Abstract Submitted
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**Polydot at the interface with DPPC membrane: A Molecular Dynamics Simulation Study**[1] SIDATH WIJESINGHE, DVORA PERAHIA, Clemson University, GARY GREST, Sandia National laboratories, CHRISTOPH JUNGHANS, Los Alamos National laboratories — Luminescent polymers confined into long lived polydots are of potential interest because of their tunable properties and biocompatibility. These desired properties of polydots make them potential candidates for target drug delivering agents and bio markers. The first and foremost step in such applications is introducing these polydots to biological membranes which consist of different lipids whose collective dynamics mediate the cell membrane functions. Experimental studies suggest that their ability to penetrate cells depend on the polydot morphology, charge and the environmental characteristics including the type of the cell membrane. Here we report the results of an all atom molecular dynamics simulation of a carboxylate substituted dinonyl poly para phenylene ethynylene (PPE) polydot in one-component bilayer composed 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC). Introduction of a polydot into the DPPC membrane initially results in deformation of the membrane however after equilibrated, the membrane relaxes and the polydot is stable within the membrane.

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