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First-principles investigations of electronic and magnetic properties of the FeRh/MgO (001) interface

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Abstract

Ab initio calculations of the electronic and magnetic properties of FeRh/MgO (001) interface are reported, focusing on the effects of different atomic terminations. It was found that the Fe-O termination is energetically the most stable. The change in the electronic properties at the interface is analyzed using the spin-polarized layer projected density of states, which shows that the spin polarization at the Fermi level is dominated by the spin-down t_{2g} states. However, the magnetic moment of the interfacial Fe atom is not enhanced significantly compared to that of the inner layers. The difference of total energy between antiparallel (AP) and parallel (P) alignments of the magnetizations of the FeRh electrodes as function of MgO thickness shows that the AP configuration is the most stable and this interlayer exchange coupling decreases exponentially as predicted by the free-electron theory. Finally, Löwdin analysis of the electron density shows that the charge is transferred from the interface MgO layer to that of FeRh and confirm the change of the interface states at the vicinity of the Fermi level.

I. INTRODUCTION

In the last decade, equiatomic FeRh has raised growing interest both from experimental and theoretical point of view. Such interest comes in particular from its first order phase transition from antiferromagnetic (AFM) to ferromagnetic (FM) at about 350 K [1, 2], accompanied by a lattice expansion of 1%. This metamagnetic transition makes it attractive for storage media applications [3]. In addition, FeRh presents a good functional response to physical inputs such as small temperature differences, pressure or magnetic