

First-principles study of oxygen adsorption on the Cu(111) surface

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Copper is an essential material for various applications, including electronic devices and industrial components, due to its excellent electrical conductivity and ductility. However, its susceptibility to surface oxidation in air and water can degrade its properties, such as conductivity and strength. Oxidation, involving charge transfer, significantly alters the electronic structure and surface states of copper. Thus, first-principles calculations, which enable the analysis of material properties based on electronic structure, are a powerful tool to understand the oxidation process of copper at the atomic level. In this study, we employed first-principles calculations to investigate the oxygen adsorption behavior on copper surfaces, specifically focusing on the interaction of oxygen atoms with the Cu(111) surface at the initial stage of oxidation.

A six-layer slab model was employed for calculations, with each layer comprising four copper atoms. An oxygen atom was positioned 3 Å above the surface, and its adsorption was investigated at four distinct sites: top, bridge, fcc hollow, and hcp hollow.

When an oxygen atom was initially positioned at the top, bridge, or fcc hollow site, it eventually migrated to and adsorbed at the fcc hollow site. Conversely, starting from the hcp hollow site resulted in adsorption at the same site. The calculated adsorption energies were -6.37 eV and -6.26 eV for the fcc and hcp hollow sites, respectively. These findings indicate that the hollow sites, particularly the fcc hollow site, are more favorable for oxygen atom adsorption on the Cu(111) surface compared to the top and bridge sites, with the fcc hollow site exhibiting slightly stronger binding than the hcp hollow site.

Reference

1. Xin Lian, Penghao Xiao, Sheng-Che Yang, Renlong Liu, Graeme Henkelman; J. Chem. Phys. **2016**, 145, 044711.