Stanford

John Walters

Ph.D. Student in Chemistry, admitted Autumn 2024

Bio

BIO

I am a graduate student pursuing a Ph.D. in Physical Chemistry working under Professor James P. Cryan and Dr. Taran Driver. I received my undergraduate degree in Chemistry at Drexel University where I performed research under Professor Hai-Feng Ji studying low-dimensional semiconducting systems.

My present research uses x-ray free electron lasers to perform ultrafast x-ray spectroscopy to observe electron dynamics, which occur on attosecond timescales. These dynamics allow us to generate "molecular movies" that show how electrons are moving. These "movies" are used by theorists to better inform their models with respect to difficult problems such as electron-electron correlation and nuclear motion. Developing this understanding is essential for applications across many fields, including biology, chemistry, and material science.

I also spend time working at the Time-resolved Atomic and Molecular Optical Sciences (TMO) hutch at the LCLS-II, where I assist with preparing for experiments, running experiments, and analyzing experimental data. I am also involved analysis at the Resonant Inelastic X-ray Scattering (RIXS), Macromolecular Femtosecond Crystallography (MFX), and X-ray Correlation Spectroscopy (XCS) hutches.

HONORS AND AWARDS

- ACS Scholastic Achievement Award, Philadelphia Chapter, American Chemical Society (April 2024)
- Dr. Robert O. Hutchins Endowed Chemistry Prize, Drexel University (April 2024)
- Bruce and Cynthia Maryanoff Endowed Research Prize, Drexel University (May 2023)

EDUCATION AND CERTIFICATIONS

- Bachelor's of Science, Drexel University , Chemistry (2024)

LINKS

- Linkedin: https://www.linkedin.com/in/johntwalters/

Research & Scholarship

CURRENT RESEARCH AND SCHOLARLY INTERESTS

I am interested in the attosecond dynamics of atoms and molecules. Specifically, my interest lies in investigating the effect of electron-electron correlation and the influence of non Born-Oppenheimer dynamics on isolated quantum systems to drive understanding of both ground-state and excited-

state processes. Additionally, I am interesting in applying covariance and machine-learning based techniques to improve measurement resolution in high-repetition rate experiments.

My projects include, but are not limited to:

* Using attosecond x-ray pump, attosecond x-ray probe spectroscopy to monitor charge migration in molecular systems.

Using attosecond x-ray pulses separated by a variable time delay, we can measure coherent electron motion by using trXAS to monitor atomic site specific electron density on the hundreds of attoseconds to few femtosecond timescales. We have observed charge migration in several molecular systems, where we have attempted to determine how coherence changes in long range conjugated systems, in biologically relevant molecules, and with core level vacancies.

* Using techniques analogous to rainbow RABBITT to observe attosecond scale time delays in molecular photoionization.

Using the FERMI seeded FEL, we were able to use the LDM endstation to measure attosecond delays in molecular photoionization in Neon and CO2 with reference to Helium. This measurement resolves the phase shift near the autoionizing states in Neon by looking at intracycle phase shifts. The measurement also looks at intercycle phase shifts to investigate interchannel coupling in CO2 surrounding the C-state shape resonance.

* Using Raman wavepacket interferometry to investigate neutral state electronic coherence.

With impulsive x-ray Raman scattering, we can generate a coherent superposition of valence electronic states in a neutral molecule. The beating in the population of these states encodes information surrounding the energy spacing and coherence of the valence excited state, giving insight into the electronic structure of the neutral molecule.

LAB AFFILIATIONS

- James Cryan (4/1/2025)

Publications

PUBLICATIONS

- **Characterization of All Allotropes of Phosphorus** *SCI*
  Walters, J. T., Cao, M., Lam, Y., Schwenk, G. R., Ji, H.
  2025; 7 (3)
- **Structural Consequences of Post-Synthetic Modification of Cu₂P₃I₂** *MICRO-SWITZERLAND*
  Schwenk, G. R., Walters, J. T., Ji, H.
  2023; 3 (1): 256-263

PRESENTATIONS

- Correlation Approaches at LCLS-II - LCLS Users Meeting (September 24, 2025)