



The Hebrew University Center
for Nanoscience & Nanotechnology



Nano Seminar

Modeling of Nanoparticles Self-assembly and Coupling with Biomolecular Complexes

Prof. Petr Král

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Abstract:

We present our hybrid modeling of nanoparticles (NPs) formation and self-assembly done in collaboration with several experimental groups. First, we briefly describe our quantum modeling of multistep nucleation and growth of gold NPs in liquid cells [1], where a spinodal separation, amorphous cluster formation, and crystallization steps have been observed. Then, we present our atomistic molecular dynamics (MD) simulations [2] and mean-field Monte Carlo [3] modeling of NPs self-assembly into chiral ribbons, hollow shells, magnetic helices, and nanoreactors. Finally, we briefly mention our MD simulations of selective multivalent coupling of NPs and functionalized nanoclusters with biomolecular complexes [4], HPV capsids and lectin Concanavalin A.

[1] N. Duane Loh et al., Nat. Chem. ASAP (2016).

[2] J. Yeom et al., Nat. Mat. 14, 66 (2015); H. Zhao et al., Nat. Nanotech. 11, 82 (2016); M. Yang et al., Nat. Chem. ASAP (2016).

[3] G. Singh et al., Science 345, 1149 (2014).

[4] A. E. Qian et al., Nat. Chem. ASAP (2016); submitted.

Gathering & Refreshments at 10:50

Please contact Alexandra Bannykh at 6584919 if you are interested in meeting the lecturer.

Monday, Dec 19th 2016, 11:00 at the Seminar Hall
Los Angeles Building, entrance floor.