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First Principle Materials Design of Half-Metallic Ferromagnetic Half-Heusler Alloys

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Based on the first principle calculation, we predict the half-metallicity and ferromagnetism above room temperature in a class of Si-containing half-heusler alloys XYSi (X = Ni, Pd and Pt; Y = Cr, Mn). The structural and magnetic properties are investigated through the calculation of the electronic structure, phase stability, equilibrium lattice constant, magnetic exchange interaction J_{ij} and Curie temperature T_c. The equilibrium lattice constant is calculated by means of the ultrasoft pseudo-potential method. Density of states, minority spin gap, magnetic exchange interaction are calculated within KKR-LSDA framework. Curie temperature is predicted by performing Monte Carlo simulations (for comparison, two other statistical methods: mean field approximation, random phase approximation are also employed). The magnetic configuration dependence of J_{ij} and the latttice parameter effect are investigated. The discussion of the role of X and Y in the stabilization of half-metallicity and ferromagnetism is also given. In addition, we also show the stability of $C1_b$, tetragonal and orthohombic structures of XYZ compositions at different values of lattice parameters.

Obtained results show a possibility to achieve half-metallicity and ferromagnetism at temperatures much higher than room temperature in these alloys. Particularly, T_c of 785K and 1076K are predicted by Monte Carlo simulations for PtMnSi and NiMnSi at the equilibrium lattice constant, respectively. Furthermore, the predicted half-metallic alloys exhibit a much wider minority band gap than that of the protopical alloy NiMnSb. Under external conditions, the compositions XYZ can be reconstructed in tetragonal and orthohombic structures rather than $C1_b$.

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AC05

First-principles Study on the Ferromagnetic Phase Stabilization of $FePt_3$ Thin Films

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Controlling the local magnetic properties without altering stoichiometry or topography of a material is an intriguing subject related to the patterned media. The *3d-5d* intermetallic $FePt_3$ alloy is one of the promising ingredients of this use since it exhibits a rich variety of magnetic structures sensitively depending on environments. Its ferromagnetic single crystal, which is chemically disordered phase in $L1_2$ structure with high T_C of ~ 425 K and saturation magnetization of 720 emu/cc corresponding to an Fe magnetic moment of $4.6\mu_B$, evolves to two coexisting chemically ordered antiferromagnetic (AFM) Q1 and Q2 phases upon cooling at 160K and 100K with Fe moments of 3.3 and 2.0 μ_B, respectively. More interestingly, recent experimental reports demonstrate that the phase transitions between AFM Q1 and Q2 phases or between AFM and FM phases in nano-scale thin films can be induced in various ways, that is, by changing growth and annealing temperature, introducing film strain by substrates, or creating crystal defects by plastic deformation or ion radiations. In this study, we performed the first-principles calculations on $FePt_3$ in bulk and in thin film to investigate the magnetic phase stability change versus the structural change such as the tetragonal distortion and local atomic position changes by buckling or dimerization at surface and interfaces. In bulk alloy, the ground magnetic phase AFM Q1 indicate possible phase transition to AFM Q2 phase by +2 and －6 % tetragonal distortions from its equilibrium c/a ratio along (001) and (110), respectively, while FM phase indicates no occurrence within tetragonal distortion of ±20% in both directions. In contrast, the 0.3~0.5 nm thick thin films of $FePt_3$ on Pt(110) surface has its ferromagnetic ground state which is stabilized by a large surface relaxations up to 20% of two top most layers as well as by the decreased number of neighboring Fe atoms at $L1_2$ cubic corners which stabilizes AFM coupling in bulk phase. Also a comparison of clean surface and missing row formation and their effects on the FM stabilization will be discussed.

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