Self-assembly of functional materials: Exploration with computational experiments

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In recent years, atomistic simulations became an indispensable modeling tool for exploring the self-assembly of novel functional materials, such as molecular tools to understand, target and cure diseases, porous membranes, or bulk materials with interesting properties. In my talk, I will first present our collaborative efforts to characterize and optimize nucleic acid-wrapped carbon nanotube (CNT) sensors of molecular biomarkers. Our classical and quantum mechanical molecular dynamics simulations explore how the nucleic acid conformations affect the CNT sensing response [1]. Second, I will present our research efforts in understanding self-assembly of ligated nanoparticles (NPs) at the liquid-air interface, where a variety of binary NP superlattices were prepared in recent experiments [2]. Our simulations revealed that NP self-assembly into different superlattices is a result of several effects. First, the coupling energies of NPs to solvent are found to be significant in comparison to NP-NP coupling energies. Second, NP ligand-solvent interactions govern submergence of NPs into solvents [3]. As a result, the solvent can organize the bottom layer of NPs that faces the solvent in a different way than in the bulk solution, leading to self-assembly of previously unknown superlattices.

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[2] T. Udayabhaskararao, T. Altantzis, L. Houben, M. Coronado-Puchau, J. Langer, R. Popovitz-Biro, L. M. Liz-Marzán, L. Vuković, P. Král, S. Bals, R. Klajn, Tunable porous nanoallotropes prepared from binary nanoparticle superlattices self-assembled at the solvent-air interface, Science, 358, 514-518 (2017).

[3] T. A. Nitka, P. Král, L. Vuković*, Configurations of floating and self-assembling nanocubes on liquid surfaces, *submitted* (2019).