Theoretical investigation of high harmonic generation from liquid water

Zahra Nourbakhsh[1], Ofer Neufeld[1,2], Nicolas Tancogne-Dejean[1], and Angel Rubio[1,3,4]

[1] Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany.

[2] Physics Department and Solid State Institute, Technion - Israel Institute of Technology, Haifa, 320003, Israel.

[3] Nano-Bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del País Vasco UPV/EHU, 20018, San Sebastián, Spain.

[4] Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York, New York 10010, USA.

Liquids are promising systems in ultrafast technology since they gather the advantages of both solids and gases in one material. Liquids are condensed systems, that, like gases, can tolerate high intense driven pulses. We study the non-perturbative interaction of intense infrared laser pulses with liquid water to investigate its high-harmonic emissions. Our method is on the basis of real-time density functional theory. The liquid water structure is reproduced using Car-Parrinello molecular dynamics simulation. Our calculations predict the generation of high harmonics up to extreme ultraviolet energies. Similar to solids, the harmonic cutoff scales linearly with the peak field strength; and it is independent of pulse wavelength. In addition, we discuss the impact of nuclear dynamics during the pulse radiation on harmonic emissions. By considering two structures of ice, cubic and hexagonal, we also show how harmonic emission is reduced in liquid water due to the loss of long-range order. Our results provide deep fundamental insights on the electron dynamics in liquids, opening the door to the development of ultrafast technologies based on strong-field driven liquids.