

Magnetic and electronic properties of vanadium overlayers on Nb(001)  
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The strong overlayers-substrate hybridization has important effects on the surface electronic structure. Localized surface magnetism is a subject of considerable interest, particularly in overlayers of metals with a nonmagnetic bulk. We present an ab initio study of the electronic band structure and magnetic properties of vanadium overlayers on the niobium (001) surface. The calculations were performed within the full potential linearized augmented plane wave method and the generalized gradient approximation for the exchange-correlation energy density functional. In the monolayer case, we found that the strong hybridization between V-Nb defines the density of surface states characteristics and the emergence of non-magnetic activity. On the other hand, there is a transition from non-magnetic to magnetic in the surface layer as a function of the number of vanadium overlayers. The results are discussed in relation to the effects of strain and 3d-4d overlayer-substrate hybridization on the local electronic structure of the surface layers.