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Nuclear Wavepacket Propogation Model for the Retinal Chromophore in Rhodopsin BRITTANY CORN, SVETLANA MALINOVSKAYA, Stevens Institute of Technology — Rhodopsin, consisting of a retinal chromophore and a protein opsin, is responsible for the first steps in the vision process through a cis to trans photoisomerization, which is completed within 200 fs[1]. Efforts to control the ultrafast dynamics of this molecule have been carried out experimentally[2] as well as through quantum mechanical modeling of nuclear wave packet propagation[3]. We propose a two state model in which the ground electronic Potential Energy Surface (PES) is made up of two adjacent harmonic potentials, representing the cis and trans retinal saddle points, as well as an excited PES, characterized by the Morse potential, which meets the ground PES at a conical intersection. We explore the achievement of a high quantum yield of the trans retinal configuration by varying parameters of the external field and choosing the most adequate shape. Another investigation is presented in which we compare the charge distribution of cis and trans retinal in order to reveal a charge transfer mechanism behind the isomerization of rhodopsin. The results of the Lowdin and Natural Population Analyses demonstrate a significant transfer of charge in and around the isomerization region. [1] RW Schoenlein, LA Peteanu, RA Mathies, CV Shank, Science 254, 412 (1991) [2] VI Prokhorenko, AM Nagy, SA Waschuk, LS Brown, RR Birge, RJD Miller, Science 313, 1257 (2006) [3] S Hahn, G Stock, Chem Phys 259, 297-312 (2000)

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