

Abstract Submitted
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Direct Observation of Steric Effects and Non-Adiabatic Dynamics with Ultrafast Electron Diffraction¹ ELIO G. CHAMPENOIS, DAVID M. SANCHEZ, NANNA H. LIST, TODD J. MARTINEZ, XIJIE WANG, THOMAS J. A. WOLF, SLAC National Accelerator Laboratory, SLAC UED COLLABORATION — Ultrafast Electron Diffraction (UED) has emerged as a powerful tool to investigate photochemistry on its natural femtosecond timescale. We present two recent time-resolved studies in which UED, coupled with *ab initio* molecular dynamics simulations, provides two unique probing capabilities. In spectroscopically similar isomeric cyclohexadiene (CHD) derivatives, we observe steric effects which affect the mechanisms, efficiencies, and timescales of ultrafast ring opening. In ammonia (NH₃), the independent atom model for molecular diffraction breaks down as the valence electronic structure plays a substantial role. We use this to follow the ultrafast dissociation including two conical intersections following UV photoexcitation, with simultaneous sensitivity to the evolving nuclear and electronic degrees of freedom.

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