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Carbon Adsorption on Copper and Nickel Surfaces: A Comparative First-principles Study[1] QIMING ZHANG, TU HU, Uniersity of Texas at Arlington, XINGAO GONG, Fudan University, China, JACK C. WELLS, ZHENYU ZHANG, Oak Ridge National Laboratory — The goal of this work is to understand why transition metals such as Fe, Co, and Ni are good catalysts for carbon nanotube growth while others are not. Choosing Ni and Cu as prototypes, we use first-principles total energy calculations to study the adsorption of a carbon atom on the three low-index surfaces of both metals. The adsorption energies of a carbon atom at the most stable adsorption sites on the Cu and Ni surfaces have been obtained and compared. The preference order of the adsorption sites for both Cu and Ni is the same. The (100) hollow site has the highest adsorption energy. The diffusion barriers for a C atom on the three low-index surfaces have also been obtained, with the highest mobility on the (111) surface for both Cu and Ni. Our investigation shows that the adsorption energies of the C atom on Ni are significantly higher than those on Cu for all the three surfaces. This phenomenon could be explained by their electronic structures at the Fermi level.

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