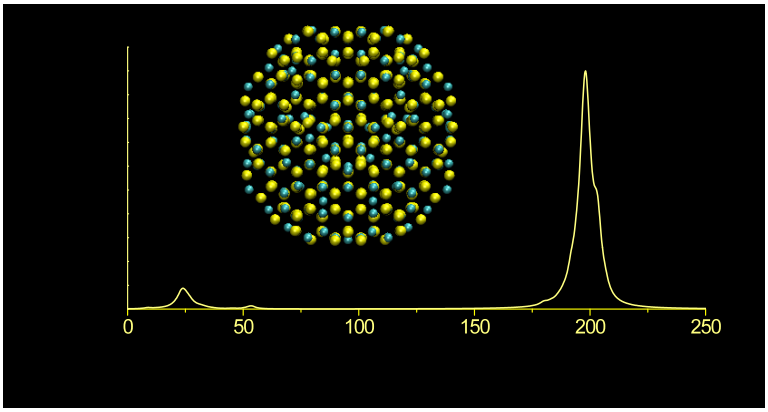
Computational study of phonons in nanocrystalline CdSe (**Mentor: Anne Myers Kelley**). The effects of quantum confinement on the electronic properties of semiconductor nanocrystals have been widely studied and are quite well understood, but far less attention has been paid to the phonons (vibrational modes). As electron-phonon coupling influences the optical spectra of these materials and helps to determine the rates of processes such as charge transfer across interfaces, hot carrier relaxation, and multiple exciton generation, it is important to have an accurate description of the phonons. This would also aid our ongoing experimental studies of the resonance Raman excitation profiles of CdSe nanocrystals.[1] Calculations of the phonons using an explicitly atomistic model[2] allow us to understand the Raman scattering lineshapes of CdSe nanocrystals in a way that was not achievable through traditional dielectric continuum theories. In this project, the student will extend our previous work to examine the phonon modes of CdSe nanocrystals with different shapes (*e.g.* rods versus spheres) and with semiconductor shells of varying thickness and composition. The Generalized Utility Lattice Program (GULP) used in our previous work will be employed to optimize the geometry and calculate the phonon frequencies and modes for each of a number of structures, and the Normal Mode Wizard plug-in to the University of Illinois Visual Molecular Dynamics program will allow the student to visualize the motions involved in each normal mode. This project could be suitable for students at any level and little background is required, although it is helpful for the student to have studied harmonic oscillators both classically and quantum mechanically.



(1) Baker, J. A.; Kelley, D. F.; Kelley, A. M. Resonance Raman and Photoluminescence Excitation Profiles and Excited-State Dynamics in CdSe Nanocrystals. *J. Chem. Phys.* **2013,** *139*, 024702.
(2) Kelley, A. M. Electron-Phonon Coupling in CdSe Nanocrystals from an Atomistic Phonon Model. *ACS Nano* **2011,** *5*, 5254-5262.