First-principles Study of the Adsorption of Carbon Atom on Nickel Surfaces and a Ni38 Cluster*

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Abstract

Significant current interest exists in the catalytic growth of carbon (C) nanotubes on transition metal clusters. We have performed first-principles calculations to investigate the adsorption energetics and mobility of carbon atoms interacting with low-dimensional systems of Ni chosen as a model element. Two extreme cases of surface curvature, a magic-sized Ni cluster (Ni38) and several low-index Ni surfaces, have been studied. Our methods are based on density-functional theory using the plane wave formalism with ultra soft pseudopotentials. The binding energies of a C atom on Ni sur- faces and the corresponding facets on Ni clusters have been obtained and compared. In spite of the huge difference in the curvature, the preference order of the sites for the C atom is unchanged. A Ni(100) facet is favored for C adsorption versus Ni(110) and Ni(111) surfaces. The diffusion barriers for a C atom on these surfaces have also been obtained, with the highest mobility on the Ni(111) surface.

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