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The surface passivation effects on the optical response of small CdTe quantum dots OSMAN BARIS MALCIOGLU, JEAN-YVES RATY, University of Liege — In this work, the optical properties of various small-sized CdTe based quantum dots are investigated using time dependent density functional formalism. `turboTDDFT`, an implementation of the Lanczos-Liouville approach to linearized time-dependent density-functional theory, designed to simulate the optical spectra of molecular systems made of up to several hundreds atoms and distributed as a part of the open source `QUANTUM ESPRESSO` project is used. The response of the clusters at ambient temperature is estimated by performing averages of the optical spectra along the molecular dynamics trajectories. Different types of surface passivation schemes are considered in forming the quantum dot structures. Solvent effects on the surfaces that result from different passivation schemes are considered in detail using an explicit solvent approach.

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