MAR17-2016-020166

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Large Scale Molecular Simulation of Nanoparticle-Biomolecule Interactions and their Implications in Nanomedicine

RUHONG ZHOU, IBM Research and Columbia University

Nanoscale particles have become promising materials in various biomedical applications, however, in order to stimulate and facilitate these applications, there is an urgent need for a better understanding of their biological effects and related molecular mechanism/physics as well. In this talk, I will discuss some of our recent works, mostly molecular modelling, on nanotoxicity and their implications in de novo design of nanomedicine. We show that carbon-based nanoparticles (carbon nanotubes, graphene nanosheets, and fullerenes) can interact and disrupt the structures and functions of many important proteins. The hydrophobic interactions between the carbon nanotubes and hydrophobic residues, particularly aromatic residues through the so-called π-π stacking interactions, are found to play key roles. Meanwhile, metallofullerenol Gd@C82(OH)22 is found to inhibit tumour growth and metastases with both experimental and theoretical approaches. Graphene and graphene oxide (GO) nanosheets show strong destructive interactions to E. coli cell membranes (antibacterial activity) and Aβ amyloid fibrils (anti-AD, Alzheimer's disease, capability) with unique molecular mechanisms, while on the other hand, they also show a strong supportive role in enzyme immobilisation such as lipases through lid opening. In particular, the lid opening is assisted by lipase's sophisticated interaction with GO, which allows the adsorbed lipase to enhance its enzyme activity. The lipase enzymatic activity can be further optimized through fine tuning of the GO surface hydrophobicity. These findings might provide a better understanding of "nanotoxicity" at the molecular level with implications in de novo nanomedicine design.