Development of AI Methods for Finding Hidden Dimensions - the Physics of Correlated Atomic Motions from "Molecular Movies"

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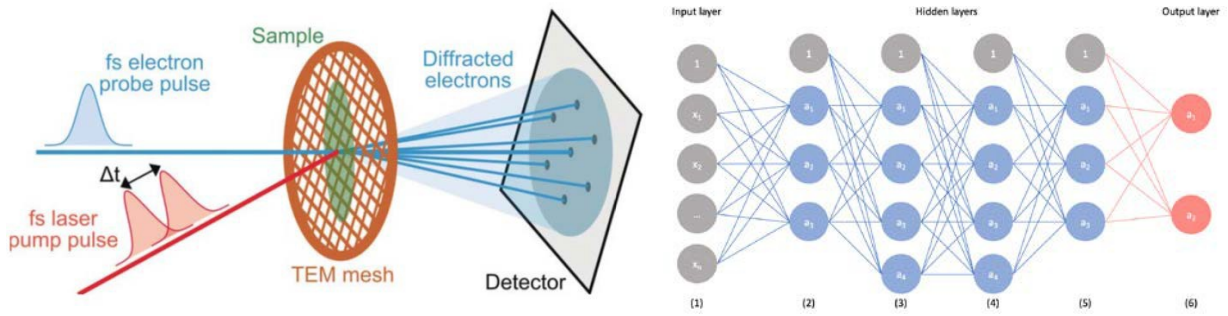
Ultrafast electron diffraction (UED) is a pump-probe technique that combines the spatial resolution of x-ray crystallography with the time resolution of traditional optical spectroscopies. This powerful tool is capable of capturing atomic motions in real time by observing changes in diffraction patterns over time. From inorganic molecules and their relevant photophysical processes and associated bond length changes, to condensed matter systems undergoing laser excitation near the band gap, UED captures chemistry and physics in action. Understanding the diffraction patterns requires a thorough analysis of the changes in intensity and position of diffraction peaks and rings and matching these changes to dynamical changes in the structure of the studied samples.



(left) General schematic for UED pump-probe experiment *(right) Schematic of a neural network*

The goal in this project is to explore how Artificial Intelligence (AI) can aid in matching changes in diffraction pattern to those of structural changes. It is a challenging project but can be very rewarding. The student will work closely with a senior graduate student on this project. Prior knowledge of AI is not required but the student should be highly motivated. A good command of Python is recommended.

The student is expected to perform the following tasks:

- In the first 4-6 weeks, the student will take the Deep Learning specialization on Coursera.org. This will give the student the foundational knowledge necessary for this project.
- The student is then expected to explore the publicly available electron diffraction machine learning algorithms on the web, train them with group's diffraction data to extract information about the structural changes induced by photoexcitation of the samples.

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