

Supplementary information for Imaging Conical Intersection Dynamics during Azobenzene Photoisomerization by Ultrafast X-Ray Diffraction

Daniel Keefer^a, Flavia Aleotti^b, Jérémy R. Rouxel^a, Francesco Segatta^b, Bing Gu^a, Artur Nenov^b, Marco Garavelli^b, and Shaul Mukamel^{a,1}

^a*Department of Chemistry and Physics and Astronomy, University of California, Irvine, California 92697-2025, USA*

^b*Dipartimento di Chimica Industriale, Università degli Studi di Bologna, Viale del Risorgimento 4, I-40136 Bologna, Italy*

*smukamel@uci.edu

Diffraction movies

The electronic supplement contains movies of the time-resolved diffraction signal according to the figures presented in the main manuscript. The movie captions are given in the following.

Movie S1: Nuclear wavepacket motion on the adiabatic potential energy surface for azobenzene isomerization according to Eq. (10). This movie corresponds to Fig. 2 of the main manuscript and gives the full time-resolved picture.

Movie S2: Time evolution of the full \mathbf{q} -space diffraction pattern according to Eq. (3), and dissected into the corresponding terms. This movie corresponds to Fig. 3 of the main manuscript and gives the full time-resolved picture.

Movie S3: Two-dimensional diffraction patterns of all three molecular planes after integration of the respective third spatial direction. Orientational axes are given in Fig. 1. This movie corresponds to Fig. 4 of the main manuscript and gives the full time-resolved picture.

Movie S4: Two-dimensional diffraction patterns of the coherence term (v) in Eq. (3) in all three molecular planes and after integration of the respective third spatial direction. Orientational axes are given in Fig. 1. This movie corresponds to Fig. 5 of the main manuscript and gives the full time-resolved picture.

Movie S5: Real-space movie of the electronic transition density $\langle \chi_e(t) | \sigma_{ge}(\mathbf{r}) | \chi_g(t) \rangle$ during the non-adiabatic passage. This movie corresponds to Fig. 8(d)–(f) of the main manuscript and gives the full time-resolved picture.