Abstract Submitted
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Ligand-modulated interactions between charged monolayer-protected Au144(SR)60 gold nanoparticles in physiological saline[1] OSCAR VILLARREAL, LIAO CHEN, ROBERT WHETTEN, MIGUEL YACAMAN, Univ of Texas, San Antonio — We studied the interactions of functionalized Au144 nanoparticles (NPs) in a near-physiological environment through all-atom molecular dynamics simulations. The AuNPs were coated with a homogeneous selection of 60 thiolates: 11-mercapto-1-undecanesulfonate, 5-mercapto-1-pentanesulfonate, 5-mercapto-1-pentane-amine, 4-mercapto-benzoate or 4-mercapto-benzamide. These ligands were selected to elucidate how the aggregation behavior depends on the ligands' sign of charge, length, and flexibility. Simulating the dynamics of a pair of identical AuNPs in a cell of saline of 150 mM NaCl in addition to 120 Na+/Cl- counter-ions, we computed the aggregation affinities from the potential of mean force as a function of the pair separation. We found that NPs coated with negatively charged, short ligands have the strongest affinities mediated by multiple Na+ counter-ions residing on a plane in-between the pair and forming "salt bridges" to both NPs. Positively charged NPs have weaker affinities, as Cl counter-ions form fewer and weaker salt bridges. The longer ligands' large fluctuations disfavor the forming of salt bridges, enable hydrophobic contact between the exposed hydrocarbon chains and interact at greater separations due to the fact that the screening effect is rather incomplete.

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