# Electronic Structure of CdSe Quantum Dots and Ru Complexes

Victor V. Albert, Svetlana Kilina, and Sergei Tretiak
*T Division, Los Alamos National Laboratory*

We have attempted to determine the effect of ligands on the electronic structure and phonon-induced relaxation in semiconductor quantum dots (QDs). This includes creation and geometry optimization of QD systems passivated by different ligands [COO-, $OPCH_3$, $NH(CH_2)$, pyridines, and others]. We have also determined the effect of COOH and $CH_3$ ligands on the linear response spectra of Ru-based complexes. I am focusing primarily on calculations of the electronic structure and optical spectra of the systems. Binding energies and ionization potentials have also been calculated to analyze the effect of ligands on the opt-electronic properties of the QDs.