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APPLICATION/TECHNOLOGY-INSPIRED DESIGN OF QUANTUM DOT MODELS FOR ELECTRON DYNAMICS SIMULATIONS

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Quantum dots (QDs) are semiconducting nanoparticles important due to their size-tunable excitation energy and other optical properties. Self-assembled (SA) QDs are one of the most promising building blocks for future quantum information processing, as they can host optical, electronic, or spin qubit states with a decent lifetime1,2.
Qubit switching itself is a dynamical process which is, e.g., driven by external electromagnetic fields. Various electronic decay processes may shorten the lifetime of qubit states in QDs. To model such processes in QDs we seek to apply the multiconfiguration time-dependent Hartree (MCTDH)3 algorithm in an antisymmetrized version for describing electronic processes as the Auger decay4 known for SA-QDs and the interatomic Coulombic decay (ICD)5.
The intent of this initiating study is to develop a model system for SA-QDs 6. Given previous results, Gaussians are suitable, because such finite binding potentials can capture the continuum-like properties of the environment of a QD embedded in an extended wetting layer. Its parametrization is benchmarked with respect by experimental sizes and energies.
We are also aiming, for future projects, in the description of silicon QDs, colloidal QDs because if we want to include an exciton recombination in our description, we have to adjust the model to observables in the experiment (QD size, optical gap, etc.)

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Category

Solid State (Experiment)

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