Ground and Excited State Properties of Cadmium Phosphide Quantum Dots

Omolola Eniodunmo and Svetlana Kilina

Department of Chemistry and Biochemistry, North Dakota State University

Semiconductor Quantum dots (QDs) are nanomaterials which have tunable optical properties and hold great promise as photoluminescent materials. These materials have the potentiality to span the visible red through the near-infrared spectral region which has attracted a lot of interests as it can be well adapted for use in many applications such as solar-cell devices, multiphoton imaging, electronic and photoelectronic devices. So far, only a few semiconductor materials can be tuned by their nano size to address this spectral range (600nm-1200nm), and cadmium phosphide (Cd_3P_2) is among them. The Cd_3P_2 semiconductor has a small direct band gap, relatively high dielectric constant, and large exciton Bohr radius. However, limited knowledge on the optical properties of Cd_3P_2 QDs is currently available. We computationally study the ground and excited state properties of Cd_3P_2 QDs (~ 1.5 nm in size) using density functional theory-based methods. We consider carboxylic and phosphine groups as the surface passivation ligands of these QDs since the electronic structures of QDs surface has been highlighted as a key to understanding their photoactivity. We investigate how the electronic structure and optical response of Cd_3P_2 QDs are affected by varying their size and the surface passivation ligands. Obtained insights into the QD's surface chemistry will help to guide the control of their optical properties via chemical means.