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절반금속 Fe_2TX 화합물의 전자구조 연구 (T = 3d 전이금속; X = Al, Si)

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Electronic Structures of half-metallic phase of ternary Fe_2TX (T = 3d transition metal and X = Al, Si)

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초록

Electronic structures of ordered Fe$_3X (X = Al, Si), and their derivative ternary alloys of Fe_2TX (T = 3d transition metal) have been investigated by using the linearized muffin-tin orbital (LMTO) band method.
The role of the coupling between substituted transition metal and its neighbors is investigated by calculating the magnetic moments and local density of states (LDOS).
It is shown that it is essential to include the coupling beyond nearest neighbors in obtaining the magnetic moment of Fe alloy .
The preferential sites of T impurities in Fe_3X are determined from the total energy calculations. The derivative ternary alloys of Fe_2TX have characteristic electronic structures of semi-metal for Fe_2VAl and (nearly) half-metal for Fe_2TAl (T = Cr, Mn) and Fe_2TSi (T = V, Cr, Mn).