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First-Principles Description of Strong Electromagnetic Fields in Solids

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Interactions between light and matter are usually described by two theories: Macroscopic Maxwell equations describe propagation of a light in a medium, while quantum calculation of susceptibilities such as dielectric function is one of central issues in the first-principles calculation. Recent progresses of laser technologies, however, require theories beyond it. Strong electromagnetic fields of a laser pulse induce extremely nonlinear electron dynamics which no more allows perturbative separation between macroscopic electromagnetic fields and microscopic electron dynamics. We have recently developed a multi-scale theory for this problem, describing electron dynamics in solid using real-time time-dependent density functional theory. This theory provides a quite general and computationally feasible basis for the problem, including ordinary macroscopic electromagnetism in a weak field limit and being applicable to problems involving arbitrarily intense fields. In my presentation, I will discuss the basic theory, computational implementation, and physics applications of our new approach.