Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Computational Analysis of Core/Shell-like Structure Formation through Equilibrium Segregation in Ternary Compound Semiconductor Nanocrystals SUMEET C. PANDEY, TEJINDER SINGH, TRIANTAFILLOS J. MOUNTZIARIS, DIMITRIOS MAROUDAS, Dept. of Chemical Engineering, Univeristy of Massachusetts, Amherst — We present a computational analysis of equilibrium surface segregation in nanocrystals of $In_xGa_{1-x}As$, $ZnSe_{1-x}Te_x$, and $ZnSe_{1-x}S_x$. The analysis is based on coupled compositional, structural, and strain relaxation employing Monte Carlo and conjugate-gradient methods according to proper parameterizations within the valence-force-field (VFF) description. The VFF parameterizations are validated by comparisons of their segregation energy predictions with first-principles density functional theory (DFT) calculations. We report results for the equilibrium concentration distributions in the nanocrystals as a function of the compositional parameter x and nanocrystal size; the nanocrystal morphologies are polyhedral with distinct facets of low-index surface orientation as determined from DFT calculations of equilibrium crystal shapes. The results identify the particle-size and composition ranges that allow for assembly of core/shell-like nanocrystal structures with increased band-gap tunability.

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Date submitted: 25 Nov 2009 Electronic form version 1.4