Cellulose degrading oxidative enzymes: structural insights from neutron diffraction and scattering

Sensitivity to hydrogen/deuterium and lack of observable radiation damage make cold neutrons an ideal probe for structural studies of redox enzymes. Neutron protein crystallography (NPC) is a powerful tool for investigating protein chemistry because it directly locates hydrogen atom positions [1,2]. Small-angle scattering (SAS) provides low resolution information on protein dimensions. Combined with contrast variation techniques and modeling, small angle neutron scattering (SANS) further allows the structural investigation of individual components within protein-protein complexes. I will first introduce the neutron facilities at ORNL before presenting recent results from my lab.

My lab focuses on metallo-enzymes with a specific interest in cellulose degrading oxidative enzymes. Fungal lytic polysaccharide monooxygenases (LPMOs) are copper containing metallo-enzymes involved in biomass oxidation. LPMO-catalyzed monooxygenation requires input of two electrons from LPMO redox partners, the cellobiose dehydrogenase enzymes (CDHs), and of one oxygen molecule to achieve hydroxylation of one carbon in the glycosidic bond [3]. I will discuss our recent X-ray and neutron crystallographic studies that provide new insight into the LPMO monooxygenation mechanism [4,5]. Redox complexes such as the LPMO-CDH complex, are often transient, and their structural characterization can be challenging. We are using SANS to characterize the interaction between CDH and LPMO [6].