First-principles Simulation for Attosecond Optical Response of Solids

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We develop a novel simulation method in the field of optical science that describes light-matter interactions in strongly coupled systems of light and electrons. It is based on first-principles calculations in materials science. We develop our computer code SALMON (Scalable Ab-initio Light-Matter simulator for Optics and Nanoscience) as an open source software and is available through the web site, http://salmon-tddft.jp. We expect SALMON will be widely used among researchers in optical science and will be recognized internationally as a basic and useful tool in the field.

At the core of our simulation, we calculate electron dynamics in matters induced by a pulsed electric field, employing real-time and real-space method in the first-principles framework. We further combine the electron dynamics calculation with the propagation calculation of light electromagnetic fields.

Among frontiers of optical science in which SALMON is expected to be useful, we have applied it to fundamental physics and applications including attosecond science and nonthermal laser processing. Experimental studies in these fields have been actively carried out in laboratories in universities and large experimental facilities such as XFEL. Recently, we have explored changes of optical properties of diamond in a time scale less than a femtosecond. Fig. 1 shows computational scheme of our calculation, and Fig.2 shows comparison between experiments and calculations of ultrafast changes of absorptive property of diamond induced by a few cycle pulsed light.

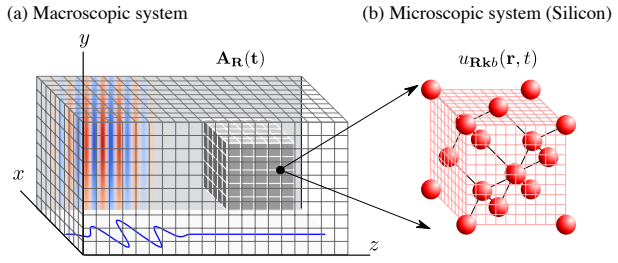

Fig.1: Grid systems to be used in the multiscale first-principles calculations that describe dynamics of electrons and electromagnetic fields simultaneously.

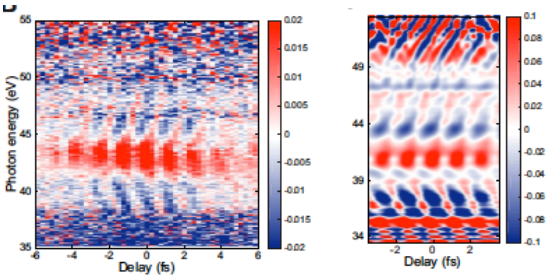

Fig.2: Absorption change of diamond in time scale less than a femtosecond. (Left) Experiment done at ETH, (Right) Our simulation.

Bibliography

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[3] M. Lucchini et.al; Science **353**, 916 (2016).

External links

http://salmon-tddft.jp