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Combining Structural and Spectroscopic Probes of Molecular Dynamics[1] YUSONG LIU, SPENCER HORTON, Stony Brook University, JIE YANG, THOMAS WOLF, SLAC National Laboratory, PEDRO NUNES, University of Nebraska, RUARIDH FORBES, University College London, University of Ottawa, VARUN MAKHIJA, University of Ottawa, PAUL HOCKETT, RUNE LAUSTEN, National Research Council, Canada, ALBERT STOLOW, University of Ottawa, National Research Council, Canada, PHILIPP MARQUETAND, University of Vienna, TAMAS ROZGONYI, Hungarian Academy of Sciences, XIJIE WANG, SLAC National Laboratory, THOMAS WEINACHT, Stony Brook University — We combine ultrafast electron diffraction (UED) measurements with time resolved photoelectron spectroscopy (TPRES) measurements of excited state molecular dynamics. Both measurements are compared with trajectory surface hopping calculations of the dynamics, which can produce the measurement observables in both cases. The measurements highlight the non-local dynamics captured by different groups of trajectories in the calculations. This is the first time that both structural and spectroscopic measurements are combined with a theory capable of calculating the measurement observables in both cases, and the combination yields an unprecedented view of the multidimensional coupled electron nuclear dynamics involved in the molecular relaxation.

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