Abstract Submitted
for the DAMOP20 Meeting of
The American Physical Society

Unraveling the Photochemical Ring-Opening Dynamics of 1,3-cyclohexadiene with Ultrafast Electron Diffraction and *Ab initio* Multiple Spawning[1] DAVID SANCHEZ, Stanford PULSE Inst and Stanford Univ, THOMAS WOLF, Stanford PULSE Inst, JIE YANG, Stanford PULSE Inst and SLAC Natl Accelerator Lab, ROBERT PARRISH, Stanford PULSE Inst and Stanford Univ, JOAO NUNES, Univ of York and Univ of Nebraska Lincoln, MARTIN CENTURION, Univof Nebraska Lincoln, RYAN COFFEE, SLAC Natl Accelerator Lab, JAMES CRYAN, Stanford PULSE Inst, MARKUS GUHR, Stanford PULSE Inst and Univ Potsdam, KAREEM HEGAZY, Stanford PULSE Inst and Stanford Univ, ADAM KIRRANDER, Univ of Edinburgh, RENKAI LI, SLAC Natl Accelerator Lab, JENNIFER RUDDOCK, Brown Univ, XIAOZHE SHEN, THEODORE VECCHIONE, STEPHEN WEATHERSBY, SLAC Natl Accelerator Lab, PETER WEBER, Brown Univ, KYLE WILKIN, Univ of Nebraska Lincoln, HAI-WANG YONG, Brown Univ, QIANG ZHENG, XIJIE WANG, MICHAEL MINITTI, SLAC Natl Accelerator Lab, TODD MARTINEZ, Stanford PULSE Inst and Stanford Univ
— While the photoinduced ring-opening of 1,3-cyclohexadiene (CHD) has been the topic of numerous experimental and theoretical studies, none have achieved the temporal and spatial resolution needed to unambiguously observe its ring-opening dynamics. Here, we directly observe the photoinduced ring-opening of CHD on the femtosecond and sub-Ångström scales using MeV Ultrafast Electron Diffraction (UED) and Ab Initio Multiple Spawning (AIMS). We show that CHD experiences a substantial acceleration of the ring-opening motion upon relaxation to the ground state via a conical intersection, which is transformed into rotation of the terminal ethylene groups in 1,3,5-hexatriene (HT). Additionally, we observe a coherent oscillation between the cZc, tZc/cZt, and tZt rotamers of HT upon relaxation to the ground state.

David Sanchez
Stanford PULSE Inst and Stanford Univ

[1]NSG GRFP and EDGE Diversity

Date submitted: 03 Feb 2020 Electronic form version 1.4