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Enhanced binding between metals and CNT surface mediated by oxygen

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In the present work, we present the optimized the hybrid structures of carbon nanotubes (CNTs) and metal nanocomposites including Cu, Al, Co and Ni using the first principle calculations based on the density functional theory.

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 application of defective or functionalized CNTs has thus attracted great attention to enhance the interfacial strength of CNT/metal nanocomposites.

Herein, we design the various hybrid structures of the single wall CNT/metal complexes and characterize the interaction between single wall CNTs and various metals such as Cu, Al, Co or Ni. First, differences in the binding energies or electronic structures of the CNT/metal complexes with the topological defects, such as the Stone-Wales and vacancy, are compared. Second, the characteristics of functionalized CNTs with various surface functional groups, such as -O, -COOH, -OH interacting with metals 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 metal. The binding energy is also greatly increased when it is absorbed on the defects of CNTs. 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[1].

1. Kim, K.T.; Cha, S.I.; Gremming, T.; Eckert, J.; Hong, S.H. *Small* **2008**, 4(11), 1936.