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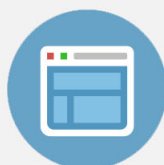Ab initio study on stability of half-metallic Co-based full-Heusler alloys
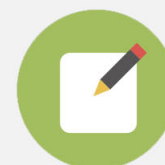J. Appl. Phys. **99**, 08J112 (2006); 10.1063/1.2176907

Slater-Pauling behavior in LiMgPdSn-type multifunctional quaternary Heusler materials: Half-metallicity, spin-gapless and magnetic semiconductors

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We employ *ab-initio* electronic structure calculations to study 60 LiMgPdSn-type (also known as LiMgPdSb-type) quaternary Heusler compounds. All compounds obey the Slater-Pauling rule with diverse electronic and magnetic properties. 41 compounds are found to be half-metals, 8 spin-gapless semiconductors, and 9 semiconductors. CoVTiAl and CrVTiAl compounds are identified as ferromagnetic and antiferromagnetic semiconductors, respectively, with large energy gaps in both spin directions. All magnetic compounds are expected to have high Curie temperatures making them suitable for spintronics/magnetoelectronics applications. © *2013 AIP Publishing LLC*.
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I. INTRODUCTION

The growth of magnetic nanomaterials and their incorporation in functional devices is a central issue in modern materials science.[1] The simultaneous development of computer modelling of materials and nanoscale growth techniques triggered the study of a huge variety of magnetic materials like the Heusler compounds or the diluted magnetic semiconductors.[2,3] Especially, computational materials science enabled the study of well-known materials in the nanoscale, where their properties are completely altered with respect to the known stable lattice structures.

Multifunctional materials integrating a variety of properties are of particular interest for spintronics/magnetoelectronics since they can enhance the functionality of devices. To this respect, Heusler compounds are widely studied due to their variety of diverse magnetic phenomena. Extensive databases on Heusler compounds using first-principles calculations have appeared in literature offering a bird-eye view of the properties of Heusler compounds.[4,5] Such studies have been complemented by more detailed materials-specific investigations.[6–10] Almost all compounds crystallize in a cubic close-packed structure which is actually a fcc structure with four equidistant sites along the cube's diagonal as basis. Several Heusler compounds (NiMnSb was the first)[11] have been predicted to be half-metallic magnets, e.g., the electronic band-structure is metallic along one spin-direction, while it is semiconducting along the other spin-direction leading to a perfect spin-polarization of the electrons at the Fermi level.[2] An important property of half-metallic Heusler magnets is the so-called Slater-Pauling rules which connect the total spin magnetic moment in the unit cell to the total number of valence electrons.[12] In the case of full-Heusler alloys with four atoms per unit cell, such relations have been

derived both for the usual full Heusler compounds (chemical formula is X_2YZ, where X and Y are transition-metal atoms and Z a sp-element) as well as the so-called inverse Heusler compounds (same chemical formula but the valence of X is lower than Y and the sequence of the atoms in the basis changes).[13,14] Slater-Pauling rules connect directly the electronic to the magnetic properties of half-metallic magnets and thus allows to determine the half-metallic character through magnetization measurements. Moreover, some of the inverse Heusler compounds have been identified to be also spin-gapless semiconductors (SGSs) where the spin-up band structure instead of being metallic presents a zero-gap semiconducting behavior;[15] Mn_2CoAl a predicted SGS has been successfully synthesized.[16] The advantage of SGS with respect to usual half-metallic magnets is that no-energy is required to excite electrons from the valence to the conduction band, and excited carriers (both electrons and holes) can be 100% spin-polarized simultaneously leading to new functionalities of spintronics devices and potential applications in logic gates.[17]

Except the usual and inverse full-Heusler compounds, another full-Heuslers family are the LiMgPdSn-type ones, also known as LiMgPdSb-type Heusler compounds.[18] These are quaternary compounds with the chemical formula $XX'YZ$, where X, X', and Y are transition metal atoms. The valence of X' is lower than the valence of X atoms, and the valence of the Y element is lower than the valence of both X and X'. The sequence of the atoms along the fcc cube's diagonal is X-Y-X'-Z which is energetically the most stable.[19] A few LiMgPdSn-type half-metallic compounds have been studied,[18,20,21] and a recent study showed that one can also find SGS among them.[22] In this communication, we have used the full-potential nonorthogonal local-orbital minimum-basis band structure scheme (FPLO)[23] within the generalized gradient approximation (GGA)[24] to study the electronic and magnetic properties of all the LiMgPdSn-type $XX'YZ$

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compounds where X = Co, Fe, Mn, or Cr, Z = Al, Si or As and Y is a transition-metal atom with valence smaller than X and X′ in each case. We have determined the equilibrium lattice constants using total energy calculations. We focus first on the occurrence of Slater-Pauling rules in these compounds and second on the existence of spin-gapless and magnetic semiconductors among them. Note that we have not employed spin-orbit coupling in our calculations but its effect is negligible for the half-metallic magnets.[25]

II. RESULTS AND DISCUSSION

A. Slater-Pauling behavior

In Tables I–III, we have gathered the calculated equilibrium lattice constants, the atom-resolved and total spin magnetic moments, and the number of valence electrons, Z_t, per formula unit for all LiMgPdSn-type Heusler compounds under study. All compounds included in the tables follow a Slater-Pauling behavior since their total spin magnetic moments, M_t, in μ_B scales linearly with the total number of valence electrons. The compounds presented in Tables I and II are half-metals and the ones in Table III show either spin-gapless or magnetic semiconducting behavior. Note that we have chosen in all cases the gap to be in the spin-down band (in the case of magnetic semiconductors discussed later, the larger of the two energy gaps was chosen to be in the spin-down band). The compounds in Table I follow a $M_t = Z_t - 18$ law, the ones in Table II a $M_t = Z_t - 24$ rule, while the compounds in Table III are either spin-gapless or magnetic semiconductors and they are dispersed between the two variants of the Slater-Pauling rule. The relative orientation of the spin magnetic moments of the nearest neighboring atoms follows the Bethe-Slater curve[26] and the equilibrium lattice constants are larger when early transition-metal atoms are present since their d-wavefunctions are more extended in space with respect to the late transition-metals.

To understand the Slater-Pauling behavior, we should first quickly revise the Slater-Pauling rules in the other full-Heusler compounds. In the usual X_2YZ full-Heuslers, the Z atoms offers a single s and a triple-degenerated p band per spin direction which are located low in energy (below the d bands).[13] These bands are important since they accommodate charge from the transition-metal atoms reducing the effective d-charge

TABLE I. Calculated equilibrium lattice constant and spin magnetic moments in μ_B for the LiMgPdSn-type Heusler compounds under study obeying the $M_t = Z_t - 18$ Slater-Pauling rule. Note that the chemical formula is XX′YZ but the sequence of the atoms in the unit cell is X-Y-X′-Z. The total spin magnetic moment is given per formula unit (which coincides with the per unit cell value).

XX′YZ	a (Å)	m^X	$m^{X'}$	m^Y	m^{total}	Z_t
			$M_t = Z_t - 18$			
CrVTiSi	5.96	0.97	0.30	−0.22	1.00	19
MnVTiAl	6.11	−2.06	2.37	0.73	1.00	19
CrVTiAs	6.02	0.32	1.74	−0.04	1.95	20
MnVTiSi	5.92	−0.09	1.97	0.17	2.00	20
FeVTiAl	6.04	−0.54	2.23	0.39	2.00	20

TABLE II. Similar to Table I for the compounds obeying the $M_t = Z_t - 24$ Slater-Pauling rule.

XX′YZ	a (Å)	m^X	$m^{X'}$	m^Y	m^{total}	Z_t
			$M_t = Z_t - 24$			
MnCrTiAl	6.04	−2.11	−2.52	0.59	−3.85	20
MnCrVSi	5.74	−1.27	−1.55	0.76	−1.98	22
MnCrTiAs	5.90	−1.07	−1.51	0.50	−1.99	22
FeCrVAl	5.84	−0.97	−1.98	0.87	−2.00	22
FeMnTiAl	5.89	−0.87	−1.79	0.55	−1.99	22
FeCrTiSi	5.81	−0.65	−1.75	0.30	−2.00	22
FeVTiAs	5.96	−0.64	−1.59	0.15	−2.00	22
CoCrTiAl	5.95	−0.23	−2.15	0.28	−2.00	22
CoVTiSi	5.90	−0.26	−1.67	−0.12	−2.00	22
MnCrVAs	5.79	−0.74	−0.78	0.51	−0.96	23
FeMnVAl	5.75	−0.65	−0.98	0.58	−0.99	23
FeCrVSi	5.70	−0.58	−0.90	0.45	−0.99	23
FeMnTiSi	5.74	−0.51	−0.77	0.25	−0.97	23
FeCrTiAs	5.86	−0.50	−0.79	0.26	−0.99	23
CoCrVAl	5.82	−0.34	−1.28	0.59	−1.00	23
CoMnTiAl	5.86	−0.23	−1.03	0.23	−0.98	23
CoCrTiSi	5.80	−0.21	−0.92	0.09	−1.00	23
CoVTiAs	5.97	−0.13	−0.90	−0.03	−1.00	23
FeMnCrSi	5.59	0.11	−0.33	1.22	0.98	25
FeMnVAs	5.74	0.70	−0.17	0.43	0.95	25
CoMnCrAl	5.71	0.66	−1.09	1.50	1.00	25
CoFeVAl	5.73	0.61	0.51	−0.09	0.97	25
CoMnVSi	5.65	0.67	−0.05	0.38	0.97	25
CoFeTiSi	5.73	0.58	0.65	−0.19	1.00	25
CoCrVAs	5.80	0.72	−0.41	0.68	1.00	25
CoMnTiAs	5.83	0.62	0.54	−0.15	1.00	25
FeMnCrAs	5.73	0.42	−0.72	2.32	2.00	26
CoFeVSi	5.66	1.06	0.76	0.18	1.97	26
CoMnVAs	5.77	1.15	0.47	0.35	2.00	26
CoFeMnAl	5.68	0.73	−0.18	2.59	3.00	27
CoFeCrSi	5.61	1.00	0.33	1.79	3.00	27
CoMnCrAs	5.75	1.06	−0.44	2.38	3.00	27
CoFeVAs	5.78	1.05	1.19	0.75	3.00	27
CoFeMnSi	5.60	0.79	0.55	2.81	4.00	28
CoFeCrAs	5.75	0.91	0.80	2.34	4.00	28
CoFeMnAs	5.74	0.94	0.99	3.12	5.00	29

TABLE III. Similar to Table I for the compounds being magnetic semiconductors or spin-gapless semiconductors. The last column is the sum of the absolute values of the atom-resolved spin magnetic moments.

XX′YZ	a (Å)	m^X	$m^{X'}$	m^Y	m^{total}	Z_t	m^{abs}
			$M_t = Z_t - 18$				
CrVTiAl	6.20	−3.10	2.50	0.58	0.00	18	6.20
FeCrTiAl	5.97	0.65	2.89	−0.38	3.00	21	4.07
FeVTiSi	5.91	0.66	2.33	0.08	2.99	21	3.14
CoVTiAl	6.04	0.23	2.55	0.32	3.00	21	3.18
			$M_t = Z_t - 24$				
MnCrVAl	5.90	−1.91	−2.39	1.18	−2.99	21	5.60
MnCrTiSi	5.86	−1.21	−2.38	0.48	−2.98	21	4.21
MnVTiAs	5.99	−1.09	−2.12	0.23	−2.87	21	3.54
CoFeCrAl	5.70	0.94	−0.63	1.78	2.00	26	3.45
CoMnCrSi	5.63	0.91	−0.77	1.93	2.00	26	3.67
CoFeTiAs	5.85	1.02	1.21	−0.29	2.00	26	2.57

and stabilizing the structure.[27] Concerning the hybridization between the d-orbitals of the transition-metal atoms, one should first consider the X-X interactions. The d orbitals of the X atoms hybridize strongly creating (i) 5 bonding d-hybrids (the double-degenerated e_g and the triple-degenerated t_{2g} hybrids) which obey the tetrahedral symmetry and can in their turn hybridize with the d-orbitals of the Y atom creating at the end five bonding and five antibonding hybrids and (ii) five non-bonding d-states (the double-degenerated e_u states and the triple-degenerated t_{1u} states), which are of octahedral symmetry, cannot couple with the d-orbitals of the Y atoms since the latter obey the tetrahedral symmetry. The energy gap in the spin-down band is between the occupied t_{1u} and the unoccupied e_u states and thus in total in the spin-down band, there are exactly 12 occupied states leading to the $M_t = Z_t - 24$ Slater-Pauling rule.[13] In the case of inverse Heuslers, it is possible to get a $M_t = Z_t - 18$ rule when X is Sc or Ti (and in some X = V compounds also) since the t_{1u} states are high in energy and are unoccupied.[14] The same occurs for the LiMgPdSn-type compounds under study. When X′ = V, Y = Ti, and Z = Al or Si, the t_{1u} states are high in energy and are unoccupied leading to the $M_t = Z_t - 18$ variant of the rule. When Z = As, the s and p states are deeper in energy and thus the spin-down d-states are shifted also deeper in energy leading to the occupation of the t_{1u} states and the XVTiAs compounds follow the $M_t = Z_t - 24$ rule. In all other cases of X, X′, and Y combinations, the compounds behave like the usual full-Heusler compounds. We should note here that when $Z_t = 24$ or 18, it is possible to get a half-metallic antiferromagnet or an antiferromagnetic semiconductor since the total spin magnetic should be zero but the constituents are magnetic.[9] In the case of CrVTiAl which has 18 valence electrons, we really get an antiferromagnetic semiconductor as shown in Table III. But all the 24 valence electron compounds which we have studied [FeMnCrAl(5.67 Å), FeMnVSi (5.63 Å), FeCrVAs (5.77 Å), FeMnTiAs (5.79 Å), CoMnVAl (5.74 Å), CoFeTiAl (5.81 Å), CoCrVSi (5.69 Å), CoMnTiSi (5.73 Å), CoCrTiAs (5.87 Å)] prefer to be semiconductors as the well-known Fe$_2$VAl Heusler compound.[28]

B. Spin-gapless and magnetic semiconductors

Among the LiMgPdSn-type Heusler compounds, which we have studied, we have identified ten compounds which behave like spin-gapless or magnetic semiconductors. In Fig. 1, we have gathered their total density of states (DOS) for a narrow energy window around the Fermi level. For all ten compounds, we have also examined in detail the band structure (not presented here). MnCrVAl and MnCrTiSi belong to the family of SGSs since they have a large energy gap in the spin-down gap, while the Fermi level falls within a zero-energy gap in the spin-up band structure. CoFeCrAl, CoMnCrSi, and CoFeTiAs are almost SGS since in the spin-up electron band structure, there is a small overlap of the bands being located above and below the Fermi level although no band-crossing occurs. In the case of FeVTiSi, there is a large gap in both spin directions but the two gaps are not located at the same energy region and the Fermi level touches the left edge of the spin-up gap and the right edge of the spin-down gap. It is similar for also FeCrTiAl; a close
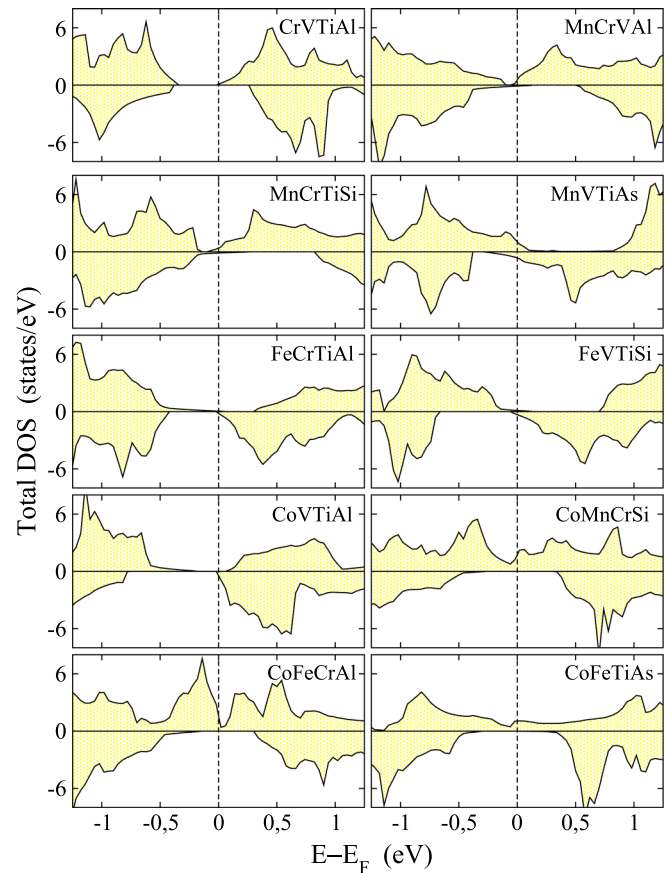

FIG. 1. Total DOS per formula unit for the compounds being magnetic/spin-gapless semiconductors. Positive DOS values correspond to the spin-up states and negative DOS values to the spin-down states. The zero of the energy axis corresponds to the Fermi level.

look at its band structure reveals that there is a wide band below the Fermi level in the spin-up band which touches the Fermi level resulting in an almost vanishing DOS below the Fermi level. MnVTiAs has a band structure similar to FeVTiSi and FeCrTiAl but now the Fermi level slightly crosses the spin-up valence band and the spin-down conduction band; all three compounds can be classified as indirect spin-gapless semiconductors. CrVTiAl and CoVTiAl are two special cases since there is a large energy gap in both spin directions, and the gaps are located at the same energy region resulting in an antiferromagnetic and a ferromagnetic semiconducting behavior, respectively; CrVTiAl has a zero total spin magnetic moment, while CoVTiAl has as a spin magnetic moment of 3 μ_B as shown in Table III. Moreover as discussed in Ref. 15, the Curie temperature for these compounds should be roughly proportional to the sum of the absolute values of the atomic spin magnetic moments.[29,30] As shown in Table III, CrVTiAl exhibits the largest sum (6.20 μ_B) among all studied magnetic semiconductors and thus we expect a Curie temperature approaching the 1000 K based on the results in Ref. 15.

All compounds being spin-gapless semiconductors have 21 or 26 valence electrons per unit cell as presented in Table III, while magnetic semiconductors have either 18 (CrVTiAl) or 21 (CoVTiAl) valence electrons. To understand the origin of the spin-gapless/magnetic semiconducting

behavior in Fig. 2, we present a schematic representation of the energy levels of the majority- and minority- spin electronic band structure for the 21 and 26 valence-electrons spin-gapless semiconductors. Below the Fermi level are located the occupied states and the numbers in front of the each orbital denote the corresponding degeneracy while we have used the nomenclature introduced above for the orbital names. We will start our discussion from the case of the 21-valence electrons compounds which follow the $M_t = Z_t - 18$ rule (see Table III). In their case in the minority spin-down band structure, the t_{1u} states are not occupied and the minority-spin gap is created between the non-bonding t_{1u} and the bonding t_{2g} states. In the majority spin-up band structure, the t_{1u} states are occupied while the e_u states are above the Fermi energy and we have in total 12 occupied majority spin-up states and 9 minority spin-down states and thus a total spin magnetic moment of $3 \mu_B$. When the 21 valence electron follow the $M_t = Z_t - 24$ rule, the situation is as discussed above but now the majority are the spin-down electrons and the minority the spin-up states resulting in a total spin moment of $-3 \mu_B$. For the 26 valence electron compounds, the minority spin-down band structure is similar to the usual full-Heusler compounds and contains exactly 12 electrons. The remaining 14 electrons in the majority spin-up band structure occupy also the e_u states and in order to have a spin-gapless semiconductor the non-bonding e_u bands should not overlap with the antibonding e_g states.

Finally, we should also comment on the comparison between the results obtained in the present study and the ones by Xu *et al.* in Ref. 22. In the latter study, five SGS have been identified: CoFeMnSi, CoFeCrAl, CoMnCrSi, CoFeVSi, and FeMnCrSb. We have not included FeMnCrSb in our study. Our calculations predict that CoFeCrAl and CoMnCrSi are SGS in agreement with the result by Xu and collaborators.[22] On the contrary, our calculations suggest that CoFeVSi and CoFeMnSi are usual half-metallic magnets and no zero-width energy gap exists in the majority spin-band but instead there is a region of low DOS. The prediction of the spin-gapless semiconducting property is a very sensitive study since small details in the calculations can easily result in a small overlap of the bands around the Fermi level in the majority-spin band structure. We believe that the discrepancy comes from the different electronic structure methods employed in the two

studies. We have used an all-electron full-potential first-principles electronic structure method while in Ref. 22 a pseudopotentials method is employed. The latter methods, although the progress made during the last years, depend strongly on the choice of the pseudopotentials, especially for magnetic systems, and do not possess for magnetic systems the accuracy of the all-electron electronic structure methods.

III. CONCLUSIONS

In conclusion, based on first-principles electronic structure calculations, we have studied the electronic and magnetic properties of the 60 LiMgPdSn-type (also known as LiMgPdSb-type) multifunctional quaternary Heusler compounds. All compounds obey the Slater-Pauling rule, the origin of which can be explained in terms of orbitals hybridization. Among the considered compounds, we have identified 41 half-metals, 8 spin-gapless semiconductors which have either 21 or 26 valence electrons per unit cell, 2 magnetic semiconductors (CrVTiAl is an antiferromagnetic and CoVTiAl a ferromagnetic semiconductor), and 9 semiconductors. All magnetic compounds are expected to have high Curie temperatures making them suitable for spintronics/magnetoelectronics applications. The effect of deformations and defects on the properties of these alloys still remains an open issue to be addressed in future studies.
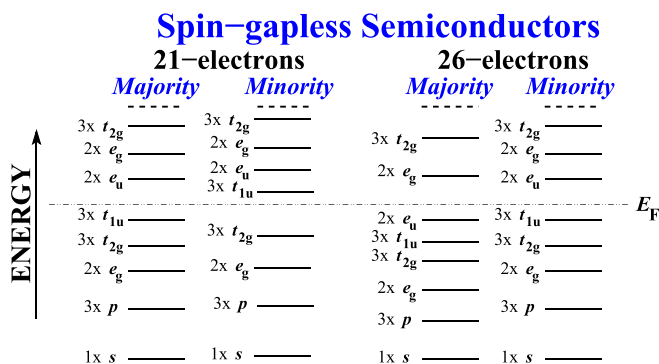

FIG. 2. Schematic representation of the energy levels of the majority- and minority- spin electronic band structure for the 21 and 26 valence-electrons spin-gapless semiconductors.

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