Modeling the self-assembly of nanoparticle and nanorod superlattices

ALEXEY TITOV, PETR KRAL, University of Illinois at Chicago, PROF. KRAL'S RESEARCH GROUP TEAM — Colloidal semiconductor PbSe/CdSe nanoparticles (NP) of the sizes of 3-10 nm can self-assemble in fcc, hcp and single-hexagonal (sh) superlattices [1]. We model the Coulombic, van der Waals and steric interactions between these NPs to understand the exact conditions under which they can self-assemble in these lattice structures. Our simulations show that non-local dipoles of the NPs and their screening by the conducting substrate are both crucial for the sh lattice formation. We model analogously the self-assembly of semiconducting CdSe nanorods (NRs), realized also in the presence of electric fields [2], and the binary semiconducting-metallic nanoparticle superlattices [3].