

Pd bonded to Nb(001): from a noble metal to a ferromagnet

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We present theoretical and experimental data concerning the possibility of inducing two competing properties: nobleness and ferromagnetic order, in the same metal, *i.e.* Pd bonded on Nb(001). ARUPS measurements, confirmed by first principles, self consistent DFT calculations show that the the strong, direct bonds between a Pd monolayer and Nb(001) push the d-band center of the monolayer toward lower binding energies, which results in the Pd reactivity comparable to that of the noble metal Ag. In thicker Pd films the (11 $\bar{2}$ 0)-oriented hexagonal close-packed structure is induced by the Nb(001) substrate. First principles, self-consistent DFT calculations with spin-orbit coupling included performed at 0 K show that Pd in this structure is ferromagnetically ordered at the optimum lattice constant. Its bands at the Fermi level are flatter in comparison to those of Pd in its natural, non-magnetic, face centered cubic structure, leading to the DOS at the Fermi level which fulfills the Stoner criterion for ferromagnetism. We identify these bands in the bulk band structure and probe them with angle-resolved ultraviolet photo-electron spectroscopy in (11 $\bar{2}$ 0)-oriented hexagonal close-packed Pd films.

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