Postdoc Position

Density Functional Theory for ultrafast dynamics of photo-excited silica glasses

A postdoctoral position is available for up to 3 years (renewable each year) at Laboratoire Hubert Curien (LabHC) in Saint-Étienne, France. The postdoc will work in the framework of the international project funded by French National Research Agency in collaboration with the Max Born Institute of Berlin, Germany. LabHC is jointly run by the CNRS (The French National Center for Scientific Research) and Jean Monnet University (member of University of Lyon).

Objectives: The postdoc research program is aimed to elucidate primary pathways of light-matter energy coupling during the ultrafast laser pulse interaction with a dielectric material such as silica. The photo-excitation processes and electronic structure evolution at quantum level will be investigated by ab initio density functional theory (DFT) and time-dependent DFT (TDDFT). The ambition is to enhance our knowledge of fundamental processes at ultrashort timescale during the laser pulse which are not considered today by the commonly-used modeling approaches in laser processing of dielectrics. In particular, the band distortion and energy transfer to the lattice via polarization coupling and vibrational activation will be targeted. The simulation results should be able to provide interpretation of experiments, revealing the strong field physics beyond linear response for a realistic band structure under a wide variety of thermodynamic and photo-excitation conditions.

Research program: The experiments will be performed at the Max Born Institute (time-resolved spectral interferometry for probing the band distortion during the laser pulse and time-resolved vibrational spectroscopy for energy transfer). The postdoc will work closely with the experimentalists to interpret and guide experiments. Two computing strategies will be considered:

- **DFT/TDDFT simulations.** The capacities of TDDFT will be explored to model an irradiated amorphous dielectric (silica glass). To discriminate between band distortion and excited electron-hole population effects, a many-body perturbation theory will be combined with TDDFT. TDDFT combined with molecular dynamics will allow for nonadiabatic coupling to analyze electron-phonon energy transfer.
- **Kinetics of relaxation.** To overcome TDDFT current limits in describing explicitly collisional effects, other approaches such as DFT+GW, Boltzmann transport or Maxwell-Bloch formalism could be implemented. The objective is to provide a microscopic evolution of the electron-electron (for thermalization and avalanche ionization processes), electron-hole interaction and recombination.

**Keywords:** DFT, TDDFT, Density Functional Theory, Molecular Dynamics, Ultrafast laser, Simulation, Theory

**Qualifications:** We are seeking a highly motivated candidate for working at the interface between condensed matter physics and photonics. The candidate should hold a PhD in physics or closely related field no later than May 2020. The candidate must have academic records/publications in the field of quantum mechanics, solid-state physics or nonequilibrium thermodynamics. Additional programming skills (C, Python, Fortran, Matlab, etc.) are requested.

**Start date:** April-May 2020

**Salary conditions:** monthly net salary 2000-2500€ depending on experience and skills.

**How to apply:** Interested candidate should send a CV and a short cover letter to:
Pr. Jean-Philippe Colombier (jean.philippe.colombier@univ-st-etienne.fr) & Dr. Elena Silaeva (elena.silaeva@univ-st-etienne.fr)

**Application deadline:** March 1st, 2020.