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Optical properties of semiconductor nanocrystals in the tight-binding (TB) approximation ANDREW SHABAEV, EUGENE TSIPER, ALEXANDER EFROS, DIMITRIS PAPACONSTANTOPOULOS, Naval Research Laboratory and George Mason University — Tight-binding (TB) approach is very attractive for computing electronic properties of semiconductor nanocrystals since it can handle large numbers of atoms, and since nanocrystals of arbitrary shape can be studied. TB approach provides realistic boundary conditions at the surface, which are often defined with uncertainty in the effective mass approximation. This is especially important in small nanocrystals, where a large fraction of atoms belongs to the surface. For example, in a 1000-atom Si nanocrystal about 2/3 of all atoms have less than four nearest neighbors. Successful TB approaches, such as NRL-TB method, exist to compute electronic structure of various bulk materials. We use NRL-TB to compute electronic transitions in nanocrystals of arbitrary shape. It appears, that a given TB parameterization that yields adequate electronic structure is incomplete in terms of predicting oscillator strengths of the transitions, in contrast to a common belief. Such TB parameterization must be augmented with additional quantities that contribute to the transition dipole matrix elements between localized orbitals. We thus resolve the existing controversy, despite the arguments that these extra contributions are problematic and should not be incorporated into TB. We also discuss practical ways to calculate the extra quantities, which are not supplied by the conventional TB parameterizations.

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