Probing Biologically Relevant Solubility Parameters for Selected Nanoscale Building Blocks using Molecular Dynamics

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Recent reports have highlighted the potentially hazardous nature of nanomaterials. It has, for example, been shown that carbon nanotubes can accumulate in the lungs of rats and that buckminsterfullerenes (C60) can bind to and deform DNA sequences. For a particular substance to exhibit adverse physiological or environmentally adverse effects, it must energetically prefer an organic phase to an aqueous phase. In this work, calculating the Gibbs free energy of inserting such a particle in both phases, and comparing the energies in each solvent will help elucidate the compound's toxic potential from a thermodynamic point of view. In this work, nanoparticles from the fullerene and POSS family will be considered. POSS are of the molecular formula (SiO1.5R)8 where R is typically an organic functional group used to tether the POSS molecule to a polymer chain. POSS molecules have been proposed as building blocks for novel organic-inorganic hybrid nanocomposite materials. As a result a rapidly increasing number of POSS monomers are being synthesized and novel applications are continuously being proposed. However, at present, neither the thermodynamic properties of systems that contain POSS monomers, nor the environmental impact of POSS-based materials are satisfactorily understood. Fullerenes are carbon-based materials, very similar to graphite, with the exception that they contain 5-carbon unit rings in addition to 6 carbon unit rings. This prevents the planarity seen in graphite, resulting in spherical or cylindrical carbon structures.

We report molecular dynamics simulations to evaluate both the thermodynamic properties of both C60 and H-POSS molecules, and their potential environmental impact. We concentrate on the properties of nannoparticle systems at infinite dilution in order to compute the octanol/water partition coefficient, which is obtained

from the change in free energy for a particle being transferred from water to octanol. The change in free energy is prototypical to that of transferring the particle from water to a lipid bilayer.