Ab inito study of the magnetic stability of Mn nanostructures on Fe(001)

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Nanostructured magnetic materials such as 3d transition metals on metallic surfaces have attracted considerable attention due to novel magnetic properties reported [1,2]. One of the magnetic properties of nanostructures which play an important role in the design of new magnetic devices is the magnetic interaction between the constituent atoms. Depending on the strength and sign of the exchange interaction, the nanostructure can be driven into ferromagnetic, antiferromagnetic or very complex spin structures [3]. A complex noncollinear magnetic structure have been recently reported for reconstructed Mn films on Fe(001) [2]. Here, motivated by these results, the magnetic structures of Mn nanowires supported on top of a Fe(001) surface, or within the surface layer have been investigated with noncollinear first-principles theory. The calculations have been performed using the real-space linear muffin-Tin orbital method (RS-LMTO-ASA) [3,4]. The Mn nanowires supported on top Fe(001) surface are found to order ferromagnetically regardless of the wire size. Mn dimmers located within the first Fe(001) surface were found to be antiferromagnetically coupled. Larger nanowires embedded in Fe (001) are also investigated and the complex magnetic behavior is discussed.

References

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