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Time-Dependent Density Functional Calculations for Optical Excitations in Nanoscale Materials.[1]

IGOR VASILIEV, New Mexico State University

Optical properties play a crucial role in our understanding of the electronic structure of nanoscale materials. Despite significant progress in the development of computational methodologies, first principles calculations for optical excitations in nanomaterials remain extremely difficult. While the ground-state electronic structure formalism is relatively well established, calculations for excited states present major challenges to theoretical methods traditionally employed by condensed matter physics and quantum chemistry. This talk focuses on recent advances in a computational technique based on time-dependent density functional theory (TDDFT). Within the TDDFT method, electronic transition energies and oscillator strengths are obtained in the framework of linear response theory by solving a frequency-dependent equation for the dynamic polarizability. The linear-response TDDFT formalism is applied to compute the excitation energies and absorption spectra for a variety of nanoscale systems, including molecules, atomic clusters, semiconductor quantum dots, functionalized carbon nanotubes, and nanotube-polymer composites. The TDDFT approach is compared to other first principles computational methods for excited states and discussed in terms of accuracy, efficiency, and computational cost.

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