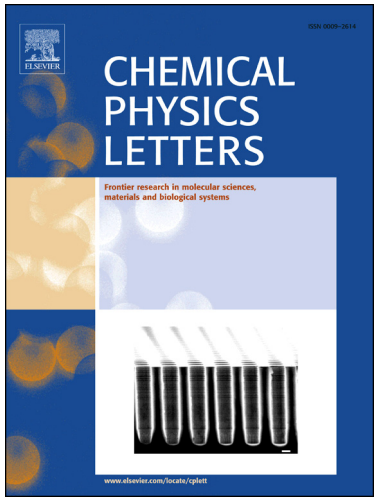

Research paper

(10, 10) Single Walled Carbon Nanotube Consisted of Chemisorbed Oxygen Atoms as a Promising Supercapacitor Electrode Material: A First Principles Study

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(10, 10) Single Walled Carbon Nanotube Consisted of Chemisorbed Oxygen Atoms as a Promising Supercapacitor Electrode Material: A First Principles Study

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Abstract

The effects of atomic oxygen chemisorption on the electronic structures and quantum capacitance of (10, 10) CNT have been studied in this article. The results indicated that the chemisorption on bonds aligned with nanotube axis is more favorable than other position. The most efficient configuration for enhancing quantum capacitance is the nanotube with oxygen atoms chemisorbed on axial bonds. Specifically, in water stability range, the quantum capacitance of (10, 10) CNT before and after chemisorption of six oxygen atoms (aligned with nanotube axis) were found to be 222.6 (anode) −117.6 (cathode) and 306.9 (anode) −217.2 (cathode) F/g, respectively.

Keywords: Quantum Capacitance; Supercapacitors; Chemisorption; Ab-initio Study.