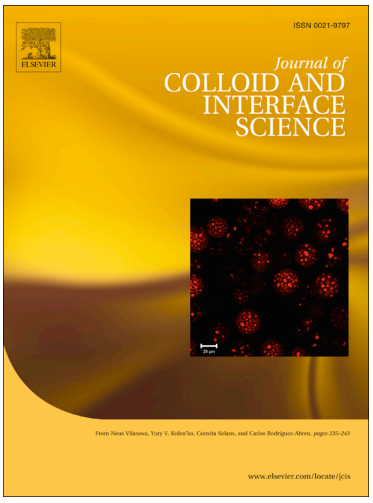

Regular Article

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PII: S0021-9797(17)30566-0
DOI: http://dx.doi.org/10.1016/j.jcis.2017.05.046
Reference: YJCIS 22353

To appear in: *Journal of Colloid and Interface Science*

Received Date: 2 April 2017
Accepted Date: 15 May 2017

Please cite this article as: J. Lin, H. Zhang, R. Dargazany, PEGylation on Mixed Monolayer Gold Nanoparticles: Effect of Grafting Density, Chain Length, and Surface Curvature, *Journal of Colloid and Interface Science* (2017), doi: http://dx.doi.org/10.1016/j.jcis.2017.05.046

PEGylation on Mixed Monolayer Gold Nanoparticles: Effect of Grafting Density, Chain Length, and Surface Curvature

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KEYWORDS: PEGylation, chain length, grafting density, surface curvature, aggregation, shielding ability

ABSTRACT PEGylation on nanoparticles (NPs) is widely used to prevent aggregation and to mask NPs from the fast clearance system in the body. Understanding the molecular details of the PEG layer could facilitate rational design of PEGylated NPs that maximize their solubility and stealth ability without significantly compromising the targeting efficiency and cellular uptake. Here, we use molecular dynamics (MD) simulation to understand the structural and dynamic the PEG coating of mixed monolayer gold NPs. Specifically, we modeled gold NPs with PEG grafting densities ranging from 0-2.76 chain/nm^2, chain length with 0-10 PEG monomers, NP