Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Self-assembly of polydisperse nanoparticles into monodisperse supraparticles: a computer simulation study TRUNG D. NGUYEN, University of Michigan, YUNSHENG XIA, National Center for Nanoscience and Technology, BYEONGDU LEE, Argonne National Laboratory, MING YANG, AARON SANTOS, University of Michigan, PAUL PODSIADLO, Argonne National Laboratory, ZHIYONG TANG, National Center for Nanoscience and Technology, SHARON C. GLOTZER, NICHOLAS A. KOTOV, University of Michigan — Experiments have shown that polydisperse inorganic nanoparticles such as CdSe, CdS and PbS self-assemble into highly uniform supraparticles with a core-shell morphology[1]. The self-assembly process is believed to be self-limiting as indicated by the time evolution of the measured surface potential and supraparticle size distribution. We performed molecular dynamics simulations to demonstrate that the balance between van der Waals attraction and Coulombic repulsion leads to the self-limiting growth of the supraparticles[2-4]. That the uniform supraparticles are stable over a wide range of density indicates that they are thermodynamically stable, rather than consequences of limited diffusion. Our simulation results further reveal that the broad nanoparticle polydispersity leads to the core-shell morphology of the supraparticles. The generic nature of the governing interactions suggests great versatility in the composition, size and shape of the constituent building blocks, and allows for a large family of hierarchical self-assembled structures, including colloidal crystals. References 1. Y. Xia et al, Nat. Nano. 6, 580, 2011. 2. Gonzalez-Mozuelos et al, J. Chem. Phys. 103, 3145, 1995. 3. Van Hyning et al, Langmuir 17, 3120, 2001. 4. J. Ramsden, Proc. R. Soc. Lond. A 413, 407, 1987

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Date submitted: 11 Nov 2011 Electronic form version 1.4