

Abstract Submitted
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Dynamical simulations of photochemical reactions of *trans*-stilbene, and coherent control of C₆₀ vibrational response¹ CHENWEI JIANG, Texas A&M University, Xi'an Jiaotong University, FULI LI, RUIHUA XIE, Xi'an Jiaotong University, ROLAND ALLEN, Texas A&M University — *Trans*-to-*cis* photoisomerization of stilbene, induced by a femtosecond-scale laser pulse, has been observed in simulations employing semiclassical electron-radiation-ion dynamics (SERID). Our results demonstrate that *trans*-to-*cis* and *cis*-to-*trans* isomerization involve the same basic mechanism. We also predict that another photochemical reaction, photocyclization of *trans*-stilbene to 4a,4b-dihydrophenanthrene (DHP), can be achieved using an ultrashort laser pulse. Specifically, the *trans*-stilbene molecule is observed first to isomerize to *cis*-stilbene (as an excited-state intermediate) after more than one picosecond, and then to form a new bond to become DHP, after a few hundred additional femtoseconds. For C₆₀ at low temperature, we predict that specific vibrational modes can be excited by optimally choosing the delay between two femtosecond-scale pulses.

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