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Ligand Chemistry and the Low-Frequency Vibrations of Semiconductor Nanocrystals[1] ANNA JOLENE MORK, WILLIAM TISDALE, Massachusetts Institute of Technology — A variety of phonon-mediated processes centrally contribute to heat dissipation in colloidal quantum dot (QD) solids, and a method to tailor the QD vibrational spectrum may allow engineering of more efficient QD devices. Organic ligands, molecules attached to the surface of the inorganic core, are known to affect QD electronic transitions through the energy level alignment and degree of passivation; however, we demonstrate for the first time that ligands also affect the QD vibrational spectrum. We use low-frequency non-resonant Raman spectroscopy to non-destructively probe the acoustic phonon vibrational structure of CdSe QD cores with a variety of different attached ligands. The frequencies of the confined acoustic modes shift depending on the size and structure of the ligand, with more massive ligands resulting in red-shifted phonon energies. We develop a mathematical model based on vibrations of an elastic sphere to understand ligand-dependent shifts in the QD Raman spectrum upon ligand exchange. These data further our understanding of the factors affecting phonon energies and heat transport in QD solids.

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