First-principles electron dynamics calculations under strong electromagnetic fields

A TALK BY PROF. KAZUHIRO YABANA

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The time-dependent density functional theory (TDDFT) is known to provide a fair description of light-matter interaction with reasonable computational costs. We have been developing a first-principles computational method for electron dynamics in crystalline solid induced by light pulses based on the TDDFT. In my presentation, I would like to present our computational method and applications to electron dynamics in dielectrics induced by intense and ultrashort laser pulses. In theoretical side, I discuss time-dependent calculations of orbitals and polarization [1]. I also discuss a multiscale implementation for a coupled dynamics of macroscopic electromagnetic fields and microscopic Kohn-Sham orbitals [2]. As applications, I will show analyses of coherent phonon generation [3], dense electron-hole pair generation and optical breakdown [4], and propagations, reflections, transmissions of intense laser pulses [2].

[1] G.F. Bertsch, J.-I. Iwata, A. Rubio, K. Yabana, Phys. Rev. B62, 7998 (2000).
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[3] Y. Shinohara, K. Yabana, Y. Kawashita, J.-I. Iwata, T. Otobe, and G.F. Berstch, Phys. Rev. B 82, 155110 (2010)
[4] T. Otobe, M. Yamagiwa, J.-I. Iwata, K. Yabana, T. Nakatsukasa, G.F. Bertsch, Phys. Rev. B77, 165104 (2008).