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# The interface of the ferromagnetic metal CoS<sub>2</sub> and the nonmagnetic semiconductor FeS<sub>2</sub>

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The electronic and magnetic properties of the cubic pyrite CoS<sub>2</sub>/FeS<sub>2</sub> interface are studied using the all-electron full-potential linearized augmented plane wave method. We find that this contact between a ferromagnetic metal and a nonmagnetic semiconductor shows a metallic character. The CoS<sub>2</sub> stays close to half-metallicity at the interface, while the FeS<sub>2</sub> becomes metallic. The magnetic moment of the Co atoms at the interface slightly decreases as compared to the bulk value and a small moment is induced on the Fe atoms. Furthermore, at the interface ferromagnetic ordering is found to be energetically favorable as compared to antiferromagnetic ordering. © 2010 American Institute of Physics. [doi:10.1063/1.3511684]

Interfaces between perovskite transition metal oxides have attracted great attention in recent years due to the discovery of remarkable electronic and magnetic properties, see Refs. 1–4, for example. Half-metallic ferromagnetic (FM) materials are of special interest because of possible applications in spintronics. For pyrites, few interface studies have been performed so far, even though they are similarly important for device applications as oxide perovskites. The pyrite structure has a cubic symmetry with space group 205 ( $Pa\bar{3}$ ), in which the metal ions form an fcc lattice, being coordinated octahedrally by six S anions.<sup>5</sup> The properties of transition-metal pyrites  $MS_2$  ( $M=\text{Fe, Co, Ni, Cu, ...}$ ), in particular, are governed by the 3d electronic states and their different fillings.<sup>6,7</sup>

In this context, we will address an interface between a metallic ferromagnet and a nonmagnetic semiconductor: CoS<sub>2</sub>/FeS<sub>2</sub>. This system has been proposed as a possible candidate for a half-metallic interface, which would be highly desirable from the spintronics application point of view. It is known that the transport properties of metal-semiconductor interfaces strongly depend on the local electronic states at the interface.<sup>8</sup> After discussing the details of our calculations, we will address the structure of the component materials CoS<sub>2</sub> and FeS<sub>2</sub>. Afterwards, we will deal with the CoS<sub>2</sub>/FeS<sub>2</sub> interface and study its electronic and magnetic properties in detail.

The calculations are performed using the full-potential linearized augmented plane-wave plus local orbital method implemented in the WIEN2K code.<sup>9</sup> It is based on the framework of spin-degenerate and spin-polarized density functional theory. The exchange-correlation potential is computed in the local density approximation. Fully relativistic effects are taken into account for the core states, whereas the scalar relativistic approximation is applied to the valence states, neglecting the effects of the spin-orbit coupling. We have optimized the structure of the CoS<sub>2</sub>/FeS<sub>2</sub> interface by relaxing the atomic forces.

The wave function expansion inside the atomic spheres is based on a maximum value of  $l_{\text{max}}=10$  and a plane-wave cutoff of  $R_{\text{mt}}K_{\text{max}}=6.0$  with  $G_{\text{max}}=18$ . For the self-consistent

calculations, a  $9 \times 1 \times 9$  k-space grid containing 25 points within the irreducible region of the Brillouin zone is used. The valence states consist of Fe 3d<sup>6</sup>, Co 3d<sup>7</sup>, and S 3p<sup>4</sup> orbitals. The muffin-tin sphere radii  $R_{\text{mt}}$  (in atomic units) are chosen 2.0 for both Fe and Co and 1.8 for S. For ensuring a good convergence, all these parameters have been checked carefully.

The bulk electronic structures of the two pyrites, FeS<sub>2</sub> and CoS<sub>2</sub>, are very well studied. The Co 3d and Fe 3d electronic configurations are  $t_{2g}^6 e_g^1$  and  $t_{2g}^6 e_g^0$ . Both transition metal ions are in low-spin states,  $S=1$  for FeS<sub>2</sub> and  $S=0$  for CoS<sub>2</sub>.<sup>10</sup> FeS<sub>2</sub> is a nonmagnetic semiconductor with a small band gap of  $E_g=0.9$  eV.<sup>11</sup> The crystal structure of this compound has been reported in Refs. 12 and 13. Recently, experimental studies on the structure, the electronic structure, and the optical properties have been performed for FeS<sub>2</sub> in bulk and surface configurations using a wide range of techniques.<sup>14–16</sup> Due to a high specific energy density and the low cost of the material it is used in lithium batteries as positive electrode.<sup>17</sup>

CoS<sub>2</sub> is an itinerant system which is metallic and orders ferromagnetically at a critical temperature of  $T_c \approx 120$  K. It has a saturated magnetic moment of 0.84  $\mu_B$  per Co atom at 0 K.<sup>18–20</sup> Electronic structure calculations for CoS<sub>2</sub> predict close proximity to a half-metallic ferromagnet.<sup>12,20</sup> Experimentally, the compound remains in a high spin state but shows no half-metallicity up to the Curie temperature in the range of 116–120 K. It can be alloyed with the nonmagnetic narrow band gap semiconductor FeS<sub>2</sub> to obtain the highly spin polarized ferromagnet  $\text{Fe}_{1-x}\text{Co}_x\text{S}_2$ , which has a half-metallic ground state.<sup>21</sup>

The interface of the two pyrite compounds is modeled by a supercell consisting of eight layers of FeS<sub>2</sub> and eight layers of CoS<sub>2</sub>, as shown in Fig. 1, where each layer comprises two inequivalent Co/Fe atoms. The experimental lattice parameters of cubic FeS<sub>2</sub> and CoS<sub>2</sub> are 5.416 Å and 5.508 Å, respectively,<sup>21,22</sup> i.e., the lattice constant mismatch is less than 2%. Thus, we can use the averaged lattice constant of CoS<sub>2</sub> and FeS<sub>2</sub> for the ab-plane of our supercell. It is observed that the calculated magnetic properties at the interface depend critically on structural details. As a consequence, it is crucial that the structural relaxation is taken into account in the calculation.

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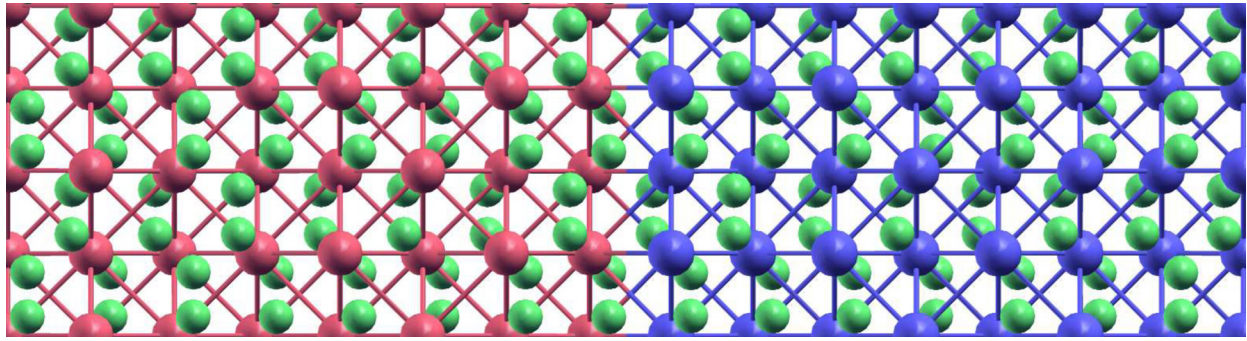


FIG. 1. (Color online) Schematic representation of the  $\text{CoS}_2/\text{FeS}_2$  interface. Large and small spheres represent Fe/Co and S, respectively.

Interesting changes affect the bond lengths and bond angles. We find that the Fe–Fe and Co–Co bond lengths are virtually the same in the bulk-like regions of the supercell before and after the structural relaxation ( $3.830 \text{ \AA}$ ). On the contrary, in the vicinity of the interface there are following deviations: while the Fe–Fe bond length shrinks to  $3.825 \text{ \AA}$ , the Co–Co bond length grows to  $3.832 \text{ \AA}$ . A different behavior is observed for the Fe–S and Co–S bond lengths which amount to  $2.256 \text{ \AA}$  in the bulk-like regions. At the interface they shrink to  $2.249 \text{ \AA}$  (Fe–S) and  $2.255 \text{ \AA}$  (Co–S). Furthermore, the Fe–S–Co bond angle decreases at the interface from  $116.17^\circ$  to  $115.18^\circ$  during the structural optimization, supporting the FM exchange.

We start our discussion of the electronic structure by showing in the top and bottom panels of Fig. 2 the density of states (DOS) of bulk  $\text{CoS}_2$  and bulk  $\text{FeS}_2$ , respectively. The Co  $3d$  states exhibit a distinct spin splitting, resembling the FM ordering. In contrast, there is no spin splitting observed for the Fe  $3d$  states. The semiconducting nature of  $\text{FeS}_2$  is clearly reflected.

We next turn to the interface. The DOS projected on Fe/Co layers with different distances to the  $\text{CoS}_2/\text{FeS}_2$  interface is depicted in Fig. 3 in order to obtain a qualitative description of the atomic and orbital origin of the electronic states. The states in the energy interval from  $-1.7$  to  $-0.5$

eV mainly trace back to the Fe  $3d$  orbitals with some S  $4p$  contribution. The most interesting feature, however, is that the first layer next to the interface, denoted as Fe(1,2), becomes metallic with a very small Fe magnetic moment of  $0.05 \mu_B$  since the Fermi energy ( $E_F$ ) shifts slightly to higher energy at the interface. The DOS shows that toward the  $\text{FeS}_2$  bulk the semiconducting nature is recovered.

On the other hand,  $\text{CoS}_2$  preserves its metallic FM nature. However, at the interface the Co(1,2) layer almost develops a half-metallic character. In this case,  $E_F$  shifts slightly toward lower energy. In the energy range from  $-2.5$  to  $-1.2$  eV the DOS is dominated by the Co  $3d$  states with finite S  $4p$  contributions. The DOS between  $-0.5$  and  $0.5$

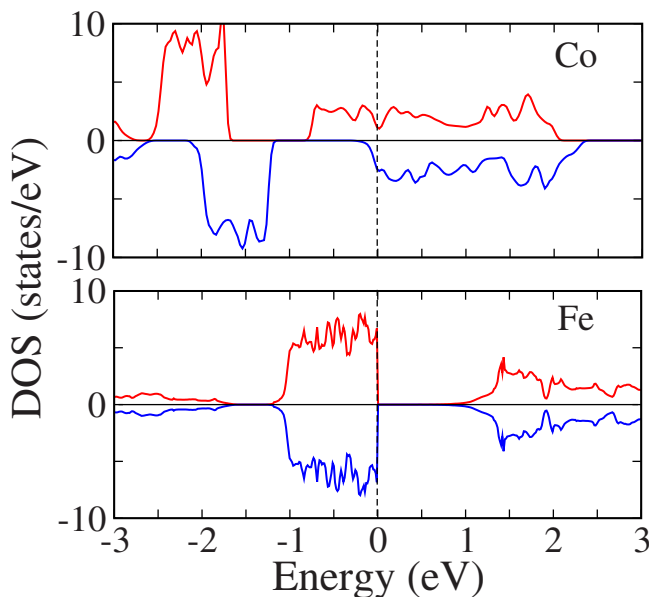


FIG. 2. (Color online) Partial Co DOS per atom of  $\text{CoS}_2$  (top) and partial Fe DOS per atom of  $\text{FeS}_2$  (bottom).

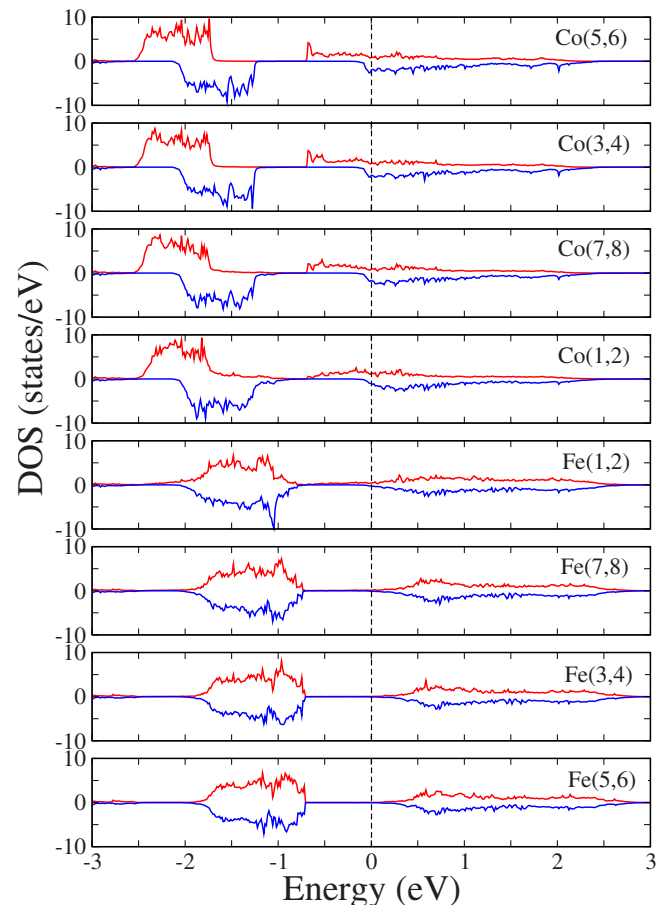


FIG. 3. (Color online) Partial DOS of the  $\text{CoS}_2/\text{FeS}_2$  interface, projected on different Fe/Co layers. The Co moments and induced Fe moments are aligned ferromagnetically. Numbers in brackets denote the separation of the different layers from the interface.

eV almost completely traces back to the Co  $3d$  states. The Co moment near the interface is  $0.63 \mu_B$ , i.e., slightly smaller than the bulk value of  $0.80 \mu_B$ .

In order to judge the stability of the FM ordering, we have also analyzed an antiferromagnetic ordering at the interface. To this end, we enforced antiparallel ordering between the first two Co layers directly at the interface, whereas keeping all other Co spins parallel to the second Co layer. We find that the FM interface is energetically more favorable than the AFM interface, with an energy difference of  $0.07$  eV per supercell.

In summary, we have studied the electronic and magnetic properties of  $\text{CoS}_2/\text{FeS}_2$ , which is an interface of a metallic ferromagnet and a nonmagnetic semiconductor, employing all-electron band structure calculations based on spin-polarized density functional theory. Structural optimization of the atomic coordinates indicates significant alterations in the bond lengths and bond angles between the atoms at the interface. Our results show that a FM ordering of the Co spins at the interface is energetically favorable as compared to an antiferromagnetic ordering.

We have discussed the behavior of the local densities of states as a function of the distance to the interface. We observe that the  $\text{FeS}_2$  develops a metallic state in the vicinity of the interface, whereas the electronic structure of the  $\text{CoS}_2$  gets close to a half-metallic state. However, our calculations clearly show that a finite spin minority DOS is maintained at the Fermi energy. For this reason a half-metallic state has to be excluded. The charge transfer occurring at the  $\text{CoS}_2/\text{FeS}_2$  interface thus is simply not strong enough to induce such a state. The system therefore is strongly restricted in its applicability in the field of spintronics.

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