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Magnetic and electronic structures of FeAs by first principles calculations ©

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Recently, much theoretical and experimental attention is paid to the half metallic ferromagnetism in the zincblende compounds such as MAs and MSb (M is a transition− metal element) which are structurally and chemically compatible with the important III−V and II−VI semiconductors. These binary compounds do not exist naturally in the zincblende structure but the nonequilibrium growth by MBE has facilitated the fabrication of these compounds with novel magnetic properties. The zincblende structure is maintained when grow on a zincblende semiconductor substrate. Although the zincblende phases of the compounds [1−4] have been successfully fabricated as nanodots, ultrathin films, and multilayers, it has not been possible to grow the zincblende half−metallic ferromagnetic phases as high−quality layers or thick films. One of the reasons the much higher energy ($\triangle E \approx 1$ eV per formula unit) of the ground state NiAs(*B*81) phase. Therefore, it is still required to find out proper half−metallic ferromagnetic materials, which on the one hand are compatible with the binary tetrahedral−coordinated semiconductors, and on the other hand are comparable in energy with the corresponding ground−state structures.

We performed the precise ab−initio full−potential linearised augmented plane wave (FLAPW) method within density function theory in generalized gradient approximation (GGA) to investigate electronic and magnetic properties of FeAs in zincblende structure. We found that FeAs stabilizes itself in a antiferromagnetic state compared to a ferromagnetic state in zincblende structure for the lattice constant of 5.653Å (the GaAs lattice constant). We will also discuss the variation of electronic and magnetic properties of the FeAs in NiAs structure with different lattice constants. The motivation of this work is to design materials in a crystal structure that is stable for spin electronics applications and provide a guideline for experimental works that attempt to grow these materials.

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References

[1] K. Ono, J. Okabayashi, M. Mizuguchi, M. Oshima, A. Fujimori, and H. Akinaga, J. Appl. Phys. **91**, 8088(2002).

[2] H. Akinaga, T. Manago, and M. Shirai, Jpn. J. Appl. Phys., Part 2 **39**, L1118 (2000).

[3] M. Mizuguchi, H. Akinaga, T. Manago, K. Ono, M. Oshima, M. Shirai, M. Yuri, H. J. Lin, H. H. Hsieh, and C.T. Chen, J. Appl. Phys. **91**, 7917 (2002).

[4] J. H. Zhao, F. Matsukura, K. Takamura, E. Abe, D. Chiba, and H. Ohno, Appl. Phys. Lett **79**, 2776 (2001).