Quantifying the detectability of surface defects in $CuInS_2$ quantum dots through DFT-informed electron microscopy simulations

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Surface defects in semiconductor nanocrystals, such as reconstructions, vacancies, and adatoms, govern structural and electronic properties, and thereby their overall functionality. In $CuInS_2$ (CIS) quantum dots (QDs), these defects induce only subtle local lattice distortions that lie at the limits of what electron microscopy can detect, leaving a key question unanswered: Under what imaging conditions do these distortions become experimentally visible? Here, first-principles calculations are combined with electron microscopy (EM) image simulations to evaluate the detectability of surface defects in CIS QDs under experimentally relevant conditions. Representative CIS surface defect motifs are generated and relaxed using density functional theory (DFT). The resulting structures serve as the basis for multislice simulations of EM imaging modalities, including HR-TEM/HR-STEM and diffraction-based approaches such as 4D-STEM. Using a practical experimental parameter space, including accelerating voltage, probe size, convergence angle, detector geometry, and realistic electron dose limits corresponding to low signal-to-noise ratios, we calculate quantitative performance criteria for defect detection. By directly comparing pristine and defect-containing surface structures and quantitatively evaluating both real-space image contrast and reciprocal-space signatures, we generate a matrix of detectability describing the conditions under which subtle structural distortions in CIS QDs become experimentally resolvable. This matrix will allow for the selection of imaging modes that maximize sensitivity to specific defect classes at electron dose levels compatible with radiation-sensitive QDs. The result is a transferable, DFT-informed approach for predicting detection limits prior to experiments, providing clear guidance for the selection of imaging techniques and acquisition strategies when investigating subtle surface distortions in semiconductor quantum dots.