Photochemistry of the Water Molecule: Adiabatic versus Nonadiabatic Dynamics
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CONSPECTUS

Water and light are two common constituents of both the earth’s
atmosphere and interstellar space. Consequently, water photo-
dissociation is a central component of the chemistry of these environ-
ments. Electronically excited molecules can dissociate adiabatically (on
a single potential energy surface, or PES) or nonadiabatically (with
transfer between PESs), and water serves as a prototype for under-
standing these two processes in unimolecular dissociation. In recent
years, extensive experimental and theoretical studies have been focused
on water photolysis, particularly on the primary product of the
dissociation, the OH radical. The use of the high-resolution H-atom
Rydberg tagging technique, in combination with various vacuum ultra-
violet (VUV) sources, has spurred significant advances in water photo-
chemistry. As the excitation energy increases, different excited electronic
states of water can be reached, and the mutual interactions between these states increase significantly. In this Account, we present
the most recent developments in water photodissociation that have been derived from the study of the four lowest electronic
excited states.

The 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 single repulsive surface, with only vibrational excitation of the OH(X2Π) product. In contrast, the dissociation of the
B′1A1 state was found to proceed via two main routes: one adiabatic pathway leading to OH(A2Σ+) + H, and one nonadiabatic
pathway to OH(X2Π) + H through conical intersections between the B state and the ground state X1A1. An interesting quantum
interference between two conical intersection pathways has also been observed. In addition, photodissociation of H2O between
128 and 133 nm has been studied with tunable VUV radiation. Experimental results illustrate that excitation to the different
unstable resonances of the state has very different effects on the OH(X2Π) and OH(A2Σ+) product channels.

The C′2B1 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. There are two kinds of
nonadiabatic dissociation routes on the C state. The first involves Renner–Teller (electronic Coriolis) coupling to the B state,
leading to rotationally hot and vibrationally cold OH products. The second goes through a newly discovered homogeneous
nonadiabatic coupling to the A state, leading to rotationally cold and vibrationally hot OH products. But the D′1A1 state shows no
rotational structure and leads to a fast, homogeneous, purely electronic predissociation to the B state.

These studies demonstrate the truly fascinating nature of water photochemistry, which is extremely variable because of the
different electronic states and their interactions. The results also provide a rather complete picture of water photochemistry and
should be helpful in the modeling of interstellar chemistry, with its abundant VUV radiation.

I. Introduction
Molecular photodissociation has long been viewed as an interesting and challenging area of chemical physics, the results of which are essential to our understanding of important processes in vision chemistry, atmospheric chemistry, and interstellar chemistry. Adiabatic dissociation (occurring on the single potential energy surface (PES)) and nonadiabatic dissociation (transferring from one PES to another) processes may occur when a molecule is electronically excited. The H2O molecule is one of the most
The ground state water molecule has $C_2v$ symmetry, and the electronic configuration is $(1a_1)^2(2a_1)^2(3a_1)^2(1b_1)^2; \bar{X}^1A_1$. It has rich electronic absorption bands in the vacuum ultraviolet (VUV) region below 200 nm (Figure 1) induced by excitations of one electron from the $1b_1$ or $3a_1$ orbital to higher orbitals. The water photochemistry has been studied at many different wavelengths. Excitation in its longest wavelength ultraviolet absorption band around 150–200 nm leads to the lowest excited singlet state (3$A_1$), which arises as a result of electron promotion from the $1b_1$ molecular orbital to an antibonding orbital with $a_1$ symmetry. Dissociation on this state is a rare prototype of direct dissociation processes that can be studied from first principles. During the last decade or so, photodissociation of H$_2$O has been extensively studied both theoretically and experimentally. Good agreements have been found between theory and experiment in the rotational distributions of the OH product. This is attributed to a conical intersection at a collinear (H–O–H) geometry. This conical intersection arises because a linear approach of H to OH on the repulsive potential curve from H + OH(X$^2\Sigma^+$) can cross an attractive potential curve from H + OH(A$^2\Sigma^+$), whereas there is an avoided crossing of these curves in the lower symmetry of a bent geometry. In addition to the conical intersection for the H–O–H geometry, there is a second symmetry-determined conical intersection on the $B$ state for the collinear O–H–H geometry. The importance of this second conical intersection in the O(1D, 3P) + H$_2$ reaction system has been illustrated before. However, only recently has its possible influence on the H$_2$O photochemistry been seriously addressed. Mordaunt et al. pointed out, in a recent wavepacket calculation, that a small part of the dissociative flux on the $B$ surface goes toward the second conical intersection (O–H–H), thus indicating that this second intersection might also play a role in the $B$ state photo-dissociation and cause quantum interference.

The $C^3B_1 \rightarrow \bar{X}^1A_1$ band of H$_2$O is located around 124 nm. Electronic structure calculations reveal that the $C$ state wave function is dominated by the 3p Rydberg configuration (1$b_1$)$_1(3p_a^1)$ in the vertical Franck–Condon region. From spectroscopic studies, the $C$ state was found to be nonbonding $3a_1$ orbital to the $3sa_1$ Rydberg orbital. The diffuse progression of bands has been interpreted as unstable periodic orbits involving a combination of bending and HO–H stretching motion. Dissociation on the $B$ state has been investigated at the Lyman-$\alpha$ wavelength (121.6 nm) which exhibits much more complicated and interesting dynamics largely due to the conical intersection between the $B$ and $X$ surfaces. Coupling between $B$ and $A$ states is also possible near the linear geometry of the H$_2$O molecule because these two states are degenerate components of a $1\Pi_u$ state at the linear geometry. Adiabatic dissociation on the $B$ surface leads to an H atom and an electronically excited OH(A$^2\Sigma^+$) radical. This process is relatively minor in comparison with the dominant dissociation process that produces an H atom plus the electronically ground state OH(X$^2\Sigma^+$) via nonadiabatic transition from the $B$ state to the $A$ state or the ground state of water (X$^1A_1$).

Photodissociation of water in the deep VUV region has also been studied using tunable synchrotron radiation. Conical intersections between PESs have been recognized as playing an important role in the dynamics of excited electronic state photochemistry: the H$_2$O $B$ state is a well-known example. One of the notable observations from experimental studies is the extremely high rotational excitation of the OH product. This is attributed to a conical intersection at a collinear (H–O–H) geometry. This conical intersection arises because a linear approach of H to OH on the repulsive potential curve from H + OH(X$^2\Pi$) can cross an attractive potential curve from H + OH(A$^2\Sigma^+$), whereas there is an avoided crossing of these curves in the lower symmetry of a bent geometry. In addition to the conical intersection for the H–O–H geometry, there is a second symmetry-determined conical intersection on the $B$ state for the collinear O–H–H geometry. The importance of this second conical intersection in the O(1D, 3P) + H$_2$ reaction system has been illustrated before. However, only recently has its possible influence on the H$_2$O photochemistry been seriously addressed. Mordaunt et al. pointed out, in a recent wavepacket calculation, that a small part of the dissociative flux on the $B$ surface goes toward the second conical intersection (O–H–H), thus indicating that this second intersection might also play a role in the $B$ state photo-dissociation and cause quantum interference.
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The experimental apparatus used for the H$_2$O photodissociation experiments, dissociation dynamics at different photolysis wavelengths were studied. The experimental apparatus used for the H$_2$O photodissociation study has been described in ref 43. In addition to the 157 and 121.6 nm used for photolysis, we have also used a tunable VUV source for the photolysis source. The tunable VUV light is generated using DFWM of the same $\lambda_1$ (212.5 nm) light for generating 121.6 nm light used for the first step of the H-atom Rydberg tagging and another tunable source from 532 to 750 nm. A molecular beam of H$_2$O was generated by expanding a mixture of H$_2$O/Ar through a pulsed nozzle. The rotational temperature of the H$_2$O molecules in the molecular beam is around 10 K.38 The detector in the photodissociation experiment is fixed in a direction perpendicular to that of the molecular beam. The molecular beam and the photolysis laser beam are perpendicular to each other.

III. H$_2$O Photochemistry via the $\tilde{A}^1B_1$ Surface: Direct Dissociation

Photodissociation of H$_2$O on the $\tilde{A}^1B_1$ surface has been studied at 157.6 nm using the HRTOF technique.39–41 The TOF spectrum of the H-atom product from H$_2$O photodissociation was measured and then converted into the product translational energy spectrum. Figure 2 shows the product TE spectrum of H$_2$O photodissociation at 157.6 nm with a molecular beam. Five vibrational features have been observed in the spectrum, which can be assigned to the vibrational excited OH($v = 0, 1, 2, 3, 4$) products. Rotational structures with higher rotational quantum number are partially resolved. By simulating and integrating each individual peak in the TE spectrum, the OH product vibrational distributions for the molecular beam and the water vapor can be obtained (Figure 3). Experimental results by the laser-induced fluorescence (LIF) method and theoretical results are also shown for comparison. By comparison of the cold molecular beam result with the room temperature vapor result, it seems that the rotational excitation of the parent
molecule has a negligible effect on the OH product vibrational distribution from H₂O photodissociation at 157.6 nm.

The OH product vibrational distributions obtained by HRTOF are significantly different from the one measured using the LIF method, especially for the higher vibrational states. This indicates that the vibrational distribution of OH obtained by previous LIF measurements may have serious errors. There are a few problems involved when one uses LIF to measure relative OH product vibrational populations. For example, propagation errors caused by changing laser dyes to cover all vibrational states, the errors caused by saturation effects, and the inaccurate off-diagonal Franck-Condon factors used in calibrating the LIF intensities. Predissociation of OH in the excited electronic state in the LIF scheme can also cause serious errors.

From Figure 3, the vibrational state distributions of the OH product obtained under the two experimental conditions are in good agreement with the theoretical results, suggesting that the overall accuracy of the theoretical calculations are fairly good for the \( v \leq 4 \) levels. There is, however, a large discrepancy between the previous theoretical results and experimental measurement at \( v = 5 \). This could come from the inaccuracies of the H₂O \( A \) state PES on which all previous theoretical calculations are based. Recent theoretical studies based on an improved PES have shown that this is truly the case. The agreement between the product state distributions from theory and experiment is much improved for H₂O. This improved \( A \) state PES is now believed to be one of the most accurate model potentials for direct dissociation processes in triatomic molecules.

Photodissociation of D₂O via the \( A \) state at 157.6 nm has also been investigated. Seven vibrational features have been observed. These features can be assigned to the vibrational excited OD products with \( v = 0 - 6 \). Because of the smaller OD rotational constant, the rotational structures are not as well resolved as in the H₂O case. It is interesting to point out that even though more vibrational states of the OD product in the D₂O photodissociation are populated in comparison with the OH product from H₂O photodissociation, the vibrational energy deposited into the OD product is quite similar to the OH product. The averaged vibrational energy deposited in the OH product is about 4170 cm⁻¹, while that deposited in the OD product is about 4310 cm⁻¹.

IV. H₂O photochemistry via the \( B^1A_1 \) Surface: Dissociation through Conical Intersections

Dissociation of H₂O on the \( B^1A_1 \) surface is a much more complicated case than on the \( A \) surface. Three electronic
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states have been implicated in the photochemistry of H₂O at 121.6 nm. Figure 4 shows the TE distribution of the products from H₂O photodissociation at 121.6 nm using two different laser polarization schemes. The three-dimensional (3D) contour of the TE distribution has also been shown in Figure 4. It is obvious that the most important pathway leads to the OH ground electronic state products in the ν = 0 state. Figure 5a shows the rotational distributions of the OH(X, ν = 0) product obtained from the simulations. Most of the OH(X, ν = 0) products are extremely rotationally excited with a peak at N ≈ 45, corresponding to about 32 000 cm⁻¹ rotational excitation. This is truly a phenomenal case in that almost 75% of the available energy is deposited into purely rotational excitation. Dynamical calculations using time-dependent wavepackets have shown that the high average rotational angular momentum of the OH product is the consequence of a high torque acting in the vicinity of the conical intersection at a collinear (H–O–H) geometry between B and X surfaces.

The most interesting observation in 121.6 nm photodissociation of H₂O is the intensity oscillations of the OH(X, ν = 0) rotational distribution. Figure 5a shows a clear oscillation around N = 40, with the odd N levels having enhanced population with respect to the neighboring even N levels. There is also another oscillation in the weaker peaks of the rotational distribution near N = 16. The two oscillations have also been observed in exactly the same region of the distribution for the rotational-dependent angular anisotropy parameter (Figure 5b). Two-dimensional quantum dynamical calculations, which span the regions that include both H–O–H and O–H–H conical intersections between the B and X surfaces, show that the even/odd intensity alternation in the OH(ν = 0) rotational distribution arises through a quantum interference between components of the wave function emanating on the X surface from these two conical intersections. The recent 3D dynamical calculations by Dixon also show the quantum interference between waves emanating from the two dissimilar conical intersections on the X surface. The interference pattern and the OH product rotational distribution are sensitive to the positions and energies of the conical intersections. This interesting feature provides a chemical analog of Young's well-known double-slit experiment.

The substitution of a hydrogen atom in H₂O by one deuterium atom often leads to significant changes in dynamics, particularly where nonadiabatic dissociation is involved. An HOD photodissociation experiment has recently been carried out to investigate such a dynamical effect. The observed highest peak in the product TE spectrum below the dissociation limit is the N = 47 level of OH(X²Π, ν = 0), which has a rotational energy of 33 400 cm⁻¹, already 94% of the bond dissociation energy of the OH molecule. Even more interesting, OH rotational states (N = 49, 50) above its dissociation limit have been detected. These extremely rotationally excited levels are clearly quasibound through the support of a centrifugal barrier. Rotational levels that are only slightly above the dissociation limit have a substantial centrifugal barrier to dissociation; therefore the tunneling probability is extremely small. However, as rotational excitation further increases, the centrifugal barrier is significantly reduced, and thus the tunneling probability through the centrifugal barrier is dramatically increased.

The photodissociation process, HOD + hν → OD + H, has also been studied at the 121.6 nm. Figure 6 shows the 3D contour of the H-atom product at 121.6 nm excitation. The rotational state distribution shows that the population of the OD(A³Σ⁺) product at ν = 0, N = 28, is much larger than that of
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OD in any other rotational states. This is a very interesting and unusual phenomenon. Based on a classical–quantum calculation, this single rotational state product propensity is attributed to a dynamically constrained threshold effect in the HOD photodissociation process.

Recently, van Harrevelt et al. have used their new PESs for water to carry out a complete 3D quantum mechanical description of its photodissociation at a number of energies following excitation. Those calculations show that both the absorption spectrum and the product state distributions are strongly influenced by transient resonances on the adiabatic potential energy surface, which probably involve both stretching and bending motions. Excitation of the H$_2$O to different unstable resonances in the $\tilde{B}$ state using HRTOF has recently been performed in our laboratory.

It is interesting that the rotational distributions of OH($A^2\Sigma^+$) products are dramatically different at five photolysis wavelengths. These features clearly indicate that different unstable resonance excitation on the $\tilde{B}$ state of H$_2$O has a different effect on the dynamics of OH($X^2\Pi$) and OH($A^2\Sigma^+$) products.

V. H$_2$O Photochemistry via the $\tilde{C}^1B_1$ Surface: Rotational Dependent Predissociation

The dissociation on the $\tilde{A}$ and $\tilde{B}$ states occurs extremely rapidly, typically in tens of femtoseconds, while the predissociation of the $\tilde{C}^1B_1$ state near 124 nm is much slower. This can be seen by its fully resolved rotational structure. The $\tilde{C}$ state predissociation lifetime is on the order of a few picoseconds. This is much longer than the rotational period of the H$_2$O molecule, which might result in variable dissociation dynamics. A recent study of the dissociation of H$_2$O via its $\tilde{C}$ state did indeed reveal rotational-state-specific dissociation dynamics. Figure 8 shows the photodissociation action spectrum for the $\tilde{C} \rightarrow \tilde{X}$ absorption band in which a few rotational lines are clearly resolved. The line widths are rotationally dependent and show an increase that is approximately proportional to $J(J+1)$ for the excited states. The TOF spectra of the H-atom product for all observed rotational lines were measured. Figure 9 shows the TOF spectra of the H-atom product for two rotational transitions, $0_0 \leftarrow 1_{10}$ and $1_{10} \leftarrow 0_0$. For the $0_0 \leftarrow 1_{10}$ transition, the two TOF spectra are virtually identical, as is expected for $J' = 0$, which has an isotropic wave function. The OH radicals
produced via this transition are vibrationally excited in the $X^2Π$ ground electronic state, with little rotational excitation. The vibrational state distribution for this rotational transition (Figure 10) extends to as high as $ν = 13$, with its peak around $ν = 7$. No OH products were observed in the $A^2Σ^+$ state via this transition. For the $1_{10} → 0_{00}$ transition, however, the two TOF spectra for the parallel and perpendicular directions are dramatically different from one another. Most of the OH $(X^2Π)$ products for this transition are in the $ν = 0$ state with extremely high rotational excitation, as are the OH $(A^2Σ^+)$ products.

An explanation for this dramatic variation in the rovibrational product distributions has been given by wavepacket calculations on 3D \textit{ab initio} PESs. Nonadiabatic coupling 

![Figure 8](image8.jpg)  
**FIGURE 8.** The rotational state resolved photodissociation action spectrum of the $\tilde{C}−\tilde{X}$ band.

![Figure 9](image9.jpg)  
**FIGURE 9.** Time-of-flight spectra of the H-atom product from H$_2$O photodissociation via the $0_{00} → 1_{10}$ and $1_{10} → 0_{00}$ rotational transitions of the $\tilde{C}−\tilde{X}$ band with the detection axis parallel and perpendicular to the laser polarization.

![Figure 10](image10.jpg)  
**FIGURE 10.** The total OH($X$) vibrational state distribution produced from the different rotational transitions of the $\tilde{C}−\tilde{X}$ band.
between the $\tilde{C}$ state and $\tilde{B}$ state surfaces is mediated by the electronic Coriolis interaction around the $\alpha$-axis of the water molecule, which has $a_2$ symmetry permitting transfer from $1B_1$ to $1A_1$. The dissociation dynamics via this route is quite similar to the direct excitation on the $\tilde{B}$ state. Despite the large vertical energy difference between the $\tilde{C}$ state and $\tilde{A}$ state, the homogeneous coupling route between these two PESs through electronic momentum coupling is still significant. Theoretical analysis shows that the wavepacket on the $\tilde{A}$ surface is completely diverted by the rising potential on the diagonal toward the two low-energy exit valleys, each leading to $H + \text{OH}(X^2\tilde{I})$. The slalom-like oscillation across these exit valleys is very evident, indicating high vibrational excitation of the $\text{OH}(X^2\tilde{I})$ products.

Figure 11 illustrates these two dynamically distinctive pathways. The $\tilde{C} \rightarrow \tilde{A}$ pathway is a direct dissociation process through homogeneous coupling that produces vibrationally hot and rotationally cold $\text{OH}$ product. The $\tilde{C} \rightarrow \tilde{B}$ pathway proceeds via Coriolis-type coupling that yields extremely rotationally hot and vibrationally cold ground-state $\text{OH}$ molecules, as well as rotationally hot $\text{OH}(A^2\Sigma^+)$ molecules. Based on experimental results, the branching ratios between the $\tilde{C} \rightarrow \tilde{A}$ and $\tilde{C} \rightarrow \tilde{B}$ pathways were derived. The branching ratio ($\tilde{C} \rightarrow \tilde{B}/\tilde{C} \rightarrow \tilde{A}$) is dependent on the $k_{a'}$ quantum number, but more slowly than quadratic, suggesting that there is some rotational enhancement of the $\tilde{C} \rightarrow \tilde{A}$ rate. This remarkable dynamical picture of $\text{H}_2\text{O}$ photodissociation provides an excellent case of nonadiabatic dynamics involving at least four electronic surfaces.

**VI. $\text{H}_2\text{O}$ Photochemistry via the $\tilde{D}^1\tilde{A}_1$ Surface: Fast Electronic Predissociation through the $\tilde{B}$ State**

The absorption band arising from the $\tilde{D}^1\tilde{A}_1$ state with its electronic origin around 122 nm shows no rotational structure. A strong interaction with the $\tilde{B}$ state due to avoiding crossing at bent geometries can explain this feature. The predissociation $\tilde{D} \rightarrow \tilde{B}$ is of purely electronic nature and therefore shows no isotope effect. Two-photon photodissociation dynamics of $\text{H}_2\text{O}$ via the $\tilde{D}$ state around 122 nm have been investigated recently.\(^5\) The width of the two-photon photodissociation action spectrum of the $\tilde{D} \rightarrow \tilde{X}$ transition gives an estimated lifetime of about 13.5 fs for the state. The $\text{OH}$ product TE distributions and angular distributions are qualitatively similar to those of 121.6 nm $\text{H}_2\text{O}$ photodissociation. This implies that photodissociation of $\text{H}_2\text{O}$ on the $\tilde{D}$ state proceeds via fast electronically nonadiabatic conversion to the $\tilde{B}$ state and the main dynamical features observed eventually are determined by the topography of the $\tilde{B}$ surface. The similar dynamics between 121.6 and 122 nm suggest that the initial excitation of $\text{H}_2\text{O}$ at the Lyman-$\alpha$ wavelength might also be through the $\tilde{B} \rightarrow \tilde{X}$ transition rather than the underlying $\tilde{B} \rightarrow \tilde{X}$ continuum. In any case, the dynamics at these two wavelengths are essentially controlled by the $\tilde{B}$ surface. The large discrepancies of branching ratios between experiment and theory suggest that the most recent calculated PESs of $\text{H}_2\text{O}$ are still inaccurate, especially in describing the nonadiabatic dissociation dynamics.
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VII. Concluding Remarks

The photochemistry of the water molecule has been studied using the HRTOF technique in a molecular beam. State-to-state dissociation dynamics have been carefully investigated at different excitation wavelengths. The A state photodissociation of H$_2$O has been studied at 157.6 nm and was found to be a fast and direct dissociation process on the single PES. The second excited singlet state (B) has been investigated at 121.6 nm and between 128 and 133 nm. Direct dissociation on this surface that leads to electronically excited OH(A$^2\Sigma^+$) fragments is a minor channel, while the dominant dissociation on this surface that leads to an H-atom plus a rovibrationally excited ground state OH molecule occurs via two conical intersections between B and X states. The strong quantum interference observed from the two dissimilar conical intersection pathways provides a chemical analogue of Young's well-known double-slit experiment. Dissociation on the C state presents an excellent example of rotational dependent predissociation. The C state decays via electronic Coriolis coupling to the B state or through a newly discovered homogeneous nonadiabatic coupling to the A state. Dissociation on the D state has also been studied and shows a fast electronic predissociation to the B state. Through the detailed investigations described above, a clear dynamical picture of H + OH channels from water photochemistry through excitation to its lowest four electronically excited states has been firmly established, providing an excellent case of polyatomic molecular photodissociation. It is necessary to point out that the O(1D) + H$_2$ channel is not detectable by HRTOF; therefore the importance of this channel is not discussed in this Account. Theoretical evidence in the QCT calculation suggest that this is not a major channel.43

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Biographical Information

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Richard N. Dixon was born in 1930 in Borough Green, Kent, England, and received his B.Sc. degree in physics from London University in 1951. He received his Ph.D. (1955) and D.Sc. (1976) degrees from Cambridge University. After a spell with the UKAEA, he was a postdoctoral fellow in Canada at the University of Western Ontario (1956–1957) and the National Research Council (1957–1959). He returned to England to a lectureship in chemistry at the University of Sheffield in 1959 and was appointed to a Professoral Chair at the University of Bristol in 1969. He was the Sorby Research Fellow of the Royal Society (1964–1969) and was elected FRS in 1986. He has won many awards, most recently the Rumford Medal of the Royal Society. His main research interests are in molecular spectroscopy, theoretical chemistry, and molecular reaction dynamics.

Xueming Yang was born in 1962 in Zhejiang, China, and received his B.S. degree in physics from Zhejiang Normal University in 1982 and his M. S. degree in chemical physics from Dalian Institute of Chemical Physics, CAS, in 1985. He obtained his Ph.D. in chemistry from University of California at Santa Barbara in 1991. After postdoctoral work at Princeton University and University of California at Berkeley, he became an associated research fellow in the Institute of Atomic and Molecular Sciences in Taipei in 1995 and was promoted to a full research fellow with tenure in 2000. In 2001, he made a move to the Dalian Institute of Chemical Physics, Chinese Academy of Sciences, and became the director of the State Key Laboratory of Molecular Reaction Dynamics. His main research interests are in the area of experimental chemical dynamics in the gas phase and at interfaces.

References