

Evidence of surface magnetism in the V/Nb(001) system : A total energy pseudopotential calculation

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Résumé / Abstract

We determine that an overlayer of vanadium (V) on Nb(001) shows ferromagnetic activity, using the pseudopotential method with a local spin density approximation (LSDA), under the density functional theory (DFT). Precisely calculated total energy, with and without relaxation shows the ferromagnetic (FM) state to have lower energy than the paramagnetic one. The non-relaxed V overlayer has appreciable magnetism of $0.76 \mu_B$. On relaxation, due to the large values of relaxation (-22.5%) obtained there is complete hybridization of the V and Nb d bands and the magnetism is drastically reduced to $0.2 \mu_B$. Since we know, that the LSDA under estimates the magnetism, a finding of magnetism, however weak, represents the physical reality. This is in qualitative agreement with our previous work and contradicts the results of Kim and Lee.