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Nonadiabatic Dynamical Studies of Lead Chalcogenide Quantum Dots ($Pb_{16}X_{16}$; X = S, Se, Te) Passivated with thin Cadmium Chalcogenide Shells PATRICK TAMUKONG, SVETLANA KILINA, North Dakota State University — DFT and TDDFT studies of $Pb_{16}X_{16}/Cd_{52}Y_{52}$ (X, Y = S, Se, Te) Core/Shell quantum dots (QDs) have been performed to assess their ground (i.e., the optimized geometries, density of states, projected density of states, and optical absorption spectra), and excited state properties. Most of the heterostructures were analyzed for the first time (e.g., $Pb_{16}S_{16}/Cd_{52}Te_{52}$ and $Pb_{16}Te_{16}/Cd_{52}Se_{52}$). The thin shell core/shell QDs proved to be largely borderline type II with much similarly between QDs containing $Cd_{52}S_{52}$ and $Cd_{52}Se_{52}$ shells, whereas core/shell QDs with a $Cd_{52}Te_{52}$ shell appeared to be borderline type-I. Nonadiabatic DFT-based dynamics, coupled with the surface hopping method, have been done to investigate fates of excited electrons or holes in these systems.

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