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Separation of chiral nanotubes with an opposite handedness by oligopeptide adsorption: A molecular dynamics study

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The separation of enantiomeric chiral nanotubes that can form non-covalent complexes with an unlike stability upon adsorption of chiral molecules is a process of potential interest in different fields and applications. Using fully atomistic molecular dynamics simulations we can study the adsorption and denaturation of an oligopeptide taken from human serum albumin formed by 16 chiral amino acids having a helical structure in the native state on both the inner and the outer surface of the chiral (10, 20) and (20, 10) single-walled carbon nanotubes having an opposite handedness, and of the armchair (16, 16) nanotube with a similar diameter for comparison. In the final adsorbed state, the oligopeptide loses in all cases its native helical conformation, assuming elongated geometries that maximize its contact with the surface through all the 16 amino acids. We find that the complexes formed by the two chiral nanotubes and the chosen oligopeptide have a strongly unlike stability both when adsorption takes place on the outer convex surface of the nanotube, and on the inner concave surface. Thus, the molecular simulations indicate that separation of chiral enantiomeric carbon nanotubes for instance by chromatographic methods can indeed be carried out using oligopeptides of a sufficient length. Moreover, membranes formed by aligned chiral single-walled carbon nanotubes of a given handedness might also act as chromatographic chiral selectors for appropriate racemic mixtures, with also possible application in the field of proteomics. The favorable protein–nanotube interaction would yield significantly different retention times.

Biography

Giuseppina Raffaini has received her Bachelor's degree in Chemistry and the Post-graduate Diploma at Advanced School in Polymer Science G. Natta; the inter-university Master's in Biomaterials in 2005 and PhD in Materials Engineering from Politecnico di Milano. In 2008, she became an Assistant Professor and Associate Professor in 2014 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. She is the co-author of 40 original peer-reviewed ISI papers (H-index Scopus=17), 2 invited reviews and 5 contributions to books.

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