First-principles explorations of dynamics in materials - from attoseconds to nanoseconds - aided by X-ray spectroscopy

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The understanding and control of physical processes relevant to our societal energy needs, encompasses a range of time-scales spanning several orders of magnitude. Here we discuss preliminary work within two limits in this space: light-matter interactions at attosecond timescales and beyond and molecular-scale electrochemical processes at solid-liquid interfaces. Predominantly, we make use of density functional theory approaches, with various extensions designed to model the intrinsic excited states and those of an amazingly versatile probe - X-ray spectroscopy. This talk will focus on our direct interpretations of measurements made using X-ray absorption spectroscopy of the biased gold-water interface [1] and photo-excited silicon [2].