**The Birth of an Excited State and Beyond: Does Ultrafast Science Meets Photochemistry?**

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Short laser pulses undeniably gave traditional chemical concepts new physical content, most famously by direct observation of atomic motion during chemical reactions. Do even shorter, brighter, and more energetic photons deliver a similar promise for photochemistry? Ultrafast X-ray sources now provide new windows on electronic structure, element specificity, and local environments and attosecond HHG pulses can in principle track the electronic motion. Yet it is not obvious that the resulting observables automatically translate into traditional chemical concepts. For example, organic chemists speak about electron flow, in ultrafast physics the same phrase can refer to something rather different. In that sense, the question behind this talk is: does ultrafast science meet (photo)chemistry?

As a computational chemist, I will approach this question by focusing on the earliest photochemical event that is often treated as instantaneous: the formation of the excited state during photoexcitation. I will argue that a central early photochemical event is the birth of the excited state itself, a dynamical process that can shape everything that follows. I will present time-domain simulations of electronic excitations in solution, focusing on charge-transfer-to-solvent (CTTS) states of solvated ions and what they reveal about the emergence of delocalized electronic character during excitation. I will then discuss how vibronic structure forms on ultrafast timescales and how such a viewpoint helps connect ultrafast (including X-ray) observables to chemically useful descriptions. Finally, I will outline practical strategies for incorporating finite-pulse excitation into trajectory-based molecular dynamics built on classical nuclear motion. Along the way, I will use “attochemistry” in the broad sense often adopted in the field: not only sub-femtosecond electron motion, but also the few-to-tens of femtoseconds regime where electronic and nuclear degrees of freedom become entangled in ways that matter for photochemistry. I will end with a critical look at the scope and limits of computational photochemistry as a predictive tool.