UV DYNAMICS OF CIS-STILBENE STUDIED BY ULTRAFAST ELECTRON DIFFRACTION

S. K. SAHA, *Department of Physics and Astronomy, University of Nebraska - Lincoln, Lincoln, NE, USA*; PEDRO NUNES, *HeXI, Diamond Light Source, Didcot, United Kingdom*; HAYLEY WEIR, MONIKA WILLIAMS, *Department of Chemistry, Stanford University, Stanford, CA, USA*; ANDREW ATTAR, *Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, CA, USA*; BRYAN MOORE, *Department of Physics and Astronomy, University of Nebraska - Lincoln, Lincoln, NE, USA*; DUAN LUO, MING-FU LIN, MATTHIAS HOFFMANN, FUHAO JI, MATTHEW R WARE, *Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, CA, USA*; SHASHANK PATHAK, *J.R. Macdonald Laboratory, Kansas State University, Manhattan, KS, USA*; THOMAS JA WOLF, *Stanford PULSE Institute, SLAC National Accelerator Laboratory, Menlo Park, CA, USA*; JIE YANG, *Department of Chemistry, Tsinghua University, Beijing, China*; KEITH JOBE, *Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, CA, USA*; TODD MARTINEZ, *Department of Chemistry, Stanford University, Stanford, CA, USA*; MARTIN CENTURION, *Department of Physics and Astronomy, University of Nebraska - Lincoln, Lincoln, NE, USA*.

Stilbene is a prototype molecule for studying photoisomerization and photocyclization mechanisms which are pivotal to converting light into chemical and mechanical energy in nature. Despite multiple decades of research, the exact details of the photoisomerization of cis-stilbene into trans-stilbene and/or its cyclization into 4a,4b-dihydrophenanthrene (DHP) have remained a topic of debate. We have used mega-electronvolt ultrafast electron diffraction (UED) to capture and spatially resolve the photoexcitation dynamics with sub-angstrom resolution. At the SLAC MeV-UED beamline, cis-stilbene was optically pumped with 267 nm ultraviolet light with different pulse energy and probed with 3.7 MeV electrons. We compare our experimental difference-diffraction signals with Ab initio multiple spawning simulations (AIMS) for single-photon excitation dynamics and molecular dynamics simulation for two-photon excitation leading to ionization. We found that with 80uJ pulse energy, the single and two-photon excitation channels are comparable, while with 130uJ pulse energy the two-photon channel dominates. Our data and simulations revealed very different dynamics and end products in the one-photon and two-photon channels.