

Abstract Submitted
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Molecular simulations of PEGylated lipids at interfaces: size selective dispersion of nanoscale objects MARIA SAMMALKORPI, SAMPISA VIERROS, Department of Chemistry, Aalto University, Finland, PAUL R. VAN TASSEL, Department of Chemical & Environmental Engineering, Yale University, USA, JUKKA MÄÄTTÄ, Department of Chemistry, Aalto University, Finland — Phospholipids and phospholipid derivatives offer efficient, noncovalent functionalization and dispersion of hydrophobic objects, e.g. therapeutic molecules and nanoparticles including carbon nanotubes (CNTs). However, the relation of lipid aggregates in bulk solution and in the presence of the object, and the resulting dispersion remain important questions. We employ here molecular dynamics simulations to explore PEGylated lipid aggregates at interfaces and the resulting dispersion efficiency. By varying lipid and substrate curvature, and the PEG chain length, we find 1) lipid-CNT and PEGylated lipid-CNT aggregation behavior consistent with recent experiments, 2) the assembled morphology to vary from micellar-like to tubular coating (phospholipids) and micellar to monolayer-like (PEGylated lipids) with the transition depending on lipid curvature and for PEGylated lipids also on the PEG chain length and CNT diameter, 3) aggregation morphology dependent CNT dispersion ability, and 4) good agreement between simulation and scaling theories of a brush-type PEG [1,2]. Finally, we discuss the implications to size-selective separation of hydrophobic particles and experimental observations.

[1] J. Chem. Eng. & Data 59 (10), 3080-3089 (2014).

[2] Soft Matter 9, 2136-2144 (2013).

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