Predicting semiconductor's behavior upon ultrashort laser irradiation using quantum simulations, supercomputers and machine learning.

Thibault J.-Y. Derrien – Group of Ultrafast Photonics (Department of Scientific Laser Applications)

Developing controllable applications based on intense laser light requires a deep knowledge of the physical processes taking place after but also *during* the intense irradiation. For example, laser structuring of materials by femtosecond laser pulses usually involves laser field strengths close to 1 V/nm, a situation known as "strong field" or "beyond perturbative" regime that calls for quantum analyses [1]. In this context, *ab-initio* simulation methods, such as time-dependent density functional theory (TDDFT) are powerful for gaining quantitative knowledge about dynamics of such processes from a quantum perspective and for predicting material's reaction to intense laser light.

In this seminar, with the aid of national and European supercomputers, I will show how the dynamics of electrons in band-gap materials irradiated by ultrashort laser pulses can be revealed using the TDDFT. In a first example, the TDDFT was employed for describing the excitation dynamics of silicon by powerful ultrashort laser pulses in a wide range of irradiation parameters [2] using a realistic band structure. This work resulted in a dataset on the excitation rates which are valid for the regimes of laser-matter interaction where widely spread two-band theories are not applicable. This work enables to introduce the TDDFT simulated parameters with quantum features into simplified classical models, thus considerably improving them for addressing the real experimental scales. In particular, training an algorithm with the obtained dataset [3] enabled to establish a direct bridge between the quantum and the large scale simulations at reduced cost.

As a second example, TDDFT was employed to predict the ultrafast electrical current resulting from the ultrashort laser irradiation of silicon. Using this current, the spectrum of photons that are emitted by the sample upon phase-stabilized few-cycle laser irradiation was predicted. The simulation results were in very good agreement with the experiments performed by the Charles University [4], enabling the capacity for HiLASE to predict spectra of high harmonics generation from solids irradiated by ultrashort laser pulses. It also demonstrates the reliability of the TDDFT for predicting behavior of materials under powerful laser irradiation in the regimes that cannot be addressed by widely known simplified approaches.

The obtained results demonstrate the adequacy of quantum simulation techniques for revealing new control parameters that can be useful for development of novel applications based on ultrashort laser pulses. As a whole, high-power computing (HPC) and *ab-initio* theories are proving to be a solid ground for studies and applications of ultrafast photonics.

[1] Derrien, T. J.-Y.; Levy, Y. & Bulgakova, N. M. Chapter 1 in *Ultrafast Laser Nanostructuring - The Pursuit of Extreme Scales*, *Springer*, 2023.
[2] Derrien, T. J.-Y.; Tancogne-Dejean, N.; Zhukov, V.; Appel, H.; Rubio, A. & Bulgakova, N. M. *Phys. Rev. B* **104**, L241201 (2021).
[3] Special session "Machine Learning and Simulation for Laser Processing", Laser Precision Microfabrication (LPM), Japan (2023).
[4] Suthar, P.; Trojánek, F.; Malý, P.; Derrien, T. J.-Y. & Kozák, M. *Comm. Phys.*, **5**, 288 (2022).

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