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Zahra Nikfar, Zahra Shariatinia



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## ACCEPTED MANUSCRIPT

DFT computational study on the phosphate functionalized SWCNTs as efficient

drug delivery systems for anti-osteoporosis zolendronate and risedronate drugs

Zahra Nikfar, Zahra Shariatinia\*

Department of Chemistry, Amirkabir University of Technology (Tehran Polytechnic), P.O.Box:15875-

4413, Tehran, Iran.

\*Corresponding author. Tel.: +98 2164545810. E-mail address: shariati@aut.ac.ir

**Abstract** 

The pristine (4,4)-armchair SWCNT as well as its three phosphate functionalized (CNT-nH<sub>2</sub>PO<sub>4</sub>, n=1-3)

forms were studied as novel drug delivery systems for the two commercially famous anti-osteoporosis

drugs including risedronate (RIS) and zolendronate (ZOL) using the density functional theory (DFT)

computations at both B3LYP and B3PW91 levels. Results revealed that the binding energy was

increased by increasing number of H<sub>2</sub>PO<sub>4</sub> moieties attached on the CNT with the most negative binding

energy was measured for the CNT-3H<sub>2</sub>PO<sub>4</sub> carrier. The dipole moments of all phosphate containing

CNTs were much greater (~1.5–4.5 D) than that of pristine CNT (~0 D). The contour maps verified that

when the CNT was functionalized by H<sub>2</sub>PO<sub>4</sub> groups, the symmetric distribution of electric charge was

vanished so that the highest and the lowest asymmetric charge distributions were achieved for the CNT-

2H<sub>2</sub>PO<sub>4</sub> and CNT-3H<sub>2</sub>PO<sub>4</sub>, respectively, leading to the greatest and the smallest dipole moments for the

CNT-2H<sub>2</sub>PO<sub>4</sub> (4.177 D) and the CNT-3H<sub>2</sub>PO<sub>4</sub> (1.614 D). The compounds RIS-CNT-3H<sub>2</sub>PO<sub>4</sub> and ZOL-

CNT-3H<sub>2</sub>PO<sub>4</sub> displayed the greatest electronegativity and electrophilicity index which were appropriate

for the binding of drugs onto the bone surface (having partial positive charge due to the presence of

Ca<sup>2+</sup>) and therefore effectively inhibiting the osteoporosis. Consequently, it was proposed that the drug-

CNT-3H<sub>2</sub>PO<sub>4</sub> was the most appropriate drug-carrier system for both of the RIS and ZOL drugs which

could be employed as the most efficient vehicle.

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