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Realistic adsorption behaviors of the copper onto the functionalized CNTs

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Introduction of CNTs into a metal matrix has been considered to improve the mechanical properties of the metal matrix. However, the binding energy between metals and pristine CNTs wall is known to be so small that the interfacial slip between CNTs and the matrix occurs at a relatively low external stress. The interfacial strength between CNT and metal matrix is thus one of the key factors for successful development of the CNT/metal composites. Defective or functionalized CNT has been considered to enhance the interfacial strength of nanocomposites.

In the present work, we design the various realistic hybrid structures of the single wall CNT/Cu complexes and characterize the interaction between single wall CNTs and Cu nano-particle and Cu13 cluster using first principle calculations. The characteristics of functionalized CNTs with various surface functional groups, such as −COOH, −OH, and −O interacting with Cu are investigated. We found that the binding energy can be enhanced by the surface functional group including oxygen since the oxygen atom can mediate and reinforce the interaction between carbon and Cu. These results strongly support the recent experimental work which suggested the oxygen on the interface playing an important role in the excellent mechanical properties of the CNT/Cu composite.

Keywords: composite, functionalized CNT