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Agenda for the visit of
Prof. Kazuhiro Yabana
Center for Computational Sciences, University of Tsukuba, Japan

September 2023, 18th

13:45   Arrival

14:00 – 14:15   Welcome words & presentation of HiLASE Centre,
                MSc. Sanin Zulić, International Business Development Manager at HiLASE.

14:15 – 15:00   „Time-dependent density functional theory for extremely nonlinear optics" (see abstract below)
                Prof. Kazuhiro Yabana, Center for Computational Sciences, University of Tsukuba, Japan.

15:00 – 15:20   Overview of activities of the *Scientific Laser Applications (SLA) department: theory vs experiments*
                Prof. Nadezhda M. Bulgakova, head of SLA department at HiLASE.

15:20 – 15:40   Overview of TDDFT simulation activities at HiLASE
                Dr. Thibault J.-Y. Derrien, leader of „Ultrafast Photonics" group of SLA.

15:40 - 16:00   Coffee break

16:00 – 17:00   Lab tours

17:00 – 18:00   Free discussions

18:00 – End of meeting

Time-dependent density functional theory for extremely nonlinear optics

Prof. Kazuhiro Yabana

Center for Computational Sciences, University of Tsukuba, Japan

For a strong pulsed light, coupling of light electromagnetic field and motion of electrons cannot be treated by perturbation theory. Theory and computations solving simultaneously the coupled system of Maxwell's equations for light propagation and time-dependent Schrodinger equation for electronic motion are required. In my presentation, I would like to show our efforts in this direction extending the first-principles density functional theory calculations. I first explain that two schemes have been developed to describe the coupled motion, corresponding to macroscopic and microscopic descriptions in electromagnetism. We then show some applications of the scheme, taking from (1) a systematic view for the change of optical response from linear response for which the band structures of materials determine, to extremely nonlinear regimes where plasma reflection dominates. (2) energy transfer and carrier generation in intense and ultrashort laser pulse irradiation on solids, (3) generation and detection of coherent phonons, and (4) generation and propagations of high harmonics from solids.