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H₂O photochemistry and photophysics: adiabatic vs. nonadiabatic dynamics

The photochemistry of the water molecule is important in the upper atmosphere and interstellar medium. The main absorption of the water molecule lies in the vacuum ultraviolet region below 200 nm. In recent years, significant advances have been made in the study of water photochemistry by using the high resolution H-atom Rydberg tagging technique in combination with various VUV sources. The dynamics of the water photodissociation through different electronic absorption bands is extremely colorful. In this talk, we present the most recent developments in the water photodissociation via the lowest four electronic excited states. The \tilde{A} (¹B₁)-state photodissociation of H₂O has been studied at 157.6 nm, and was found to be a fast and direct dissociation process on a repulsive surface, with only vibrational excitation of the OH(X² Π) product; while the dissociation of the $\tilde{B}({}^{1}A_{1})$ -state was found to proceed via two main routes: one adiabatic pathway leading to $OH(A^2\Sigma^+) + H$ and one nonadiabatic pathway to $OH(X^2\Pi)$ + H through conical intersections between the \tilde{B} -state and the ground state (\tilde{X}^1A_1). The \tilde{C}^1B_1 state of H₂O is a predissociative Rydberg state with fully resolved rotational structures. A striking variation in the OH product state distribution and its stereodynamics has been observed for different rotational states. But the \tilde{D}^1A_1 state shows no rotational structure and leads to a fast homogeneous, purely electronic predissociation to the \tilde{B}^1A_1 state. From these studies, we found that the picture of water photochemistry is extremely colorful and truly fascinating. These studies provide rather complete understanding of water photochemistry and should be helpful for modeling interstellar chemistry with abundant VUV light radiations.