Vibrational properties of (10,10) and (8,8) SWCNT before and after albumin fragment adsorption: a molecular dynamics study

G. Raffaini*[1], M. Catauro[2]

[1]*Dipartimento di Chimica, Materiali ed Ingegneria Chimica "G. Natta" Politecnico di Milano, piazza Leonardo da Vinci 32, 20131 Milano, Italy*
[2]*Department of Engineering, University of Campania "Luigi Vanvitelli", Via Roma 29, I-813031 Aversa, Italy*

**corresponding author Giuseppina.raffaini@polimi.it*

Keywords. vibrational properties, carbon nanotube, curvature, protein adsorption, molecular dynamics

Abstract.
Single walled carbon nanotubes (SWNTs) have received great attention for their mechanical, electronic properties and possible interesting technological applications. Raman spectroscopy has proven to be a sensitive tool for studying the vibrational properties of carbon nanotubes. The frequency of the radial breathing mode (RBM) in the region of 100-350 cm^{-1} is found to be inversely proportional to the diameter of the nanotube [1].
Using Molecular Mechanics (MM) and Molecular Dynamics (MD) methods conformational properties of pure armchair SWCNT having different diameters and of a same (10,10) NT after adsorption of an albumin fragment are studied. The distances between carbon atoms in the central part of the nanotube cavity change during MD run at constant temperature (T=300 K), and the frequencies of motion are calculated. The conformational properties of armchair (10,10) and (8,8) SWCNT, having the diameter equal to 13.56 Å and 12.23 Å respectively, are here reported. The distances between carbon atoms from opposite sites in the central cavity of the nanotube are calculated during MD runs. Interesting, for the (10,10) SWCNT the frequency of Raman vibrational mode E_{2g} around 17 cm^{-1} is correctly calculated. The frequency of motion due to this motion increase decreasing the curvature of the armchair CNT. After the adsorption process of an albumin fragment on the (10,10) NT, lower frequencies of motion and the lower intensities are calculated. This theoretical work can useful to study possible periodic motion in pure nanomaterials or when they interact with protein fragments, water or molecules.

[1] A. M. Rao, E. Richter, S. Bandow, B. Chase, P. C. Eklund, K. A. Williams, S. Fang, K. R. Subbaswamy, M. Menon, A. Thess, R. E. Smalley, G. Dresselhaus, M. S. Dresselhaus, Science, 275, 187-191, (1997).