Unraveling Photochemical Mechanisms by Capturing Electrons Move in Real Time

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Savini Bandaranayake received her B.Sc. degree in Computational Chemistry from University of Colombo and completed her Ph.D. in Physical Chemistry at The Ohio State University in 2022. Her doctoral research focused on ultrafast photoexcited state dynamics in transition metal oxides and the development of advanced ultrafast spectroscopy techniques. Since 2023, she has been a Postdoctoral Scholar at Sandia National Laboratories, studying non-adiabatic dynamics in molecular systems following photoexcitation, using ultrafast X-ray, UV-visible and IR spectroscopy techniques.

Abstract: Harnessing solar energy to drive chemical reactions play a vital role in sustainable innovation and fundamental understanding of light-matter interactions remain crucial for progress. Heterogeneous photocatalysis is one such example that shows potential to convert solar energy to chemical energy. Upon photoexcitation, charge carriers are generated within the catalyst, which can follow multiple competing pathways that determine the efficiency and selectivity of the reaction. Many of these processes occur in the ultrafast time regime, accessible only through the recent advancement of transient spectroscopy techniques. Extreme Ultraviolet (XUV) transient absorption spectroscopy is one such powerful method capable of probing charge carrier dynamics with element and site specificity, with a time resolution < 100 fs, in a laboratory setting. In this talk, I will present transient XUV studies on hematite, (α-Fe_2O_3), a model photocatalyst for water splitting. These measurements reveal that polaron formation occurs within < 1 ps after photoexcitation, lowering the efficiency by trapping charge carriers. Furthermore, surface functionalization with self-assembled monolayers can be used to modulate charge transfer dynamics in hematite. Observing electron motion in real time provide insights into intrinsic properties of materials, crucial for the design and synthesis of better performing photocatalysts. Thus, continued development of ultrafast techniques is key to advancing our understanding of photochemical processes.