Semiconducting (Half-Metallic) Ferromagnetism in Mn(Fe) Substituted Pt and Pd Nitrides

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Using first principles calculations as based on density functional theory, we propose a class of so far unexplored diluted ferromagnetic semiconductors and half-metals. These latter may be very interesting as a potential candidates for spintronic applications. Here, we study the electronic properties of recently synthesized $4d$ and $5d$ transition metal dinitrides. In particular, we address Mn- and Fe-substitution in PtN_2 and PdN_2. Structural relaxation shows that the resulting ordered compounds, $Pt_{0.75}(Mn,Fe)_{0.25}N_2$ and $Pd_{0.75}(Mn,Fe)_{0.25}N_2$, maintain the cubic crystal symmetry of the parent compounds. On substitution, all compounds exhibit long-range ferromagnetic order. While both $Pt_{0.75}Mn_{0.25}N_2$ and $Pd_{0.75}Mn_{0.25}N_2$ are semiconducting, Fe-substitution causes half-metallic behavior for both parent materials.
Structural properties were investigated via the energy versus volume calculations. The obtained theoretical lattice parameters in the non spin polarized case ($Pt_{0.75}Mn(Fe)_{0.25}N_2$: a = 9.21(9.12) Bohr, $Pd_{0.75}Mn(Fe)_{0.25}N_2$: a = 9.15(9.09) Bohr) are slightly larger than the experimental one of PtN_2 (a = 9.08 Bohr). The same procedure is carried out to optimize the internal parameter u of the pyrite structure. The results ($Pt_{0.75}Mn(Fe)_{0.25}N_2$: u = 0.415(0.420), $Pd_{0.75}Mn(Fe)_{0.25}N_2$: u = 0.420(0.420)) show that the internal parameters of all the compounds are nearly equal to the PtN_2 one (u = 0.415). Furthermore, we extend our calculations to include the particular value of $u = 0.25$ (where the pyrite structure coincides with the fluorite one) which is shown to be just a *local minimum*, which indicate that the fluorite is energetically less stable compared to the pyrite.
Finally, the very interesting result concern the obtained bulk modulus of the four compounds. These latter are found to be very large, especially $Pt(Pd)_{0.75}Mn_{0.25}N_2$ with a value of 352 GPa (345 GPa) which are as high as to the PtN_2 one (360 GPa). This makes the compounds an *ultra-hard magnetic* semiconductors.