Optical control of dynamics in a simple chemical reaction: The cyclohexadiene ring-opening reaction

ROSEANNE SENSION, FOCUS Center, University of Michigan — UV excitation of 1,3-cyclohexadiene (CHD) results in an optically induced ring-opening reaction to form 1,3,5-cis-hexatriene (ZHT). The initial excited state wave packet accelerates away from the Frank-Condon region and is funneled through a conical intersection onto the 2A excited state where the nuclear ring-opening reaction occurs. Return to the ground state proceeds within a few hundred femtoseconds through two or more conical intersections between the 1A and 2A potential energy surfaces. Recent studies have demonstrated that multiphoton excitation of CHD can be used to influence the photochemical yield of ZHT. The multidimensional search of the control space for optimal pulses identified both the quadratic and cubic phase parameters of the pulse as important control parameters. These results are discussed in terms of potential physical models.