

Atomic Structure and Spin Magnetism of Self-Assembled Co Nanowires on Pt (332)

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Abstract. Atomic structure and magnetic properties of monatomic cobalt wires self-assembled on a stepped Pt surface are studied using density-functional theory. Nucleation sites and the early stages of wire growth are obtained by calculating the binding energies and diffusion barriers of Co atoms on Pt (332), and the adsorption geometries of Co dimers and trimers on the same surface. We show that experimentally observed monoatomic Co wires formed at the step edges are kinetically favored over another thermodynamically equally stable structure found in our calculations. The spin magnetic moment of monatomic wires supported by Pt (332) is $3.74\mu_B$ per Co atom, more than 50% larger than that of free-standing wires. This enhancement is explained in terms of the spin-dependent hybridization between Pt-5d and Co-3d states.