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Takashi Kumagai

Visualization of Hydrogen-Bond Dynamics

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



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Masayoshi Nakasako



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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

Gray's Anatomy E-Book Susan Standring, 2021-05-22 Selected for 2025 Doody's Core Titles in Neuroscience In 1858 Drs Henry Gray and Henry Vandyke Carter created a book for their surgical colleagues that established an enduring standard among anatomical texts After more than 160 years of continuous publication Gray's Anatomy remains the definitive comprehensive reference on the subject offering ready access to the information you need to ensure safe effective practice This 42nd edition has been meticulously revised and updated throughout reflecting the very latest understanding of clinical anatomy from the world's leading clinicians and biomedical scientists The book's acclaimed lavish art programme and clear text has been further enhanced while major advances in imaging techniques and the new insights they bring are fully captured in state of the art X ray CT MR and ultrasonic images The accompanying eBook version is richly enhanced with additional content and media covering all the body regions cell biology development and embryogenesis and now includes two new systems orientated chapters This combines to unlock a whole new level of related information and interactivity in keeping with the spirit of innovation that has characterised Gray's Anatomy since its inception The result is a more complete practical and engaging resource than ever before which will prove invaluable to all clinicians who require an accurate in depth knowledge of anatomy Each chapter has been edited by international leaders in their field ensuring access to the very latest evidence based information on topics Over 150 new radiology images offering the very latest X ray multiplanar CT and MR perspectives including state of the art cinematic rendering The downloadable Expert Consult eBook version included with your print purchase allows you to easily search all of the text figures references and videos from the book on a variety of devices Electronic enhancements include additional text tables illustrations labelled

imaging and videos as well as 21 specially commissioned Commentaries on new and emerging topics related to anatomy Now featuring two extensive electronic chapters providing full coverage of the peripheral nervous system and the vascular and lymphatic systems

Hydration Structures of Proteins Masayoshi Nakasako, 2021-10-25 This book describes hydration structures of proteins by combining experimental results with theoretical considerations It is designed to introduce graduate students and researchers to microscopic views of the interactions between water and biological macromolecules and to provide them with an overview of the field Topics on protein hydration from the past 25 years are examined most of which involve crystallography fluorescence measurements and molecular dynamics simulations In X ray crystallography and molecular dynamics simulations recent advances have accelerated the study of hydration structures over the entire surface of proteins Experimentally crystal structure analysis at cryogenic temperatures is advantageous in terms of visualizing the positions of hydration water molecules on the surfaces of proteins in their frozen hydrated crystals A set of massive data regarding hydration sites on protein surfaces provides an appropriate basis enabling us to identify statistically significant trends in geometrical characteristics Trajectories obtained from molecular dynamics simulations illustrate the motion of water molecules in the vicinity of protein surfaces at sufficiently high spatial and temporal resolution to study the influences of hydration on protein motion Together with the results and implications of these studies the physical principles of the measurement and simulation of protein hydration are briefly summarized at an undergraduate level Further the author presents recent results from statistical approaches to characterizing hydrogen bond geometry in local hydration structures of proteins The book equips readers to better understand the structures and modes of interaction at the interface between water and proteins Referred to as hydration structures they are the subject of much discussion as they may help to answer the question of why water is indispensable for life at the molecular and atomic level

Handbook on Planning and Complexity Gert de Roo, Claudia Yamu, Christian Zuidema, 2020-06-26 This Handbook shows the enormous impetus given to the scientific debate by linking planning as a science of purposeful interventions and complexity as a science of spontaneous change and non linear development Emphasising the importance of merging planning and complexity this comprehensive Handbook also clarifies key concepts and theories presents examples on planning and complexity and proposes new ideas and methods which emerge from synthesising the discipline of spatial planning with complexity sciences

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

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

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^{-11} s 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-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 coordinated 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 **The Hydrogen Bond** P. Schuster, G. Zundel, C. Sandorfy, 1976

Supramolecular Assembly via Hydrogen Bonds I David Michael P. Mingos, 2004-01-28 Hydrogen-bonding Research In Photochemistry, Photobiology, And Optoelectronic Materials Keli Han, Guangjiu Zhao, 2019-03-13 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 **Hydrogen Bonds** Peter Schuster, 2014-01-15 **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

The Hydrogen Bond and the Water Molecule Yves Marechal, 2006-12-11 The Hydrogen Bond and the Water Molecule offers a synthesis of what is known and currently being researched on the topic of hydrogen bonds and water molecules The most simple water molecular H₂O is a fascinating but poorly understood molecule Its unique ability to attract an exceptionally large number of hydrogen bonds induces the formation of a dense hydrogen bond network that has the potential to modify the properties of the surrounding molecules and their reactivities The crucial role that water

molecules play is described in this book. The author begins by providing an overview of the thermodynamical and structural properties of H bonds before examining their much less known dynamical properties which makes them appear as centres of reactivity. Methods used to observe these components are also reviewed. In the second part of the book the role played by the dense H bond network developed by H₂O molecules is examined. First in ice where it has important atmospheric consequences then in liquid water and finally in macromolecules where it sheds some original light on the fundamental question: How is it that without water and hydrogen bonds life would not exist? This book will be of interest to researchers in the fields of physics, chemistry, biochemistry and molecular biology. It can also serve as a teaching aid for students attending course in chemical physics, chemistry or molecular biology. Engineers involved in the water industry would benefit from reading this book as would scientists working in pharmaceuticals, cosmetics and materials. Overview of what is known and being researched on the topic of hydrogen bonds and water molecules. Reviews methods used to observe interactions between water molecules and hydrogen bonds. Examines role of H bond network developed by H₂O molecules.

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