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First-principles calculations of magnetic and electronic properties for Fe-Ni interface

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Abstract : We have studied the electronic structures and magnetic properties of Fe-Ni multialyers using the tight-binding(TB) linear-muffin-tin orbitals(LMTO). Furthermore, we have studied the effect of vacancies in an ordered lattice of interface. The calculation of electronic structures for the locally disordered system is carried out by a first-principle self-consistent-spin-polarized real space band method, which has the TB-LMTO method in conjunction with the recursion method.