

P039 Coarse-grained MD Simulations of Nanotube/Membrane Interactions

E.J. Wallace and M.S.P. Sansom

University of Oxford

Coarse-grained MD simulations of nanotube/membrane interactions are studied.

The motivation behind this work is in the context of e.g. insertion of nanotubes as 'pores' in biological membranes or use of nanotubes (NT) as templates to direct assembly of 'one-dimensional' lipid bilayers, both of which have clear applications in nanomedicine as potential nanosyringes.

Here we exploit recent developments in coarse-grained (CG) methodologies to explore interactions of NTs with membranes and detergents. The advantage of CG simulations is in the increase in speed, allowing the capture of NT/lipid or detergent self-assembly processes.

We have conducted preliminary CG self-assembly simulations of a simple model of a NT with detergent. Our simulations allow us to study the effect of systematically modifying the tube length and diameter on the self-assembly process.