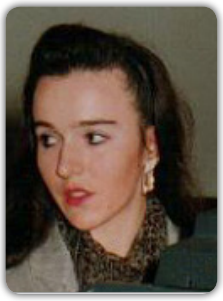
conferenceseries.com SciTechnol

Giuseppina Raffaini, J Nanomater Mol Nanotechnol 2017, 6:7(Suppl)
DOI: 10.4172/2324-8777-C1-017

2nd World Congress and Expo on

GRAPHENE & 2D MATERIALS

November 06-07, 2017 | Frankfurt, Germany



Giuseppina Raffaini

Politecnico di Milano, Italy

Importance of protein adsorption on carbon allotropes: from biomaterials to separation techniques by molecular dynamics study

Protein adsorption on carbon allotropes is an important process in different fields. Using molecular dynamics (MD) simulations, the adsorption of an albumin fragment, the most abundant blood protein, and of two fibronectin modules, important for cell adhesion, are studied to understand the first interaction when biomedical devices interact with biological fluids. Graphene favorably interacts with proteins, while two flat planes yield better interaction inducing larger conformational changes for the softer albumin, compared to fibronectin because of its stable -sheets. Interesting is the peculiar surface ordering obtained upon adsorption. Different topographies of carbon nanostructures influence protein adsorption. Armchair SWCNTs, similar to a graphene surface having different curvature, interact with proteins both on the external and on the internal surface. Using MD simulations we found that increasing the curvature, increases the interaction strength. When encapsulated in the inner nanotube surface, proteins better interact maximizing the CNTs surface adhesion, forming non-covalent complexes with larger stability. Considering finally armchair and chiral CNTs having similar curvature, the adsorption of an albumin -helix on outer convex and on inner concave surface is studied. In the final adsorbed state, the oligopeptide maximizes its contact with the surface, displaying complexes with unlike stability. Therefore, MD simulations in this theoretical study suggest the possible separation of chiral enantiomeric nanotubes by interaction with chiral oligopeptides. Also, they suggest the possible use of aligned chiral SWCNTs as stationary phase for racemic mixtures separation, and in proteomics, because favorable protein–nanotube interaction would yield different retention times.

Biography

Giuseppina Raffaini received the degree in Chemistry, the Postgraduate Diploma in "Advanced School in Polymer Science G. Natta", Inter-university Master's in Biomaterials, in 2005, and PhD in Materials Engineering at Politecnico di Milano. In 2008, she became Assistant Professor and in 2014 Associate Professor at the Politecnico di Milano. Her research interests are molecular dynamics simulations of protein adsorption on biomaterials, inclusion complexes and self-assembling of modified cyclodextrins, organic inhibitors in concrete. She is co-author of 45 original peer-reviewed ISI papers (H-index Scopus = 18), two invited reviews, and 5 contributions to books.

giuseppina.raffaini@polimi.it

Notes: