A first-principles study on the magnetism of an Fe chain on Cu(001)

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Magnetic nanowires attract much attention due to the possible applications in high-density memory storage. Previously, Weinert and Freeman [1] predicted that the linear Fe chain is "strong stoner" ferromagnet with large magnetic moment of 3.3 μ_B/atom by using the self-consistent local spin density full-potential linearized augmented plane-wave (FLAPW) method [2]. In this paper, we have investigated the electronic structures and the magnetism of an Fe chain along the [110] direction on the Cu(001) surface (Fe[110] chain) by using the all-electron FLAPW method within the generalized gradient approximation (GGA) [3]. For comparison, we also considered the free-standing Fe[110] chain and the monolayer Fe on the Cu(001) surface [1Fe/Cu(001)]. The calculated results showed that the Fe magnetic moment of the Fe[110] chain is 2.99 μ_B/atom. This value is smaller than that (3.19 μ_B) of the free-standing Fe[110] chain, but the value is larger than that (2.82 μ_B) of the 1Fe/Cu(001). These large magnetic moments of Fe atoms are understood by the localization of the Fe *d*-bands due to the reduced coordination number. The coordination numbers of Fe atoms decrease from 8 for the 1Fe/Cu(001), to 6 for the Fe[110] chain, and to 2 for the free-standing Fe[110] chain. The reduced coordination number induced localization of Fe *d*-bands is clearly seen from the calculated local density of states. The Fe *d*-band width of the Fe[110] chain is more localized than that of the 1Fe/Cu(001), and it is broaden than that of the free-standing Fe[110] chain. The magnetic moment of the Fe[110] chain is only about 4% smaller than that (3.11 μ_B) of the Fe[010] chain [4], while the intrachain Fe-Fe bond length of the Fe[110] chain is about 29% smaller than that of the Fe[010] chain [4]. From the above facts, we confirm that the magnetic moments of the Fe chains on the Cu(001) substrate are related closely with the reduced coordination number more than the intrachain Fe-Fe bond length.

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