Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

Tuesday, December 10th, 2019 – 11:00 am
CFEL Seminar room IV (Bldg. 99)

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First-principles description for light-matter interaction in thin materials: From linear response to HHG spectrum

We present a comprehensive theoretical framework for interaction of an ultrashort light pulse with a thin material based on the time-dependent density functional theory (TDDFT) [1] . We introduce a microscopic description solving the Maxwell equations for the light electromagnetic fields and the time-dependent Kohn-Sham equation for the electron dynamics simultaneously in the time domain on a common real-space grid. This scheme can simulate the light-matter interaction in thin films irrespective of the film thickness and the light intensity. For two limiting cases of extremely thin and sufficiently thick films, we develop approximate schemes. For the former, a 2D macroscopic description is developed: a 2D response functions are introduced for a weak field, while time evolution equation is derived for an intense field. For the latter, the 3D macroscopic description coincides with the ordinary electromagnetism with the 3D bulk response functions for a weak field, or the multiscale Maxwell-TDDFT scheme [2] for a strong field, which our group developed previously. In this talk, we show results for Si thin films and discuss the applicability of the microscopic and macroscopic descriptions. Furthermore, we applied the above schemes to calculation of high-harmonic generation (HHG) in reflected and transmitted waves from the Si films exposed to intense light pulse. We discuss a thickness dependence of HHG spectrum and a difference of results between the microscopic and the multiscale schemes.

[1] S. Yamada et al., PRB 98, 245147 (2018).
[2] K. Yabana et al., PRB 85, 045134 (2012).

Host: Shunsuke Sato, Angel Rubio

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