

# Materials Science and Engineering Doctoral Defense

Ultrafast electrons and X-rays as probe  
to biomolecular dynamics

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## abstract

The structure-function relation in Biology suggests that every biological molecule has evolved its structure to carry out a specific function. However, for many of these processes (such as those with catalytic activity) the structure of the biomolecule changes during the course of a reaction. Understanding the structure-function relation thus becomes a question of understanding biomolecular dynamics that span a variety of timescales (from electronic rearrangements in the femtoseconds to side-chain alteration in the microseconds and more). This presentation will focus on the study of biomolecular dynamics in the ultrafast timescales (fs-ns) using electron and X-ray probes in both time and frequency domains.

The presentation will commence with establishing the limitations of traditional electron diffraction coupled with molecular replacement to study biomolecular structure and will proceed to suggest a pulsed electron source Hollow-Cone TEM as an alternative scheme to pursue ultrafast biomolecular imaging. It will then propose the use of Energy Loss Spectroscopy as a tool to access ultrafast nuclear dynamics using monochromated NiON UltraSTEM.

The second part of the presentation will deal with X-ray as probe. It will begin by briefly highlighting the success of the GDVN and LCP sample injectors in presenting micro-biocrystals to interact with the XFEL. Finally, ultrafast X-ray spectroscopy as a tool to elucidate biomolecular dynamics will be presented with our study of photolysis of Methylcobalamin using time-resolved laser pump – X-ray absorption spectroscopy at the APS. The analysis will be compared to DFT based XAS simulations to characterize the ground state reactants and products and the intermediate state at specific laser to X-ray time delays.

Friday, October 7, 2016; 8:30AM, GWC 487