Half-metallic behavior and band alignment of Mn_2FeAl/GaAs(001) interface based on density functional theory

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Abstract

The electronic and magnetic properties and band offset of Mn_2FeAl /GaAs interface are investigated using first-principles calculations based on density functional theory and the generalized gradiant approgximation (GGA). The calculations indicate that Mn-Mn/Ga interface is stable in terms of energy. The simultaneous analysis of the Schottky barriers and the electrostatic potential for this structure indicates the type-III band alignment, where the valence band edge of Mn_2FeAl is higher than the conduction band edge of GaAs. We have found a valence band offset (VBO) of 1.54 eV and a conduction band offset (CBO) of 1.39 eV. Hence, Mn_2FeAl /GaAs (001) is recommended for GMR and TMR applications. Furthermore, there is an electrostatic potential difference of 0.056 μV and a half-metallic behavior in this interface.

Keywords: interface, band offset, DFT, Schottky barriers, half-metallic behavior

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