

Abstract Submitted
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Time-resolved molecular frame photoelectron angular distribution: Snapshots of acetylene and ethylene isomerizations¹ NICOLAS DOUGUET, University of California Davis, THOMAS RESCIGNO, Lawrence Berkeley National Lab, ANN OREL, University of California Davis — It has been proposed that chemical reactions can be imaged by detection of a photoelectron in the molecular fixed body frame (MFPAD), following either valence or K-shell photoionization. We will contrast these two techniques using acetylene and ethylene isomerization as examples. The *ab initio* calculations were carried out using the complex Kohn variational method. Our results indicate that while K-shell MFPADs are only sensitive to molecular geometry whereas valence MFPADs are sensitive to both geometry and the initial electronic state of the target. Both examples show that isomerization takes place via conical intersections. However, acetylene requires an excitation/ionization step, while ethylene undergoes isomerization following direct excitation of the neutral V state.

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