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Maxwell+TDDFT multiscale method for light propagation in thin-film semiconductor[1] MITSUHARU UEMOTO, KAZUHIRO YABANA, Center of Computational Sciences, University of Tsukuba — First-principles time-dependent density functional theory (TDDFT) has been a powerful tool to describe light-matter interactions and widely used to describe electronic excitations and linear and nonlinear optical properties of molecules and solids. We have been developing a novel multiscale modeling to describe a propagation of light pulse in a macroscopic medium combining TDDFT and Maxwell equations. In the method, the finite-difference time-domain (FDTD)-like electromagnetism (EM) calculation is carried out in a macroscopic grid. At each grid point, the time-dependent Kohn-Sham equation is solved in real time. In the presentation, we show applications of this method to the 1D/2D propagations of femtosecond laser pulses through a thin-film semiconductor.

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