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Internal Seminar

Conformational Equilibria of Organic Adsorbates on Nanostructures in Aqueous Solution: MD Simulations

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Atomistic molecular dynamics (MD) simulations of alkanethiol monolayer-protected gold nanoparticles[1,2] (GNPs) are performed in aqueous solutions at temperature 300K. Special focus has been given to the penetration depth of water and ions into the diffuse shell of alkanethiols as a function of grafting density, functionalization and chain length. Also, we focus on the formation of complexes between GNPs and surrounding ions and water. We study the orientation of water molecules inside the hydrocarbon chains (from surface of gold core to the terminal groups) and near the terminal groups. Hydrogen bonds and ionic contacts with terminal groups have been studied to observe the effect on the solvent structure of functionalization, grafting density and chain length. We modeled different types of GNPs with varying grafting density and chain length with nonpolar $-CH_3$ and polar $–COO^-$, $-NH_3^+$ and $-C(COO^-)(NH_3^+)$ termination. The solutions of GNPs with ionic terminations are neutralised by excess Na^+ and Cl^- ions. We show that the penetration of water and ions into the hydration shell increases with decreasing grafting density irrespective of the terminal group. High grafting densities leads to more extended hydrocarbon chains which behave more rigidly. Charged GNPs produce a long range effect in the surrounding solution structure. Orientation of water molecules within the hydrocarbon chain region of the solvated GNP leads to effective H-down configurations irrespective of termination.

REFERENCES

[1] A. K. Giri and E. Spohr, “Conformational Equilibria of Organic Adsorbates on Nanostructures in Aqueous Solution: MD Simulations”, Journal of Physical Chemistry C, 119, 25566-25575, (2015)
[2] E. Heikkila, et al. “Atomistic simulations of Functionalized Au144(SR)60 Gold nanoparticles in aqueous Environment”, Journal of Physical Chemistry C 116, 9805-9815 (2012)

Monday, Jul 4th 2016

4:30 PM (Tea/Coffee at 4:15 PM)

Seminar Hall, TCIS