Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Structural and Excited States Properties of Semiconductor Nanoparticle-Organic Molecule Heterocomposites: Theoretical Modelling D. S. KILIN*, University of Washington, E. I. ZENKEVICH, Institut for Molecular and Atomic Physics, NAS Belarus , O.V. PREZHDO*, University of Washington, C. VON BORCZYSKOWSKI, Chemnitz University of Technology, Germany — Long fluorescence lifetime, slow electronic relaxation, and discretization of states of the wurzite CdSe semiconductor quantum dots are calculated by the ab initio methods. The electronic structure is affected by the differece in the core/surface atoms: The inner 4-coordinated atoms maintain the crystalline structure, surface 2- and 3- coordinated atoms link to each other in vacuum [Phys. Rev. Lett. **92** 217401 (2004)] or to the TOPO/thiol ligand groups in a solvent. According to the simulations, ligand groups are preferably attached to the 2-coordinated surface atoms that increases the VB-CB gap compare to the vacuum case. In contrast, a trial attachment of ligand groups to 3-coordinated atoms creates unphysical unoccupied states on the top of the valence band so that system gains metallic properties. The information on ligand-friendly sites is used to model the anchoring of the pyridyl-substituted tetrapyrrolic organic molecules to semiconductor nanoparticles that triggers additional energy-transfer relaxation pathways of the semiconductor optical excitations as compared to the experimental results on CdSe/ZnS-porphyrin nanocomposites [E. Zenkevich et al, J. Phys. Chem. B (in print)].

Dmitri Kilin
University of Washington

Date submitted: 08 Dec 2004 Electronic form version 1.4