CORE-CM SEMINAR
Michigan State University — Department of Chemistry and Department of Physics and Astronomy

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Multiscale Modeling and Computation of Optically Manipulated Nano Devices

Abstract

We present a multiscale modeling and computational scheme for optical- mechanical responses of nanostructures. The multi-physical nature of the problem is a result of the interaction between the electromagnetic (EM) field, the molecular motion, and the electronic excitation. To balance accuracy and complexity, we adopt the semi-classical approach that the EM field is described classically by the Maxwell equations, and the charged particles follow the Schrödinger equations quantum mechanically. To overcome the numerical challenge of solving the high dimensional multi-component many-body Schrödinger equations, we further simplify the model with the Ehrenfest molecular dynamics to determine the motion of the nuclei, and use the Time-Dependent Current Density Functional Theory (TD-CDFT) to calculate the excitation of the electrons. This leads to a system of coupled equations that computes the electromagnetic field, the nuclear positions, and the electronic current and charge densities simultaneously. In the regime of linear responses, the resonant frequencies initiating the out-of-equilibrium optical-mechanical responses can be formulated as an eigenvalue problem. A self-consistent multiscale method is designed to deal with the well separated space scales. The isomerization of Azobenzene is presented as a numerical example.

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