

VISUALIZING ELECTRON DYNAMICS FOR A PHOTOISOMERIZATION REACTION

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Using time-dependent density functional theory, we probe the electron dynamics involved in the photo-chemical isomerization of 1,3-cyclohexadiene to 1,3,5-hexatriene by analyzing changes to the harmonic spectra. The reaction is often used as an analog for the photo-induced reaction of provitamin D₃ to vitamin D₃ in the skin, as that reaction proceeds through a similar scheme.

Calculations are performed for 1,3-cyclohexadiene and 1,3,5-hexatriene as well as two intermediate conformers. There are distinct changes in the harmonic spectra that could be used to mark reaction progress. As expected, the breaking of the molecular symmetry leads to peaks outside of the expected odd harmonics.

In addition to the harmonic spectra, we discuss the dynamical changes to the electron density and electron localization function (ELF). From these measures of electron probability, we can see ionization and recombination occur throughout the pulse, from each of the isomers.