been used for exchange correlation functions. The density of states, structure and magnetic parameters have been studied and analyzed. Co₂CrAl/GaAs (111) surface shows 80% spin polarization within LDA parameterizations. Variation in spin polarization with varying projections is observed due to different surface terminations and bond length. Effect of capping layers of Au and Cu on the magnetic moment and spin polarization of Co₂CrAl/GaAs for different surface projections has been studied. The DOS indicates that the spin polarization has enhanced for all surface projections within the GGA approximation for both capping layers. The magnetic moment also varies from the bulk value of $3\mu_B$ in Co₂CrAl/GaAs surfaces.

Keywords: Heusler Alloy Surfaces, Spintronics, WIEN2k, Density Functional Theory, Spin Polarization, Magnetic Moment

1. Introduction

Ab-initio study of Heusler alloy surfaces is an active area of research in the field of spintronics [1-3]. Although many materials have been identified to be half-metals in the bulk phase with a potential for 100% spin polarization, it is difficult to extract 100% spin polarization in surfaces

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