Wave Packet Propagation Model for the Retinal Chromophore in Rhodopsin

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Rhodopsin, consisting of the chromophore, retinal, and a protein opsin, is responsible for the first steps in vision through a cis to trans isomerization of retinal which occurs within 200 fs [1]. Efforts to control the ultrafast dynamics of this molecule have been carried out experimentally [2] and are now performed through quantum mechanical modeling of nuclear wave packet propagation along the ground and excited electronic potential energy surfaces (PES) of retinal. A model harmonic oscillator PES was created for the ground electronic state, using the bond stretch as the coupling mode and the torsional angle as the reaction mode. At first, retinal is in its ground state cis configuration separated by an energy barrier of 0.266eV from the all-trans retinal structure. In order to overcome this barrier, a femtosecond pulse excites 11-cis retinal up to a decaying excited state. The nuclear wave packet then travels along this excited PES, modeled by the Morse potential, until it reaches the conical intersection [3]. At this point, the wave packet bifurcates into a part which will continue along the excited surface and a portion which will jump back down onto the ground electronic PES and settle into the trans retinal saddle point. The main goal is to achieve a high target yield of the latter case by varying different parameters of the pulse and choosing which shape is the most adequate. Once an efficient pulse is created, the exact ground and excited PESs are to be calculated for retinal at the ab initio level for which the same process can be applied and compared.

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[3] H. Köppel, W. Domcke, L. S. Cederbaum, Advances in Chemical Physics, Multimode Molecular Dynamics Beyond the Born-Oppenheimer Approximation, John Wiley & Sons, Inc., Illinois, 1984.