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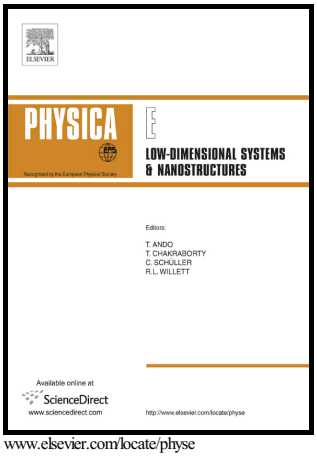

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DFT computational study on the phosphate functionalized SWCNTs as efficient drug delivery systems for anti-osteoporosis zolendronate and risedronate drugs

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Abstract

The pristine (4,4)-armchair SWCNT as well as its three phosphate functionalized (CNT-nH_2PO_4, 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_2PO_4 moieties attached on the CNT with the most negative binding energy was measured for the CNT-3H_2PO_4 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_2PO_4 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_2PO_4 and CNT-3H_2PO_4, respectively, leading to the greatest and the smallest dipole moments for the CNT-2H_2PO_4 (4.177 D) and the CNT-3H_2PO_4 (1.614 D). The compounds RIS-CNT-3H_2PO_4 and ZOL-CNT-3H_2PO_4 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^{2+}) and therefore effectively inhibiting the osteoporosis. Consequently, it was proposed that the drug-CNT-3H_2PO_4 was the most appropriate drug-carrier system for both of the RIS and ZOL drugs which could be employed as the most efficient vehicle.