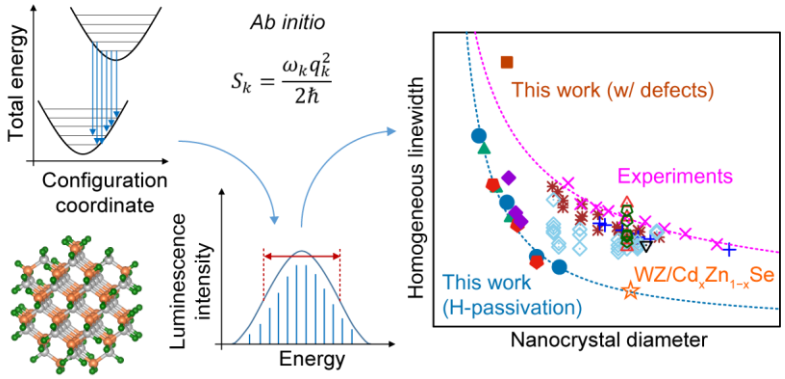
Emission lineshapes of QDs



Semiconductor nanocrystals, or quantum dots (QDs), have garnered enormous attentions in large panel displays (e.g. Samsung QLED TVs). In this application, a sharp emission spectrum is critical because it reflects monochromaticity. However, the experimental study of single-dot emission spectrum is challenging because of the small size of QD. In this work, we develop theoretical framework to calculate the emission spectra of QDs. To the best of our knowledge, this is the first attempt to evaluate the emission linewidths of NCs using ab initio methods. The role of shape, size and surface defects are studied within this framework. We find that the calculated FWHM is consistent with the result of the latest single-particle measurement for CdSe/CdxZn1−xSe core/shell QD. This work enables ones to predict the emission linewidth of QDs, which paves the way for designing QDs with an ultrasharp spectrum.