COMPUTATIONAL RESEARCH in BOSTON and BEYOND SEMINAR

Interplay of Surface and Interior Modes in Exciton–Phonon Coupling at the Nanoscale

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ABSTRACT:

Quantum dots (QDs) are semiconducting nanocrystals that have been of much interest due to their highly tunable optoelectronic properties. These properties are greatly affected by coupling between excitons and phonons, or lattice vibrations, in these systems. Despite this, a microscopic picture of exciton-phonon coupling (EXPC) is still lacking, particularly regarding the magnitude and scaling with QD size, the dependence on phonon frequency, and the role of the QD surface. The computational complexity associated with accurately describing excitons and phonons has limited previous theoretical studies of EXPC to simplified models or very small QDs, which have limited transferability to experimental systems. Here, I will describe an atomistic approach for describing EXPC in QDs of experimentally relevant sizes. We validate our approach by calculating the reorganization energies, a measure of EXPC, for CdSe and CdSe-CdS core–shell QDs, finding good agreement with experimental measurements. We demonstrate that exciton formation distorts the QD lattice primarily along the coordinates of low-frequency acoustic modes. Modes at the NC surface play a significant role in smaller QDs while interior modes dominate for larger systems. This framework provides the foundation for ongoing work to compute phonon-mediated exciton dynamics in QDs.

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