

Time-Resolved C₆₀ Femtosecond Dynamics Induced by High Intensity X-rays from the LCLS

N. Berrah^{#1}, A. Sanchez-Gonzalez[^], K. Toyota[@], Z. Jurek[@], A. Lutman^{*}, H. Xiong[#], R. Squibb[!], R. Obaid[#], T. Osipov^{*}, L. Fang[&], T. Barillot[^], J. D. Bozek[~], T. Wolf[&], J. Cryan[&], D. Ray^{*}, K. Schnorr^{**}, S. Augustin^{**}, H. Fukuzawa^{##}, K. Motomura^{##}, R. Coffee^{*}, M. Guehr[%], N. Niebuhr[%], L. J. Frasinski[^], D. Rolles^{^^}, R. Feifel[!], C-P. Schultz^{&&}, S.-K. Son[@], K. Ueda^{##}, T. Pfeifer^{**}, J. Marangos[^] and R. Santra^{@\$}

[#]University of Connecticut, Physics Department, Storrs, CT 06269, USA

[^]Department of Physics, Imperial College London, SW7 2AZ, United Kingdom

[@] Center for Free-Electron Laser Science, DESY, 22607 Hamburg, Germany

^{*}LCLS, National Accelerator Laboratory, Menlo Park, CA 94025, USA

[!]Department of Physics, University of Gothenburg, 41296 Gothenburg, Sweden

[&]Center for High Energy Density Science, University of Texas, Austin, TX 78712, USA

[~]Synchrotron SOLEIL, L'Orme des Merisiers, Saint Aubin, 91192 Gif-sur-Yvette CEDEX, France

[%]Stanford PULSE Institute, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA.

^{**}Max-Planck-Institut für Kernphysik, Heidelberg, 69117, Germany

^{##}Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan

[%]Institut für Physik und Astronomie, Universität Potsdam, 14476 Potsdam, Germany

^{^^}J.R. Macdonald Laboratory, Department of Physics, Kansas State University, Manhattan, KS 66506, USA

^{&&}Max Born Institut, 12489 Berlin, Germany

^{\$}Department of Physics, University of Hamburg, 20355 Hamburg, Germany

Synopsis: Time-resolved experimental and theoretical photoionization of C₆₀ using intense, short x-ray pulses from the linac coherent light source (LCLS) free-electron laser was studied. The aim of the work is to understand, in real time, the ionization and fragmentation dynamics induced by intense x-rays.

The real-time evolution of the photoionization and dissociation of large molecules at high x-ray intensity is unknown. Several models have been developed for studying the time evolution of the ionization of samples of increasing size irradiated by x-ray free-electron laser (FEL) pulses. We have validated in previous static work the successful use of classical mechanics to describe all moving particles in the photoionization of C₆₀ [1, 2].

We show in Fig. 1, the real-space theoretical snapshots of the time evolution of a C₆₀ molecule irradiated by an x-ray FEL pulse. The positions of the carbon atoms (red) and electrons (yellow) are shown as a function of time and spatial scale. The pulse duration used is 30 fs, with Gaussian pulse shape and a pulse energy of 345 mJ with photon energy at 485 eV.

We have carried out the time-resolved experimental and theoretical calculation of the photoionization of C₆₀ using 640 eV photons with 20 fs pulse duration and with about 4×10^{15} W/cm² pulse intensity from the LCLS FEL at SLAC National Laboratory. The measurements were conducted using a magnetic bottle spectrometer to detect the electrons or fragment ions. The time-resolved data were generated using two x-ray pulses generated by the fresh-temporal slices using the LCLS accelerator scheme [3], to measure the ions and electrons resulting from the ionization as a function of delay time between

the x-ray pump and the x-ray probe. We will present our results which will test molecular dynamics models and calculations [1, 2, 4].

This work was funded in part by the DOE-BES grants No. DE-SC0012376

Figure 1. Real-space theoretical snapshots of the time evolution of a C₆₀ molecule irradiated by an x-ray FEL pulse [1].

References

- [1] B. F. Murphy et al., 2014 Nature Comm., **5**, 4281.
- [2] N. Berrah et al., 2014 Faraday Disc., **171** (1), 471.
- [3] A. Lutman et al., 2016 Nature Photonics **10** 745.
- [4] K. Yamazaki et al., 2014 J. Chem. Phys. **141**, 121105.

