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Maxwell+TDDFT multiscale method for light-matter interaction: light propagation in the microscopic semiconducting crystal

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Due to the rapid growth of the computing resources, the large-scale simulation of the light matter interaction between the microscopic objects and intense light field becomes possible. The first principle time-dependent density functional theory (TDDFT) is a powerful tool to compute the optical properties of solids in the intense electric field. On the other hand, the finite-difference time-domain (FDTD) is also well used to solve the electromagnetic field problems by the microscopic materials. In this work, we have been developing the Maxwell+TDDFT multiscale technique combining the TDDFT and FDTD method to treat propagation and scattering of the intense laser pulses. In our approach, the light field is calculated by the FDTD-like formalism defined on the macroscopic grid. At each macroscopic point, the TDDFT based electron dynamics calculation is employed. At this time, we will introduce the demonstration of this method to problems that require 1D, 2D, and 3D description for light propagations.

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