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Ferromagnetic 1D W Atomic Chain: A Giant Magnetic Anisotropy and XMCD Studies

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Through the full potential linearized augmented plane wave (FLAPW) method, the magnetic properties of one dimensional (1D) tungsten (W) atomic chain have been investigated. Very interestingly, we have obtained that the 1D W/NiAl(110) has a ferromagnetic (FM) ground state with magnetic moment of 0.81 μ_B, while unsupported 1D Watomic chain maintains antiferromagnetic (AFM) ground state with magnetic moment of 2.76 μ_B . This implies that the hybridization significantly alters the property of exchange interaction. Typical surface buckling feature of NiAl(110) surface is found: the vertical position of Al atom is higher by 0.32 A^0 than surface Ni atom. We have obtained that the 1D W chain has a giant magnetic anisotropy of 3.509 eV/atom and the direction of magnetization is perpendicular to the chain axis, but parallel to the surface. In addition, the theoretically calculated X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD) have been presented.

SD05

Magnetic Properties of Ruthenium Monolayer Between Graphene Sheets – A First Principles Study

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The transition metal (TM) metal-graphite with a layered structure, where a TM monolayer is sandwiched between adjacent graphene layers, is expected to behave like quasi-2D magnets [1]. It is also supposed that the magnetism of TM metal-graphite may be similar to that of TM monolayer on C(0001). The magnetic properties of 4d TM monolayers on C(0001) were investigated theoretically [2,3]. It was found that magnetic properties of such systems depend strongly on the assumed structure of TM monolayer, as well as on the distance between the monolayer and the graphite sheet.

In this paper we present the results of first principles investigations of the properties of ruthenium monolayer sandwiched between two graphene sheets. Ab initio calculations were carried out with the use of full-potential linearized augmented plane wave method (FLAPW) [4] as embodied in the QMD-FLAPW code. Following the reports [2,3] we investigated the Ru monolayers of four different structures, one of them partly commensurate with the structure of graphene. Various distances between Ru and graphene layers were considered. We found that only one of the investigated structures exhibited magnetic properties. That was the system in which Ru atoms of the metal monolayer were placed partly commensurately to the graphene sheets. In that case magnetic moment of the atom placed just between two carbons of the adjacent graphene layers was close to 1.0 μ_B. In all the other cases the systems were paramagnetic, independently on the distance between the layers.

Those findings imply that the observed magnetic properties of Ru metal-graphite are due to either clustering of the metal atoms or the interactions between Ru and C atoms within the systems, and that the properties of the metal monolayer between graphene sheets are substantially different from those of the monolayer on C(0001) surface.

REFERENCES

[1] M. Suzuki, and I.S. Suzuki, Phys. Rev. B, **67**, 094406 (2003).
[2] P. Kruger, J.C. Parlebas, G. Moraitis, and C. Demangeat, Comput. Materials Sci., **10**, 265 (1998).
[3] L. Chen, R. Wu, N. Kioussis, and J.R. Blanco, J. Appl. Phys., **81**, 4161 (1997).
[4] E. Wimmer, H. Krakauer, M. Weinert, and A.J. Freeman, Phys. Rev. B, **24**, 864 (1981).