

Ultrafast Molecular Dynamics Probed by X-ray Spectroscopy (Session 4, Oral)

Ji-Cai Liu¹, Jian Wang¹, Victor Kimberg² and Faris Gel'mukhanov²

¹School of Mathematics and Physics, North China Electric Power University,
102206 Beijing, China

²Department of Theoretical Chemistry and Biology, KTH Royal Institute of
Technology, 10691 Stockholm, Sweden

Photons and photoelectrons can transfer significant linear momentum as well as angular momentum in the processes of x-ray absorption, scattering, and ionization. The related recoil-induced vibrational and rotational excitations have received significant attention in x-ray spectroscopies. However, due to the limited resolution of conventional X-ray spectrometers, the rotational structure cannot be resolved directly through x-ray spectroscopies. We proposed here several x-ray spectroscopy methods allowing for direct probing of the recoil-induced ultrafast nuclear dynamics, including recoil-induced fragmentation of the molecule, recoil-induced ultrafast molecular rotation probed by dynamical rotational Doppler effect, and time-resolved all X-ray pump-probe spectroscopy of recoil-induced rotation. It was found that the large recoil energy delivered to vibrations and rotations can not only changes the vibrational progression structure but can also breaks the chemical bond. The recoil-induced rotation can be probed by subsequent Auger electron emission shown as asymmetrical features in the Auger electron spectra or probed by a time-delayed short probe X-ray pulse visualized as the revival structures in the x-ray absorption spectra.

- [1] J.-C. Liu, F. Gel'mukhanov, S. Polyutov, et. al., *Phys. Rev. A* **109**, 023116 (2024).
- [2] J. Söderström, A. Ghosh, L. Kjellsson, et. al., *Science Advances* **10**, eadk3114 (2024).
- [3] J.-C. Liu, J. Wang, N. Ignatova, et. al., *J. Chem. Phys.* **158**, 114304 (2023).
- [4] J.-C. Liu, N. Ignatova, V. Kimberg, et. al., *Phys. Chem. Chem. Phys.* **24**, 6627-6638 (2022).
- [5] V. Savchenko, J.-C. Liu, M. Odelius, et. al., *Phys. Rev. A* **104**, 032816 (2021).
- [6] J.-C. Liu, V. Savchenko, V. Kimberg, et. al., *New J. Phys.* **23**, 063030 (2021).
- [7] J.-C. Liu, V. Savchenko, V. Kimberg, et. al., *Phys. Rev. A* **103**, 022829 (2021).
- [8] J.-C. Liu, V. V. da Cruz, S. Polyutov, et. al., *Phys. Rev. A* **100**, 053408 (2019).
- [9] D. Céolin, J.-C. Liu, V. V. da Cruz, et.al., *PNAS* **116**, 4877-4882 (2019).