Abstract Submitted
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Self-assembly of Gold Nanoparticles Directed by Lipid Nanodiscs: Molecular Dynamics Study.[1] HARI SHARMA, ELENA E. DORMIDONTOVA, University of Connecticut — Metal nanoparticles with their unique physical properties have attracted growing attention for a variety of technological applications. Gold nanoparticles (AuNPs) in combination with lipid nanocarriers are an attractive platform for biomedical applications. Using molecular dynamics simulation with the MARTINI force field, we show that, self-assembled lipid nanodiscs can be used to direct aggregation of AuNPs into ring- or string-like structures. We found that equilibrium encapsulation of hydrophobically modified 1 nm AuNPs into mixed lipid nanodisc composed of dipalmitoylphosphatidylcholine (DPPC) and dihexanoylphosphatidylcholine (DHPC) occurs at the rim of the nanodisc leading to the formation of ring-like structures along the nanodisc circumference. Upon temperature increase, the order parameter of lipid tails decreases resulting in a spontaneous transition of nanodiscs into vesicles with embedded AuNP string or into an open "round vase" structure with a ring of AuNPs along the rim. The effect of the length of hydrophobic alkane tether (C_8, C_{12} and C_{16}) grafted to the gold surface on the stability of lipid nanodisc and clustering of AuNPs will be discussed and compared with experimental and computer simulation data.

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