

## Accepted Manuscript

Title: Effects of surface functionalization on the electronic and structural properties of carbon nanotubes: A computational approach

Author: M.S. Ribeiro A.L. Pascoini W.G. Knupp I. Camps



PII: S0169-4332(17)32163-3  
DOI: <http://dx.doi.org/doi:10.1016/j.apsusc.2017.07.162>  
Reference: APSUSC 36696

To appear in: *APSUSC*

Received date: 17-3-2017  
Revised date: 13-7-2017  
Accepted date: 18-7-2017

Please cite this article as: M.S. Ribeiro, A.L. Pascoini, W.G. Knupp, I. Camps, Effects of surface functionalization on the electronic and structural properties of carbon nanotubes: A computational approach, *Applied Surface Science* (2017), <http://dx.doi.org/10.1016/j.apsusc.2017.07.162>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Title: *Effects of surface functionalization on the electronic and structural properties of carbon nanotubes. Computational approach.*

Authors: *M.S. Ribeiro, A.L. Pascoini, W.G. Knupp and I. Camps*

Journal: *Applied Surface Science*

### Highlights

- The surface functionalization produces the buckling phenomena.
- The molecular orbitals (HOMO/LUMO) energies present an oscillatory behavior with the percentage of functionalization.
- The electronic properties (gap, molecular hardness and electrophilicity) present an oscillatory behavior with the percentage of functionalization.
- The system present spin polarization for selected percentage of functionalization.

Download English Version:

<https://daneshyari.com/en/article/5349571>

Download Persian Version:

<https://daneshyari.com/article/5349571>

[Daneshyari.com](https://daneshyari.com)