

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Modeling the self-assembly of nanoparticle and nanorod superlattices ALEXEY TITOV, PETR KRÁL, University of Illinois at Chicago, PROF. KRÁL'S RESEARCH GROUP TEAM — Coloidal 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].

[1] D. Talapin, E. Shevchenko, C. B. Murray, A. Titov and P. Král, *Nano Letters* 7, 1213 (2007).

[2] A. Titov and P. Král, submitted.

[3] E. V. Shevchenko, D. V. Talapin, N. A. Kotov, S. O'Brien, C. B. Murray, *Nature* 439, 55-59 (2006).

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Date submitted: 13 Dec 2007

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