Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

Monday, January 15th, 2018 – 10:45 a.m.
CFEL Seminar room III (Bldg. 99)

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TDDFT+Maxwell multiscale method for light propagation calculation in semiconducting media

The first principle time-depend density functional theory (TDDFT) calculation has been a powerful tool to simulate the light-matter interaction in quantum mechanical level and widely used to determine microscopic optical properties (e.g., the oscillator strength and hyperpolarizability) of the molecule or solid. However, the ordinary TDDFT have not applied for the macroscopic optical problem (e.g.,light propagation and penetration and scattering in the bulk media). In this study, a multiscale simulation method, which combines the TDDFT and electromagnetics (EM) calculation, has been worked out. In our approach, the microscopic electron dynamics is provided by the TDDFT, and the macroscopic light propagation is provided by finite-difference-time-domain (FDTD)-like EM method. In the presentation, we show applications of this method to the 1D/2D propagations of femtosecond laser pulses through a thin layer crystals.The computation is performed by the open source TDDFT code SALMON [1] developed by our group.In this time, I will introduce the recent calculations in our investigation.

[1] Scalable Ab-initio Light-Matter simulator for Optics and Nanoscience (SALMON) http://salmon-tddft.jp/

Host: Angel Rubio

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