Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Doping semiconductor nanocrystals: Theory S.C. ERWIN, M.I. HAFTEL, AL.L. EFROS, T.A. KENNEDY, Naval Research Lab, L. ZU, D.J. NORRIS, U. Minnesota — The intentional introduction of impurities into semiconductor nanocrystals (NCs) is a poorly understood process whose phenomenology remains largely unexplained. For example, Mn can easily be incorporated into ZnSe NCs using simple precursors, but not into CdSe NCs—despite comparable solubility limits of 50-60 percent in the two bulk crystals. The conventional wisdom is that NCs can "self-purify" by expelling impurity atoms to the nearby surface (consistent with the fact that very small NCs cannot generally be doped). Here we propose a very different view: namely, that doping is controlled by the initial adsorption of impurities on the NC surface. For NCs with sufficiently well-defined facets, this view leads to several striking predictions. (i) Dopant incorporation should depend on crystallography. For example, we predict that Mn incorporation will be generally allowed in zinc-blende NCs (such as ZnSe) but suppressed or absent in wurtzite NCs (such as CdSe). (ii) Very small NCs are often known to form cage clusters with strongly reconstructed surfaces. We find that these surfaces do not permit strong dopant adsorption, thus precluding incorporation. (iii) If the equilibrium NC shape can be controlled, doping may be externally tunable or even switchable. Hence, for II-VI NCs grown colloidally, we predict that dopant incorporation will vary with the II:VI concentration ratio in solution.

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Date submitted: 29 Nov 2004 Electronic form version 1.4