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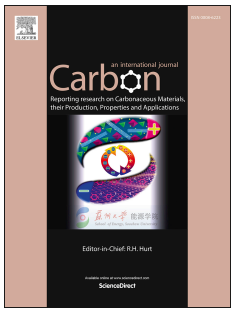

Band Gap Engineering of Carbon Nanotubes via Regular Addition Patterns of Covalent Functional Groups

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Band Gap Engineering of Carbon Nanotubes via Regular Addition Patterns of Covalent Functional Groups

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Abstract

We perform comprehensive first-principles calculations to study the addition pattern in multiply functionalized carbon nanotubes. We evaluate the relative strength of the rivaling forces between electronic effect and steric hindrance that determine whether the "cooperative addition" or the "random addition" takes place for monovalent or divalent functionalizations. We find that the electronic effect is the dominating factor and that small functional groups prefer to aggregate during successive functionalizations on CNTs. The aggregation of these functional groups leads to regular addition patterns that may drastically change the electronic properties of the original CNTs and may even result in a metallic to semiconducting transition, or vice versa.

1. Introduction

Chemical functionalization is an important method to manipulate the electrical, optical, and mechanical properties of carbon nanotubes (CNTs).[1-3] While the chemical identity of the functional groups may change from system to system, most functionalization reactions on CNT sidewalls fall into three categories: (1) Monovalent additions, such as hydrogenation, fluorination, alkylation, as well as the

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