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Theoretical investigations of two Si-based spintronic materials

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Abstract
Two Si-based spintronic materials, a Mn-Si digital ferromagnetic heterostructure (δ-layer of Mn doped in Si) with defects and dilutely doped Mn_xSi_{1-x} alloy are investigated using a density-functional based approach. We model the heterostructure and alloy with a supercell of 64 atoms and examine several configurations of the Mn atoms. We find that 25% substitutional defects without vacancies in the δ layer diminishes half metallicity of the DFH substantially. For the alloy, the magnetic moment M ranges from 1.0–9.0 μ_B/unit-cell depending on impurity configuration and concentration. Mn impurities introduce a narrow band of localized states near E_F. These alloys are not half metals though their moments are integer. We explain the substantially different magnetic moments.

1. *Introduction*

A new terminology "spintronics"[1] has been proposed recently to characterize devices that utilize the electron spin, or both charge and spin, in their basic operations and are incorporated into semiconductor technologies. Among semiconductor technologies, Si based technologies are the most advanced. Two recent developments suggest encouraging prospects for Si-based spintronic materials: First, we proposed recently a Si-based digital ferromagnetic heterostructure (Mn/Si-DFH) composed of a δ-layer of Mn in Si which exhibits two-dimensional half metallicity (HM) and high Curie temperature T_c.[2] Second, experimentally, dilutely doped Mn_xSi_{1-x} with $x \leq 10\%$ has shown T_c in excess of 400 K.[3-5] The DFH and Mn_xSi_{1-x} alloy are potential spintronic materials. The issues to be addressed are: (1) will defects destroy the HM? and (2) what are the spintronic properties of Mn_xSi_{1-x}?

In this paper, we report the results of: (1) a Si based DFH having (i) 25% substitutional defects and no vacancies in the δ-layer, (ii) a Mn in the δ-layer exchanged with a Si in a nearest-neighboring layer, and (iii) a vacancy in the δ-layer; and (2) a Mn_xSi_{1-x} alloy with $x < 10\%$.

2. *Method of calculation and models*

We used a planewave pseudopotential ab initio electronic-structure method[6] with generalized gradient approximation (GGA)[7] to exchange and correlation. The convergence of the total energy for each model is on the order of 1.0 meV. Supercells of 64 atoms were employed to model all structures. In Fig. 1, the left figure shows the supercell of an ideal Mn/Si-DFH having 4 Mn (red) and 60 Si (blue) atoms. The model with one Mn in the δ-layer replaced by a Si (25% defect) is shown in the right figure.

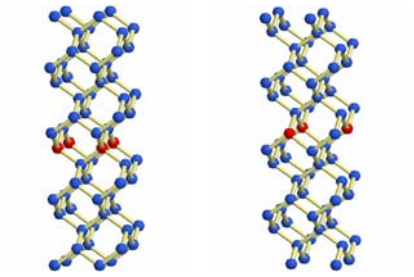

Fig. 1. Supercell models of the Mn/Si DFH with 64 atoms. Left: perfect δ-layer. Right: 25% defective δ-layer. Mn atoms are shown in red; Si atoms, in blue.

3. *Results and discussion*

a. Defects in the DFH

Table I gives the total energy, DOS at E_F, gap in the semiconducting channel, magnetic moment M, and magnetic ordering of the ideal DFH and defect cases (i)–(iii). While the integer moments are not strictly the result of integer charge transfers among species, the M values of the relaxed DFH and case (i) may nevertheless be understood in terms of a simple ionic model.[8] In this model, a Si atom takes four electrons from a Mn, leaving the Mn with three electrons in valence. Hund's first rule requires the three electron spins to align. With a g factor of 2, M is then 3 μ_B/Mn. The values in the other two cases can be understood

in terms of the d-d interaction and incomplete d-p hybridization between the Mn and Si neighbors. An integer magnetic moment/unit-cell is a necessary condition for a half-metal.

Table I. Properties of ideal relaxed DFH and defect cases (i)–(iii). ↑(↓) denote majority(minority)-spin.

Case	Total Energy (eV)	DOS at E_F (states/ eV-spin)		Gap (eV)	Magnetic Moment (μ_B/unit-cell)	Magnetic Ordering
Relaxed DFH	0.0 (ref)	↑5.69	↓0.0	0.27 ↓	12.0	Ferro
Case (i)		↑0.0	↓0.003	0.16 ↑	9.0	Ferro
Case (ii)	19.70	↑0.3	↓0.0	0.26 ↓	14.0	Ferro
Case (iii)		↑0.0	↓0.3	0.36 ↑	11.0	Ferro

b. Dilute alloys

In Table II, we give the optimized models with spin configurations indicated by arrows in the first column. Significant features in the table are: (i) Magnetic moments are integers, which may be understood in terms of a volume effect. For example, having a small volume in the isolated case, the three spins at the Mn do not align. One of them flips to give M = 1.0 μ_B/unit-cell. (ii) Small widths of the states near E_F with finite DOS. These states are localized. The alloys are not half metals though their moments are integer.

Table II. Properties of Si and dilute alloys with isolated, nearest neighbor (nn), and second-nearest neighbor (snn) impurities of two and three Mn atoms. ↑(↓) denote majority(minority)-spin.

Case	Total energy (eV)	M (μ_B /cell)	DOS ↑ (states/eV-spin)	DOS ↓ (states/eV-spin)	Width of states near E_F (eV)	Gap (eV)
Si		0.0	0.0	0.0		0.66
isolated ↑		1.0	0.0	36.3	0.055 ↓	0.97 ↑
nn ↑↓	0.0	2.0	0.06	0.0	0.090 ↑	0.29 ↓
snn(two) ↑↑	-0.03	4.0	0.0	0.015	0.092 ↓	0.40 ↑
snn(three) ↑↑↑		9.0	0.005	0.0	0.011 ↑	0.44 ↓

4. Conclusions

We find that the d-d interaction and incomplete d-p hybridization determine M in the DFH with defects. A 25% imperfection in the δ-layer can diminish HM substantially. M values of the alloys vary with volume around the Mn. Though their moments are integer, the alloys are not half metals.

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