



Contribution ID: 32

Type: Oral

Bayesian inferencing and deterministic anisotropy for molecular geometry retrieval in gas phase diffraction experiments

Monday, 13 March 2023 15:55 (20 minutes)

Ultrafast molecular gas phase diffraction is a vital tool for retrieving time dependent molecular structures. We are limited in the systems we can study as we generally require complex molecular dynamics simulations to interpret the results. We develop an alternative analysis to approximate the molecular geometry distribution $|\Psi(\mathbf{r}, t)|^2$ that does not require such complex simulations. We achieve real-space resolutions of 1 pm to 10 fm while uniquely defining the molecular structure. We demonstrate our method's viability by retrieving the ground state geometry distribution $|\Psi(\mathbf{r})|^2$ for simulated stretched NO_2 and measured N_2O . Our method expands the capabilities of ultrafast molecular gas phase diffraction to measure other variables, like the width of $|\Psi(\mathbf{r}, t)|^2$. By not relying on complex simulations and with the order 100 fm resolution, our method has the potential to effectively turn ultrafast molecular gas phase diffraction into a discovery oriented technique, exploring systems that are prohibitively difficult to simulate.

UED is supported in part by DOE BES Scientific User Facilities Division and SLAC UED/UEM program development: DE-AC02-05CH11231.

This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division.

Primary authors: HEGAZY, Kareem (STANFORD U., PHYS. DEPT.); Prof. MAKHIJA, Varun (Department of Chemistry and Physics, University of Mary Washington); Dr COFFEE, Ryan (Stanford PULSE Institute, SLAC National Accelerator Laboratory)

Co-authors: Prof. BUCKSBAUM, Phil (Department of Physics and Applied Physics, Stanford University); Dr CORBETT, Jeff (SLAC National Accelerator Laboratory); CRYAN, James (SLAC); Prof. GUEHR, Markus (Institut für Physik und Astronomie, Universität Potsdam); Dr HARTMANN, Nick (Linac Coherent Light Source); Dr ILCHEN, Markus (European XFEL); JOBE, Keith (SLAC); Prof. LI, Renkai (Department of Engineering Physics, Tsinghua University); Dr MAKASYUK, Igor (SLAC National Accelerator Laboratory); Dr SHEN, Xiaozhe (SLAC National Accelerator Laboratory); Dr WANG, Xijie (SLAC National Accelerator Laboratory); Dr WEATHERSBY, Stephen (SLAC National Accelerator Laboratory); Prof. YANG, Jie (Department of Engineering Physics, Tsinghua University)

Presenter: HEGAZY, Kareem (STANFORD U., PHYS. DEPT.)

Session Classification: Methods

Track Classification: Methods