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Insights of the Ultrafast Charge Transfer Process in CdSe Quantum Dot/Organic Molecule System: A Real-Time Time-Dependent Ab Initio Study. ZHI WANG, JAN-PHILIP MERKL, MONA RAFIPOOR, HOLGER LANGE, Institute of Physical Chemistry, University of Hamburg, LIN-WANG WANG, Lawrence Berkeley National Laboratory, GABRIEL BESTER, Institute of Physical Chemistry, University of Hamburg — We report for the first time a real-time time-dependent density function theory (rt-TDDFT) simulation on experimental size CdSe quantum dot/organic molecule system, to analyze its ultrafast (femtosecond to sub-picosecond) photoexcited charge transfer (CT) dynamics. Non-adiabatic dynamic details, such as the size-dependence of CT process, the carrier separation and cooling, the electron-phonon interaction and Auger-assisted process are presented using our high-efficient rt-TDDFT package. Our results are in excellent agreement with experiment data.

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