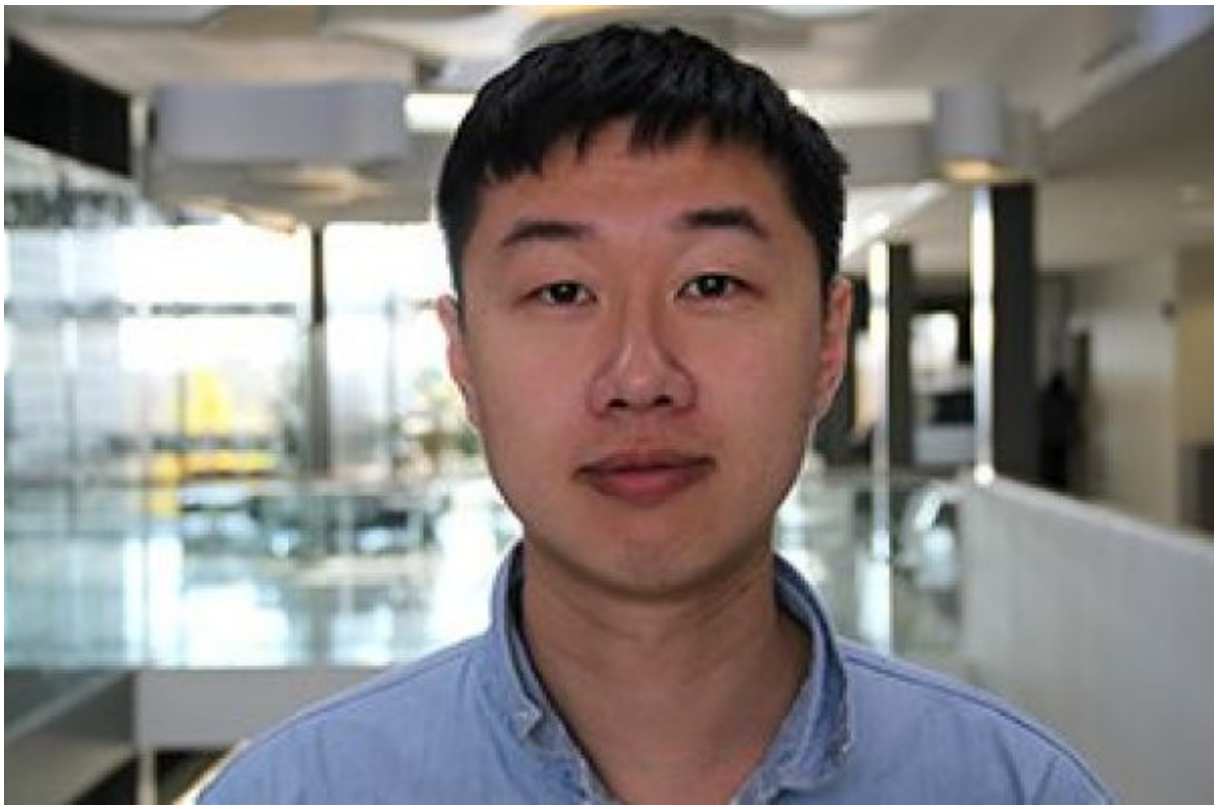
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PhD THESIS DEFENSE: Atomic imaging of complex molecular structures with laser-induced electron diffraction

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Auditorium and Online (Teams)

One of the significant challenges of modern science is to track and image chemical reactions as they occur. The molecular movies, the precise spatiotemporal tracking of changes in their molecular dynamics, will provide a wealth of actionable insights into how nature works. Experimental techniques need to resolve the relevant molecular motions in atomic resolution, which includes (10^(-10) m) spatial dimensions and few- to hundreds of femtoseconds (10^(-15) s) temporal resolution.
Laser-induced electron diffraction (LIED), a laser-based electron diffraction technique, images even singular molecular structures with combined sub-atomic picometre and femto-to attosecond spatiotemporal resolution. Here, a laser-driven attosecond electron wave packet scatters the parent's ion after photoionization. The measured diffraction pattern

of the electrons provides a unique fingerprint of molecular structure. Taking snapshots of molecular dynamics via the LIED technique is proved to be a potent tool to understand the intertwining of molecules and how they react, change, break, bend, etc.
This thesis is especially interested in exploiting advanced LIED imaging techniques to retrieve large complex molecular structures. So far, LIED has successfully retrieved molecular information from small gas-phase molecules like oxygen (O2), nitrogen (N2), acetylene (C2H2), carbon disulfide (CS2), ammonia (NH3) and carbonyl sulfide (OCS). Nevertheless, most biology interesting organic molecules typically exist as liquid or solid at room temperature. In order to accomplish the final goal to extract these larger complex molecular structural information, we need to overcome two main challenges: delivering the liquid or solid samples as a gas-phase jet with sufficient gas density in the experiment and developing a new retrieval algorithm to extract the geometrical information from the diffraction pattern. We tested one of the most simple liquid molecules - water H2O in the reaction chamber as a primary step. We traced the variation of H2O+ cation structure under the different electric fields. To solve the problem of unsatisfactory gas density, we present a novel delivery system utilizing Tesla valves that generates more than an order-of-magnitude denser gaseous beam. Machine learning is well qualified to solve difficulties with manifold degrees of freedom. We use convolutional neural networks (CNNs) combined with LIED techniques to enable atomic-resolution imaging of the complex chiral molecule Fenchone (C10H16O).

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