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강자성 Fe 내의 $s,p-$ 원소와 $3d-$원소 불순물의 전자구조

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Electronic structures of $s,p-$ and $3d-$element impurities in ferromagnetic Fe

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We have calculated electronic structures of disordered systems with $s,p-$ and $3d-$element impurities in ferromagnetic Fe. We have used the tight-binding linear-muffin-tin orbital (TB-LMTO) recursion method, which is a reliable and accurate first-principles technique for describing the electronic structure of a system without translation symmetry.

We have considered up to four shells of neighboring Fe sites around the single site impurity. We have obtained local density of states (LDOS), charge transfer, and magnetic moments. It is found that the $s-$level LDOS at the $s,p-$ impurity site has a dip in the vicinity of the bare energy of the $d-$level of the host, which is related to the Fano anti-resonance under the weak $s-d$ coupling. For $3d$-impurity, we have found that early transition metal (TM) impurities ($Ti-Cr$) favor antiferromagnetic arrangements, while late TM impurities ($Mn-Ni$) favor ferromagnetic arrangements in the host ferromagnetic Fe, as shown in Table 1. Results from the TB-LMTO-recursion method are compared with those from the conventional LMTO band method.

표 1: Local magnetic moments in μ_B at the impurity (m_{imp}) and the neighboring Fe site (m_{Fe}), using the TB-LMTO-R(recursion) and the LMTO method.

	Ti	V	Cr	Mn	Fe	Co	Ni	Cu
m_{imp} (TB−LMTO)	−0.57	−1.00	−0.94	1.90	2.12	1.69	0.90	0.18
m_{imp} (LMTO)	−0.75	−1.28	−1.69	0.29	2.26	1.75	0.89	0.12
m_{Fe} (TB−LMTO)	1.96	1.99	2.07	2.04	2.12	2.18	2.21	2.14