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].

[1] Juan-Jesus Velasco-Velez, Cheng Hao Wu, Tod A. Pascal, Liwen F. Wan, Jinghua Guo, David Prendergast, Miquel Salmeron, The structure of interfacial water on gold electrodes studied by x-ray absorption spectroscopy, Science 346, 831 (2014).
[2] Martin Schultze, Krupa Ramasesha, C.D. Pemmaraju, S. A. Sato, D. Whitmore, A. Gandman, James S. Prell, L. J. Borja, D. Prendergast, K. Yabana, Daniel M. Neumark, Stephen R. Leone, Attosecond band-gap dynamics in silicon, Science 346, 1348 (2014).