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Quantum dots – artificial atoms, large molecules, or small pieces of bulk? Insights from time-domain ab ignition studies

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Quantum dots (QD) are quasi-zero dimensional structures with a unique combination of solid-state and atom-like properties. Unlike bulk or atomic materials, QD properties can be modified continuously by changing QD shape and size. Often, the bulk and atomic viewpoints contradict each other. The atomic view suggests strong electron-hole and charge-phonon interactions, and slow energy relaxation due to mismatch between electronic energy gaps and phonon frequencies. The bulk view advocates that the kinetic energy of quantum confinement is greater than electron-hole interactions, that charge-phonon coupling is weak, and that the relaxation through quasi-continuous bands is rapid. QDs exhibit new physical phenomena. The phonon bottleneck to electron energy relaxation and generation of multiple excitons can improve efficiencies of photovoltaic devices. Our state-of-the-art non-adiabatic molecular dynamics techniques, implemented within time-dependent density-functional-theory, allow us to model QDs at the atomistic level and in time-domain, providing a unifying description of quantum dynamics on the nanoscale.