LABORATOIRE INTERACTIONS, DYNAMIQUES et LASERS
EMR9000 CEA, CNRS, Université Paris-Saclay

SEMINAIRE LIDYL

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Le Jeudi 21 Juillet 2022 à 11h00

Orme des Merisiers, Bât.701, Pièce 17 (salle de séminaires)

Participer à la réunion Zoom
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Code secret : 3yyNtT

Dynamical manifestations of the recoil effect in photoionization processes

In X-ray spectroscopy, the translational and rotational recoil effects, together with the related Doppler effect, are natural fingerprints of nuclear motion and provide deep insight into the nuclear dynamics in bound and dissociative molecular states [1]. Doppler-labeling of the dissociation products, together with the frequency-controlled duration of X-ray scattering, provide direct and detailed information about the molecular potentials and the dynamics in repulsive states. The rotational Doppler effect [2,3] in X-ray photoionization offers site-selective information on valence molecular orbitals [4,5]. The Doppler-splitting of X-ray resonances [1] also provides a unique tool to study the nonequilibrium distributions over translational and rotational degrees of freedom. For instance, the Doppler control of the amount of '*which-path*' information allowed us to address the fundamental problem of the wave-particle duality in the Einstein-Bohr recoiling double-slit *gedanken* experiment [6].
Recently, we identified for the first time the dynamical rotational Doppler effect in the high-energy Auger spectra of CO and demonstrated the quantum correlation between rotational and translational degrees of freedom [1,7]. This was performed by hard X-ray C1s photoionization of carbon monoxide accompanied by the spinning-up of the molecule via the recoil "kick" of the fast emitted photoelectron. To visualize the molecular rotation, we used the dynamical rotational Doppler effect and an X-ray "pump-probe" device offered by nature itself. The time information in our experiment [7] originates from the natural delay between the C1s photoionization initiating the rotation and the ejection of the Auger electron. I will also overview here our recent results concerning the role of translational and rotational recoil effects on nuclear dynamics of molecules and clusters in the hard X-ray region (>10 keV), including the recoil-induced dissociation [1,8]. Finally, our recent results on direct time-resolved studies of the recoil-induced rotation using time-resolved X-ray pump-probe spectroscopy will be tackled [9].

[1] F. Gel'mukhanov, M. Odelius, S. P. Polyutov, A. Föhlisch, V. Kimberg, *Rev. Mod. Phys.* **93**, 035001 (2021).
[2] Y.-P. Sun, C.-K. Wang, and F. Gel'mukhanov, *Phys. Rev. A* **82**, 052506 (2010).
[3] T.D. Thomas, E. Kukk, K. Ueda, T. Ouchi, K. Sakai, T.X. Caroll, C. Nicolas, O. Travnikova, C. Miron, *Phys. Rev. Lett.* **106** (19), 193009 (2011).
[4] C. Miron, Q. Miao, C. Nicolas, J. D. Bozek, W. Andrałojć, M. Patanen, G. Simões, O. Travnikova, H. Ågren, F. Gel'mukhanov, *Nature Communications* **5**, 3816 (2014).
[5] Q. Miao, O. Travnikova, F. Gel'mukhanov, V. Kimberg, Y.-P. Sun, T.D. Thomas, C. Nicolas, M. Patanen, C. Miron, *J. Phys. Chem. Lett.* **6**, 1568–1572 (2015).
[6] X.-J. Liu, Q. Miao, F. Gel'mukhanov, M. Patanen, O. Travnikova, C. Nicolas, H. Agren, K. Ueda, C. Miron, *Nature Photonics* **9**, 4120 (2015).
[7] D. Ceolin, J.-C. Liu, V. Vaz da Cruz, H. Agren, J.-P. Rueff, R. Püttner, T. Marchenko, R. Guillemin, R. Kushawaha, L. Journel, M.-N. Piancastelli, M. Simon, F. Gel'mukhanov, *Proc. Natl. Acad. Sci. USA* **116**, 4877 (2019).
[8] J.-C. Liu, V. V. da Cruz, S. Polyutov, A. Föhlisch, F. Gel'mukhanov, *Phys. Rev. A* **100**, 053408 (2019).
[9] J.-C. Liu, N. Ignatova, V. Kimberg, P. Krasnov, A. Föhlisch, M. Simon, F. Gel'mukhanov, *Phys. Chem. Chem. Phys.* **24**, 6627 (2022).