

Abstract Submitted  
for the MAR07 Meeting of  
The American Physical Society

**Photoinduced ring-opening mechanism in several model diarylethenes<sup>1</sup>** PETRA SAUER, ROLAND E. ALLEN, Texas A&M University —

Recent experimental results suggest that derivatives of diarylethenes may be viable candidates for switches in molecular devices. In these molecules, the ring-opening and ring-closing reactions are induced with laser pulses of different frequencies. We have shown that the ring-opening mechanism in the simplest of all diarylethenes, stilbene, occurs via a HOMO-LUMO avoided crossing and subsequent depopulation of the excited state with minimal involvement of other orbitals. We now show that the same photoinduced ring-opening process for both oxygen ( $C_{10}H_8O_2$ ) and sulfur ( $C_{10}H_8S_2$ ) containing diarylethenes involves higher order excited states. We will show simulation results in which the initial laser pulse excitation induces a transition from HOMO to LUMO. Due to both nuclear motion and symmetry changes, this laser pulse also excites some percentage of the electronic population out of orbitals lower in energy than the HOMO and into orbitals higher in energy than the LUMO. In order for the ring-opening event to occur, the electronic population in the higher excited states is first transferred, via a series of avoided crossings, into the LUMO. A subsequent avoided crossing between the HOMO and LUMO then allows ring-opening.

<sup>1</sup>This work was supported by the Robert A. Welch Foundation (Grant A-0929).

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Date submitted: 02 Dec 2006

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