

Abstract Submitted  
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**Excitonic effects and optical properties of passivated CdSe clusters**<sup>1</sup> MARIE LOPEZ DEL PUERTO, University of Minnesota, MURILO TIAGO, JAMES CHELIKOWSKY, University of Texas at Austin — We calculate the optical properties of a series of passivated non-stoichiometric CdSe clusters using two first-principles approaches: time-dependent density functional theory within the local density approximation, and many-body methods, based on computing the self-energy in the GW approximation and solving the Bethe-Salpeter equation for optical excitations. We analyze the character of optical excitations leading to the first low-energy peak in the absorption cross-section of these clusters. Within time-dependent density functional theory, we find that the lowest-energy excitation is mostly a single-level to single-level transition. In contrast, many-body methods predict a strong mixture of several different transitions, which is a signature of excitonic effects. We also find that the majority of the clusters have a series of dark transitions before the first bright transition. This may explain the long radiative lifetimes observed experimentally for these clusters. Reference: PRL 97, 096401 (2006).

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