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Polydots, Soft Nanoparticles, at Membrane Interfaces SIDATH WIJESINGHE, DVORA PERAHIA, Clemson University, CHRISTOPH JUNGHANS, Los Alamos National Laboratory, GARY GREST, Sandia National Laboratories — Luminescent polymers confined into long lived nano-configurations form dynamic nanoparticles (NPs) or polydots with a potential for new bio imaging markers and targeted drug delivery vehicles. A key step in the use of any NP for therapeutic applications is their translocation across membranes. Here we report the results of all-atom molecular dynamics simulation of a polydot that consists of carboxylate decorated dinonyl poly para phenylene ethynylene, at the interface with a 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) bilayer. The polydot size and surface charge are controlled by varying the polymer molecular weight and degree of carboxylation. The polydot structure and its effect on the membrane structure are probed. We find that the polydot remains stable as it transcends the membrane where the initial curvature of the membrane is strongly affected as polydot inserted, but it relaxes with time. The larger the polydots are the less dynamic the DPPC molecules become. Further we find that neutral-surface polydots reside in the center of the bilayer, while increasing the polydot surface charge, the polydot migrates towards the hydrophilic leaflet of the bilayer.

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