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[L] Electronic and geometry views of molecules

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The results were taken by the SLAC UED collaboration and LCLS Nucleobase collaboration (see author lists of publications below).

In this talk, I will present molecular dynamics obtained by diffraction of relativistic electrons exemplified on the rotational and vibrational modes of small model systems [1,2]. The results have been obtained at a new femtosecond ultrafast electron diffraction source at SLAC. I will point out electron-specific advantages in diffraction of small molecules and discuss future applications on larger molecular systems. In addition, I will present site specific electronic probing of molecular dynamics accomplished by soft x-ray pulses at the oxygen K-edge. We used this scheme to unequivocally observe a molecular intersystem crossing from a $\pi\pi$ state to a $n\pi$ state [3]. Combinations of the two techniques for a more complete dynamical description will be discussed.

[1] J. Yang, M. Guehr, T. Vecchione, M. S. Robinson, R. Li, N. Hartmann, X. Shen, R. Coffee, J. Corbett, A. Fry, K. Gaffney, T. Gorkhover, C. Hast, K. Jobe, I. Makasyuk, A. Reid, J. S. Robinson2, S. Vetter, F. Wang, S. Weathersby, C. Yoneda, M. Centurion, X. Wang, *Nature Comm.* 7, 11232 (2016)

[2] J. Yang, M. Guehr, X. Shen, R. Li, T. Vecchione, R. Coffee, J. Corbett, A. Fry, N. Hartmann, C. Hast, K. Hegazy, K. Jobe, I. Makasyuk, J. Robinson, M. S. Robinson, S. Vetter, S. Weathersby, C. Yoneda, X. Wang, M. Centurion, *Phys. Rev. Lett.* 115, 173002 (2016)

[3] T. J. A. Wolf, R. H. Myhre, J. P. Cryan, S. Coriani, R. J. Squibb, A. Battistoni, N. Berrah, C. Bostedt, P. Bucksbaum, G. Coslovich, R. Feifel, K. J. Gaffney, J. Grilj, T. J. Martinez, S. Miyabe, S. P. Moeller, M. Mucke, A. Natan, R. Obaid, T. Osipov, O. Plekan, S. Wang, H. Koch and M. Gühr, *Nature Communications* 8, 29 (2017)

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