Facet-Oriented Coupling for Quantum Dot Photodetectors

Zhibo Wang

Department of Chemistry, University of Toronto, ON, Email: zhibo.wang@mail.utoronto.ca

The inter-dot coupling of quantum dots strongly influences the charge carrier transport between any two adjacent dots. This coupling is naturally dependent on the nature of the interface between two dots in their contact. For PbS colloidal quantum dots, the differences in surface passivation based on facets compound to discrepancies in coupling. As [111] facets are comprised of a single atomic species, they are readily passivated by surface ligands offering a buffer to the coupling in comparison to the self-passivating bare [100] facets. Thus, depending on the shape of these quantum dots, different facings can result from the random orientations. By analyzing which and how the facets of the individual crystals couple, it is possible analyze the efficacy of a dot's shape in device performance. To isolate the contributions from each potential arrangement, the coupling strength was modeled by density functional theory. The results find the arrangement with direct [100]:[100] facets to be the strongest coupled as expected with more cubic dots also achieving higher strengths. Classical packing simulations also show preferential [100]:[100] interfaces when applied as a thin film to a flat surface for the more cubic dots.