# Optical features of ligated semiconducting quantum dots subjected to an electric field

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**Abstract:** Semiconducting quantum dots (SQDs) are attractive materials for optoelectronic applications due to the size-tunable band gaps, colloidal stability, and low-cost solution processability. In this article, we investigate the modulations in the optical features of COOH + NH3 capped tetrahedral-shape CdSe SQD in response to the external electric field. We base our calculations on an approach which combines the linear combination of atomic orbitals (LCAO) real-time-propagation-time-dependent density functional theory (*rt*-TDDFT) technique (LCAO-*rt*-TDDFT) and transition contribution maps (two-dimensional visualization of Kohn–Sham single electron–single hole transitions). Among other insights, our study indicates that electric field causes a redistribution of the oscillator strengths, early onset of absorption, and ligand-derived trap states near the top of the valence band. These theoretical findings explain the origins of the electric field induced optical features of ligated SQDs.