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Gold nanoparticle encapsulation into a mixed lipid nanodisk: molecular dynamics simulations HARI SHARMA, ZILU WANG, ELENA DORMIDONTOVA, Department of Physics and Institute of Materials Science, University of Connecticut, Storrs, CT — There is a growing interest in applications of nanoparticles in biomedicine. For practical applications of gold nanoparticles it is often desirable to encapsulate them into lipid nanocarriers. To this end it is important to understand gold-lipid interactions at the molecular level. We have performed coarse grained molecular dynamics simulations using a MARTINI force field of a lipid nanodisk composed of long and short tail lipids, DPPC and DHPC mixed in the ratio of 3:1 and studied its interaction with small gold nanoparticles (AuNP) functionalized with hydrophobic alkane tethers. We found that the inhomogeneous distribution of lipids in the nanodisk affects the outcome the AuNP-nanodisk interaction. The ordered arrangement of long chain lipids forming the interior region of the nanodisk are found to be less accessible for AuNP penetration compared to the rim of the nanodisk, where more mobile short lipids are located. Once encapsulated into a nanodisk, AuNP's have tendency to aggregate, especially if temperature is not too low. The results of computer modeling will be compared to experiment and the implications of our findings for experimental design of lipid nanocarriers for AuNP delivery will be discussed.

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