Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Molecular dynamic simulations of hydrophilically decorated poly-dots SIDATH WIJESINGHE, DVORA PERAHIA, Clemson University, GARY S. GREST, Sandia National Laboratories — The structure and interfacial characteristics of nanoparticles formed by collapsed single conjugated polymer chains decorated with hydrophilic groups, poly *para* phenylene ethynylene (PPE) with substituted carboxylate side chains, have been studied by molecular dynamic simulations. These particles constitute a new type of light emitting/harvesting entities. Their interactions with the surrounding will determine their use where for example, directed interactions with membranes are essential for penetrating into organisms as bio markers. Trapping pre-decorated polymer chains into the nano dimensions with the expectations that some of the decorated groups will statistically reside at the nanoparticle interface has opened the way to control the surface decoration and hence the interactions of these particles. The effects of the distribution of the decorating groups along the polymer backbone on the conformation of the polymer chain within the poly dot and the resulting interfacial distribution of the COONa groups will be presented. The distribution of the hydrophilic groups at the surface of the particles will direct their interactions with the environment.

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Date submitted: 18 Nov 2011 Electronic form version 1.4