First-principles Study of the Adsorption of Carbon Atoms on Copper Surfaces*

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Abstract

The adsorption and diffusion of a carbon (C) atom on several low-index Cu surfaces have been investigated by the first-principles calculations. The methods are based on density-functional theory under plane wave formalism with ultra soft pseudopotentials. The adsorption energies and diffusion barriers of a C atom on Cu surfaces are calculated. The interactions between a pair of C atoms at different separations on these surfaces are also investigated. These results are carefully compared with the results we obtained for nickel surfaces.

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