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Takashi Kumagai

Visualization of Hydrogen-Bond Dynamics

Water-Based Model Systems
on a Cu(110) Surface



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Visualization Of Hydrogen Bond Dynamics 125 Springer Theses

Ke-Li Han, Guang-Jiu Zhao



Visualization Of Hydrogen Bond Dynamics 125 Springer Theses:

Visualization of Hydrogen-Bond Dynamics Takashi Kumagai, 2012-09-02 The hydrogen bond represents an important interaction between molecules and the dynamics of hydrogen bonds in water create an ever present question associated with the process of chemical and biological reactions In spite of numerous studies the process remains poorly understood at the microscopic level because hydrogen bond dynamics such as bond rearrangements and hydrogen proton transfer reactions are extremely difficult to probe Those studies have been carried out by means of spectroscopic methods where the signal stems from the ensemble of a system and the hydrogen bond dynamics were inferred indirectly This book addresses the direct imaging of hydrogen bond dynamics within water based model systems assembled on a metal surface using a scanning tunneling microscope STM The dynamics of individual hydrogen bonds in water clusters hydroxyl clusters and water hydroxyl complexes are investigated in conjunction with density functional theory In these model systems quantum dynamics of hydrogen bonds such as tunneling and zero point nuclear motion are observed in real space Most notably hydrogen atom relay reactions which are frequently invoked across many fields of chemistry are visualized and controlled by STM This work presents a means of studying hydrogen bond dynamics at the single molecule level providing an important contribution to wide fields beyond surface chemistry *Recent Research Developments in Fluid Dynamics*, 2004 Fission-Track

Thermochronology and its Application to Geology Marco G. Malusà, Paul G. Fitzgerald, 2018-07-14 This book is focused on the basics of applying thermochronology to geological and tectonic problems with the emphasis on fission track thermochronology It is conceived for relatively new practitioners to thermochronology as well as scientists experienced in the various methods The book is structured in two parts Part I is devoted to the fundamentals of the fission track method to its integration with other geochronologic methods and to the basic principles of statistics for fission track dating and sedimentology applied to detrital thermochronology Part I also includes the historical development of the technique and thoughts on future directions Part II is devoted to the geological interpretation of the thermochronologic record The thermal frame of reference and the different approaches for the interpretation of fission track data within a geological framework of both basement and detrital studies are discussed in detail Separate chapters demonstrate the application of fission track thermochronology from various perspectives e g tectonics petrology stratigraphy hydrocarbon exploration geomorphology with other chapters on the application to basement rocks in orogens passive continental margins and cratonic interiors as well as various applications of detrital thermochronology **The Functional Nucleus** David P. Bazett-Jones, Graham

Dellaire, 2016-10-17 This book gives an in depth overview on nuclear structure and function It clearly shows that the epigenome and the three dimensional organization of the nucleus are not independent properties The intimate relationship between the location and the epigenetic modifications of gene loci is highlighted Finally it shows that the complex three dimensional organization of the nucleus is not just of academic interest The structure composition and function of virtually all

of the sub nuclear compartments identified so far can be implicated to a list of human genetic diseases Hence a detailed elucidation of how these domains are assembled and function will provide new opportunities for therapeutic intervention in clinical practice **Metals Abstracts** ,1984 **International Books in Print** ,1979 **Hydrogen Bond Networks** M.C. Bellissent-Funel,J.C. Dore,2013-04-17 The almost universal presence of water in our everyday lives and the very common nature of its presence and properties possibly deflects attention from the fact that it has a number of very unusual characteristics which furthermore are found to be extremely sensitive to physical parameters chemical environment and other influences Hydrogen bonding effects too are not restricted to water so it is necessary to investigate other systems as well in order to understand the characteristics in a wider context Hydrogen Bond Networks reflects the diversity and relevance of water in subjects ranging from the fundamentals of condensed matter physics through aspects of chemical reactivity to structure and function in biological systems Hydrogen Bonding - New Insights Slawomir Grabowski,2006-10-07 Hydrogen Bonding New Insights is an extensive text which takes numerous examples from experimental studies and uses these to illustrate theoretical investigations to allow a greater understanding of hydrogen bonding phenomenon The most important topics in recent studies are considered including Intra molecular H bonds Differences between H bond and van der Waals interactions from one side and covalent bonds from the other Bader theory to analyze H bonding Influence of weak H bonds upon structure and function of biological molecules H bonds in crystal structures With contributions from some of the foremost experts in this field this volume provides an invaluable resource for all members of the academic community looking for a comprehensive text on hydrogen bonding It will be of particular interest to physical and theoretical chemists spectroscopists crystallographers and those involved with chemical physics

Hydrogen-Bonded Liquids J.C. Dore,José Teixeira,2012-10-10 The study of liquids covers a wide range of scientific disciplines primarily in physics and chemistry As a result of this disparate activity the links between new developments in remote fields are seldom co ordinated into a single conference The objective of the present meeting was to gather together people with different forms of expertise Previous ASI meetings on the liquid state have been held over an extended period and have occurred on a three yearly basis The first meeting in this series was on Structure and Dynamics of Liquids in 1980 and was held on the island of Corsica The next meeting on Molecular liquids Dynamics and Interactions was held in Florence in 1983 and was followed by Aqueous Solutions at the Institut d Etudes Scientifiques de Cargese in 1986 It therefore seemed a natural choice to select Cargese for the next meeting in 1989 and to choose a topic which emphasised a particular area of liquid state studies Due to our own involvement in collaborative research we considered that Hydrogen bonded liquids would be an appropriate topic One of its attractions was that there was much new material coming from widely disparate investigations and it would be a convenient time to draw together the different strands The particular interest in water was clearly central to this topic but it was thought desirable to set this development in the wider context of other systems in

which hydrogen bonding plays a significant role *Supramolecular Assembly Via Hydrogen Bonds I* D. M. P.

Mingos, 2004-01-28 **Ultrafast Hydrogen Bonding Dynamics and Proton Transfer Processes in the Condensed Phase** Thomas Elsaesser, H.J. Becker, 2013-03-14 Hydrogen bonds represent type of molecular interaction that determines the structure and function of a large variety of molecular systems The elementary dynamics of hydrogen bonds and related proton transfer reactions both occurring in the ultra fast time domain between 10⁻¹⁴ and 10⁻¹¹s form a research topic of high current interest In this book addressing scientists and graduate students in physics chemistry and biology the ultra fast dynamics of hydrogen bonds and proton transfer in the condensed phase are reviewed by leading scientists documenting the state of the art in this exciting field from the viewpoint of theory and experiment The nonequilibrium behavior of hydrogen bonded liquids and intramolecular hydrogen bonds as well as photo induced hydrogen and proton transfer are covered in 7 chapters making reference to the most recent literature **Hydrogen Bonding Dynamics in Liquids** Lucas Julian Gunkel, 2025 Liquids may appear disordered compared to the structured nature of crystals but this is only true when considering long range order Unlike ideal gases most liquids exhibit local order due to molecular interactions ranging from dipole dipole to electrostatic interactions For example water forms an extensive hydrogen bond network or molecular liquids such as alcohols can form aggregates Understanding intermolecular forces especially hydrogen bonding is crucial for insights into phenomena like water's density anomalies This thesis addresses three topics within the framework of hydrogen bonding in liquids with a particular focus on the dynamics of these bonds We employ linear and two dimensional infrared spectroscopy 2DIR alongside ab initio molecular dynamics AIMD simulations to explore bonding in liquids In the first project we employ linear and two dimensional infrared 2DIR spectroscopy to investigate the correlation of the donating hydrogen bonds of water Water has previously been proposed to form asymmetric hydrogen bonds based on X ray absorption studies This supposed asymmetry has been controversially discussed Our results provide experimental evidence for dynamic anti correlations instead of static asymmetric hydrogen bonds We use 2DIR spectroscopy to isolate the inhomogeneous contributions to the lineshape for pure and isotopically dilute HOD in H₂O D₂O in dimethylformamide DMF Through the dilution in DMF each water molecule only forms two donating hydrogen bonds to the solvent This allows us to distinguish between symmetric and asymmetric stretching modes for D₂O Comparison with density functional theory calculations DFT show that the about twice broader inhomogeneous lineshape of HOD can be explained by an anti correlated distribution of hydrogen bonds Furthermore analysis of the crosspeaks for D₂O give direct experimental evidence for the anti correlation We find that this anti correlation quickly decays *Hydrogen Bonding and Transfer in the Excited State* Ke-Li Han, Guang-Jiu Zhao, 2011-03-16 This book gives an extensive description of the state of the art in research on excited state hydrogen bonding and hydrogen transfer in recent years Initial chapters present both the experimental and theoretical investigations on the excited state hydrogen bonding structures and dynamics of many organic and biological chromophores

Following this several chapters describe the influences of the excited state hydrogen bonding on various photophysical processes and photochemical reactions for example hydrogen bonding effects on fluorescence emission behaviors and photoisomerization the role of hydrogen bonding in photosynthetic water splitting photoinduced electron transfer and solvation dynamics in room temperature ionic liquids and hydrogen bonding barrier crossing dynamics at bio mimicking surfaces Finally the book examines experimental and theoretical studies on the nature and control of excited state hydrogen transfer in various systems Hydrogen Bonding and Transfer in the Excited State is an essential overview of this increasingly important field of study surveying the entire field over 2 volumes 40 chapters and 1200 pages It will find a place on the bookshelves of researchers in photochemistry photobiology photophysics physical chemistry and chemical physics

Quantum and Classical Aspects of Hydrogen Bond Dynamics Abarrul Ikram,1996 *The Hydrogen Bond* P. Schuster,G. Zundel,C. Sandorfy,1976 **Water Hydrogen Bond Structure and Dynamics in Ionic and Polymeric Aqueous Systems** Sean Anthony Roget,2022 Water is a simple molecule with many unique physical properties that are critical to life on earth Its properties arise from its extended hydrogen bonded network in which water water hydrogen bonds are constantly breaking and forming However in many biological systems and materials the water network is impacted by the presence of solutes and interfaces In this thesis the structure and dynamics of the hydrogen bond network are examined in technologically relevant materials where water plays a key role The systems studied include fuel cell membranes hydrogels and concentrated salt solutions Nonlinear infrared spectroscopy can be used to experimentally observe ultrafast motions of water as well as its structural configurations within complex chemical systems Polarization selective pump probe experiments on the OD stretch of dilute HOD in water provide information on both orientational and vibrational relaxation Orientational relaxation describes the reorientation dynamics of water molecules in the hydrogen bond network If angular diffusion is restricted orientational relaxation also provides insight into how water may be sterically hindered within its environment Vibrational relaxation describes coupling of vibrational energy absorbed by the HOD molecules to its surrounding media The vibrational lifetime provides details on the local interactions of HOD and may allow separation of distinct dynamics near different species Two dimensional vibrational echo experiments on HOD molecules observe the time scales for structural evolution of the surrounding environment through ultrafast vibrational frequency fluctuations With these experimental techniques a holistic picture of the structure and motions of the water hydrogen bond network can be acquired

Hydrogen Bonding Research in Photochemistry, Photobiology, and Optoelectronic Materials Ke-Li Han,Guangjiu Zhao,2019 As one of the typical intermolecular interactions hydrogen bonding plays a significant role in molecular structure and function When the hydrogen bond research system is connected with the photon the hydrogen bonding effect turns to an excited state one influencing photochemistry photobiology and photophysics Thus the hydrogen bond in an excited state is a key topic for understanding the excited state properties especially for optoelectronic or

luminescent materials The approaches presented in this book include quantum chemical calculation molecular dynamics simulation and ultrafast spectroscopy which are strong tools to investigate the hydrogen bond Unlike other existing titles this book combines theoretical calculations and experiments to explore the nature of excited state hydrogen bonds By using these methods more details and faster processes involved in excited state dynamics of hydrogen bond are explored This highly interdisciplinary book provides an overview of leading hydrogen bond research It is essential reading for faculties and students in researching photochemistry photobiology and photophysics as well as novel optoelectronic materials fluorescence probes and photocatalysts It will also guide research beginners to getting a quick start within this field Publisher's website

Unravelling the Ultrafast Dynamics of Aqueous Hydrogen Bond Networks with 2D IR Vibrational Echo Spectroscopy

Rongfeng Yuan, 2019 Water is one of the most important substances in the world It is used in a wide range of technologies and is an essential ingredient in all living cells we know today The structure of water molecule is simple yet it can form extended and versatile hydrogen bond HB network This ability gives water extraordinary properties such as high boiling and melting point At the same time the hydrogen bond network is not static The constant breaking and re-forming of hydrogen bond occurs on the picosecond timescale This dynamic network facilitates many functions of water including ions solvation protein folding and electricity conduction Understanding the structure and dynamics of these processes is therefore of great importance Ultrafast infrared IR spectroscopies offer a great method for accessing the sub-picosecond to picoseconds dynamics while a system is in an electronic ground state During the past two decades hydrogen bond dynamics has been investigated extensively using ultrafast IR spectroscopies But many questions still exist such as the effect of ions and confinement on the hydrogen bonding dynamics and the relation between the anomalous proton diffusion in dilute solution and hydrogen bonding In Chapter 3 we examined the nature of molecular anion hydrogen bonding The CN stretch of selenocyanate anions SeCN was used as the vibrational probe in heavy water D₂O We observed the non-Condon effect on the CN stretch whose transition dipole changes with the strength of hydrogen bonding with water In addition HB rearrangement dynamics reported by SeCN is almost the same as was that of the OH stretch of HOD molecules This result shows that this anion does not perturb the surrounding HB network significantly in the low salt concentration solution This ionic perspective is important and complements the results using OD or OH stretch of HOD molecules which can only probe the effect of ions in a high salt concentration condition In Chapter 4 we used SeCN as the probe to examine water dynamics in confinement and I focused on the nano waterpool formed in reverse micelles The water pool is surrounded by surfactants which are further solvated by organic hydrophobic solvents For large reverse micelle whose diameter is larger than 4 nm the water pool is usually divided into two regions the core region where water dynamics is like that in pure water and the interface region where water dynamics is slowed significantly due to the confinement Here we used ultrafast IR spectroscopies to measure the orientational relaxation of SeCN which reflects its interaction with water molecules and how rigid the HB

network is Based on the comparison between linear IR decomposition and ultrafast anisotropy dynamics we proposed a three component model of water in large reverse micelles The interface component should be further separated into two layers One layer corresponds to water in contact with the surfactant head group and has very slow reorientation The other layer corresponds to water molecules whose coordinating structure still resembles that of bulk but the dynamics is slowed down due to the perturbation from confinement In Chapter 5 and 6 hydrogen bonding dynamics in concentrated salt and acid solutions were investigated Through electrochemical method it was found decades ago that proton has extraordinary ion mobility about 6 times larger than that of cations of similar size such as sodium ammonium or lithium The great difference between them results from the cation transport mechanism In dilute solution the main transport mechanism of proton is through relay mechanism where the identity of proton transfers from one water molecule to another This minimizes the physical diffusion of the atoms and greatly increases the proton mobility The mechanism is generally called Grotthuss mechanism which was came up with by Grotthuss in 1806 though not on the molecular level However the step time of a single proton transfer event between two water molecules is difficult to observe experimentally Here we used the CN stretch of methyl thiocyanate MeSCN as the vibrational probe In concentrated hydrochloric solutions it has two frequency resolved states One state refers to water hydrogen bonded to the nitrogen lone pair while the other state corresponds to hydronium ion hydrogen bonded to the CN Chemical exchange phenomenon was observed between these two states Ab initio simulation done by our collaborator shows that the proton hopping is the dominate mechanism for chemical exchange The comparison experiment done in lithium chloride solution provides further contrast between hydronium and other metal ions Therefore we were able to track proton hopping in a time resolved manner for the first time Extrapolation to the dilute limit demonstrates that the HB rearrangement in pure water is the driving force of proton hopping in dilute solution

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