Interfaces In Materials Atomic Structure Thermodynamics And Kinetics Of Solid Vapor Solid Liquid

This handbook brings together, under a single cover, all aspects of the chemistry, physics, and engineering of surfaces and interfaces of materials currently studied in academic and industrial research. It covers different experimental and theoretical aspects of surfaces and interfaces, their physical properties, and spectroscopic techniques that have been applied to a wide class of inorganic, organic, polymer, and biological materials. The diversified technological areas of surface science reflect the explosion of scientific information on surfaces and interfaces of materials and their spectroscopic characterization. The large volume of experimental data on chemistry, physics, and engineering aspects of materials surfaces and interfaces remains scattered in so many different periodicals, therefore this handbook compilation is needed. The information presented in this multivolume reference draws on two decades of pioneering research on the surfaces and interfaces of materials to offer a complete perspective on the topic. These five volumes-Surface and Interface Phenomena; Surface Characterization and Properties; Nanostructures, Micelles, and Colloids; Thin Films and Layers; Biointerfaces and Applications-provide multidisciplinary review chapters and summarize the current status of the field covering important scientific and technological developments made over past decades in surfaces and interfaces of materials and spectroscopic techniques with contributions from internationally recognized experts from all over the world. Fully cross-referenced, this book has clear, precise, and wide appeal as an essential reference source long due for the scientific community. The complete reference on the topic of surfaces and interfaces of materials The information presented in this multivolume reference draws on two decades of pioneering research Provides multidisciplinary review chapters and summarizes the current status of the field Covers important scientific and technological developments made over past decades in surfaces and interfaces of materials and spectroscopic techniques Contributions from internationally recognized experts from all over the world

Computational Materials Science provides the theoretical basis necessary for understanding atomic surface phenomena and processes of phase transitions, especially crystallization, is given. The most important information concerning computer simulation by different methods and simulation techniques for modeling of physical systems is also presented. A number of results are discussed regarding modern studies of surface processes during crystallization. There is sufficiently full information on experiments, theory, and simulations concerning the surface roughening transition, kinetic roughening, nucleation kinetics, stability of crystal shapes, thin film formation, imperfect structure of small crystals, size dependent growth velocity, distribution coefficient at growth from alloy melts, superstructure ordering in the intermetallic compound. Computational experiments described in the last chapter allow visualization of the course of many processes and better understanding of many key problems in Materials Science. There is a set of practical steps concerning computational procedures presented. Open access to executable files in the book make it possible for everyone to understand better phenomena and processes described in the book. Valuable reference book, but also helpful as a supplement to courses Computer programs available to supplement examples Presents several new methods of computational materials science and clearly summarizes previous methods and results

An advanced level textbook covering geometric, chemical, and electronic structure of electronic materials, and their applications to devices based on semiconductor surfaces, metal-semiconductor interfaces, and semiconductor heterojunctions. Starting with the fundamentals of electrical measurements on semiconductor interfaces, it then describes the importance of controlling macroscopic electrical properties by atomic-scale techniques. Subsequent chapters present the wide range of surface and interface techniques available to characterize electronic, optical, chemical, and structural properties of electronic materials, including semiconductors, insulators, nanostructures, and organics. The essential physics and chemistry underlying each technique is described in sufficient depth with references to the most authoritative sources for more exhaustive discussions, while numerous examples are provided throughout to illustrate the applications of each technique. With its general reading lists, extensive citations to the text, and problem sets appended to all chapters, this is ideal for students of electrical engineering, physics and materials science. It equally serves as a reference for physicists, material science and electrical and electronic engineers involved in surface and interface science, semiconductor processing, and device modeling and design. This is a coproduction of Wiley and IEEE * Free solutions manual available for lecturers at www.wiley-vch.de/supplements/

Edited by acclaimed science writer and physicist James Trefil, the Encyclopedia's 1000 entries combine in-depth coverage with a vivid graphic format to bring every facet of science, technology, and medicine into stunning focus. From absolute zero to the Mesozoic era to semiconductors to the twin paradox, Trefil and his co-authors have an uncanny ability to convey how the universe works and to show readers how to apply that knowledge to everyday problems.

An Essential Guide to Electronic Material Surfaces and Interfaces is a streamlined yet comprehensive introduction that covers the basic physical properties of electronic materials, the experimental techniques used to measure them, and the theoretical methods used to understand, predict, and design them. Starting with the fundamental electronic properties of semiconductors and electrical measurements of semiconductor interfaces, this text introduces students to the importance of characterizing and controlling macroscopic electrical properties by atomic-scale techniques. The chapters that follow present the full range of surface and interface techniques now being used to characterize electronic, optical, chemical, and structural properties of electronic materials, including semiconductors, insulators, nanostructures, and organics. The essential physics and chemistry underlying each technique is described in sufficient depth for students to master the fundamental principles, with numerous examples to illustrate the strengths and limitations for specific applications. As well as references to the most authoritative sources for broader discussions, the text includes internet links to additional examples, mathematical derivations, tables, and literature references for the advanced student, as well as professionals in these fields. This textbook fills a gap in the existing literature for an entry-level course that provides the physical properties, experimental techniques, and theoretical methods essential for students and professionals to understand and participate in solid-state electronics, physics, and materials science research. An Essential Guide to Electronic Material Surfaces and Interfaces is an introductory-to-intermediate level textbook suitable for students of physics, electrical engineering, materials science, and other disciplines. It is essential reading for any student or professional engaged in surface and interface research, semiconductor processing, or electronic device design.

An Instructor's Manual presenting detailed solutions to all the problems in the book is available from the Wiley editorial department.

The classic book that presents a unified approach to crystallography and the defects found within crystals, revised and updated This new edition of Crystallography and Crystal Defects explains the modern concepts of crystallography in a clear, succinct manner and shows how to apply these concepts in the analyses of point, line and planar defects in crystalline materials. Fully revised and updated, this book now includes: Original source references to key crystallographic terms familiar to materials scientists Expanded discussion on the elasticity of cubic materials New content on texture that contains more detail on Euler angles, orientation distribution functions and an expanded discussion on examples of textures in engineering materials Additional content on dislocations in materials of symmetry lower than cubic An expanded discussion of twinning which includes the description and classification of growth twins The inclusion and explanation of results from atomistic modelling of twin boundaries Problem sets with new questions, detailed worked solutions, supplementary lecture material and online computer programs for crystallographic calculations. Written by authors with extensive lecturing experience at undergraduate level, Crystallography and Crystal Defects, Third Edition continues to take its place as the core text on the topic and provides the essential resource for students and researchers in metallurgy, materials science, physics, chemistry, electrical, civil and mechanical engineering.

This book describes a body of work whose ultimate goal is to optimize the design of microbatteries. It focuses on the fundamental properties of the structure and atomic diffusion in glassy materials which optimize the properties of the electrolyte. Experimental results and their phenomenological description of lithium borate glasses are extensively covered. Other chapters discuss the effects of barriers between the electrodes and the electrolyte and the book culminates with a description of actual progress in making applications of these materials to batteries, sensors and other devices. Contents:Models of Atomic Diffusion (R J Elliott)A Theory of Glass Formation (R Kerner)Structural and Vibrational Properties of B2O3 and Related Glasses (R A Barrio)Properties of Borate Glasses: Structure, Vibrational Properties and Transport Experimental Approach (M Massot)Theory of Atomic Diffusion Across Interfaces (J Deppe)Applications of Superionic Conductors in Microbatteries and Elsewhere (M Balkanski) Readership: Condensed matter physicists. keywords:Diffusion;Atomic Jump Tracer Batteries, Solid State Glasses;Borates Transition Materials;Disordered Amorphous Superionic Conductivity;Ionic Spectra;Infra-Red Raman Vibtations;Atomic

Engineering materials with desirable physical and technological properties requires understanding and predictive capability of materials behavior under varying external conditions, such as temperature and pressure. This immediately brings one face to face with the fundamental difficulty of establishing a connection between materials behavior at a microscopic level, where understanding is to be sought, and macroscopic behavior which needs to be predicted. Bridging the corresponding gap in length scales that separates the ends of this spectrum has been a goal intensely pursued by theoretical physicists, experimentalists, and metallurgists alike. Traditionally, the search for methods to bridge the length scale gap and to gain the needed predictive capability of materials properties has been conducted largely on a trial and error basis, guided by the skill of the metallurgist, large volumes of experimental data, and often ad hoc semi phenomenological models. This situation has persisted almost to this day, and it is only recently that significant changes have begun to take place. These changes have been brought about by a number of developments, some of long standing, others of more recent vintage.

The behaviour of many materials critically depends on processes at interfaces and surfaces. This volume presents up-to-date reviews on atomic structure and properties of interfaces.

Interfaces in MaterialsAtomic Structure, Thermodynamics and Kinetics of Solid-Vapor, Solid-Liquid and Solid-Solid InterfacesWiley-Interscience

Ceramic Materials: Science and Engineering is an up-to-date treatment of ceramic science, engineering, and applications in a single, integrated text. Building on a foundation of crystal structures, phase equilibria, defects and the mechanical properties of ceramic materials, students are shown how these materials are processed for a broad diversity of applications in today's society. Concepts such as how and why ions move, how ceramics interact with light and magnetic fields, and how they respond to temperature changes are discussed in the context of their applications. References to the art and history of ceramics are included throughout the text. The text concludes with discussions of ceramics in biology and medicine, ceramics as gemstones and the role of ceramics in the interplay between industry and the environment. Extensively illustrated, the text also includes questions for the student and recommendations for additional reading. KEY FEATURES: Combines the treatment of bioceramics, furnaces, glass, optics, pores, gemstones, and point defects in a single text Provides abundant examples and illustrations relating theory to practical applications Suitable for advanced undergraduate and graduate teaching and as a reference for researchers in materials science Written by established and successful teachers and authors with experience in both research and industry

This volume is a collection of papers written by the authors who were selected among the members of a project on ``Metal-Semiconductor Interfaces'' sponsored by the Ministry of Education, Science and Culture of Japan (MON-BUSHO). The M-S Interface is a problem which stems from the 1930's when the concept of surface states was first proposed by Tamm, shortly later by Shockley, and then clearly by Bardeen in 1947 to catalyze the invention of the transistor, and still exists today when one can count almost one billion M-S interfaces or contacts in a Si chip whose size is less than 1 cm square. Consequently, there have been plenty of research activities all over the world, especially over the last 15 years. The ``M-S Interfaces'' project was composed of four research branches to tackle the following subjects to be reported in the book: Theoretical Approaches, Initial Stage of M-S Interface Formation, Interface Structure of M-S Systems, Realization and Control of Contact Characterization, and Novel Characterization Techniques of Buried Interfaces.

This fifth edition of the highly regarded family of titles that first published in 1965 is now a three-volume set and over 3,000 pages. All chapters have been revised and expanded, either by the fourth edition authors alone or jointly with new co-authors. Chapters have been added on the physical metallurgy of light alloys, the physical metallurgy of titanium alloys, atom probe field ion microscopy, computational metallurgy, and orientational imaging microscopy. The books incorporate the latest experimental research results and theoretical insights. Several thousand citations to the research and review literature are included. Exhaustively synthesizes the pertinent, contemporary developments within physical metallurgy so scientists have authoritative information at their fingertips Replaces existing articles and monographs with a single, complete solution Enables metallurgists to predict changes and create novel alloys and processes

Many of the most important properties of materials in high-technology applications are strongly influenced or even controlled by the presence of solid interfaces. In this work, leading international authorities review the broad range of subjects in this field focusing on the atomic level properties of solid interfaces.

Mechanics of Carbon Nanotubes: Fundamentals, Modeling and Safety draws on the latest academic research and nanotechnology applications to provide a comprehensive guide on the most recent developments in the science of carbon nanotubes. The fundamentals of nanomechanics and mechanical behavior of carbon nanotubes are presented in initial chapters, followed by more advanced topics such as the classification of carbon nanotubes, carbon nanotubes in nanocomposites, multiwall carbon nanotubes, and recent trends. This book provides a system for the classification of carbon nanotubes into 20 classes, aiding correct selection for various applications, and includes the Atomic Registry Matrix Analysis for nanoscale interfaces, essential for design involving friction or sliding. Parametric maps are included to help readers pick the correct model for a particular CNT geometry, in addition to a thorough examination of the effective thickness paradox and safety issues related to CNTs, such as toxicity at high aspect ratio. Mechanics of Carbon Nanotubes is essential reading for anyone involved in research or engineering that includes carbon nanotubes, be they students or seasoned professionals in the field. It is particularly useful to those working with applications in the areas of microelectronics, robotics, aerospace, composites, or prosthetics. Provides a system for the classification of carbon nanotubes, aiding correct selection for various applications Includes the Matrix Registry Analysis for nanoscale interfaces that is essential for design involving friction or sliding Features parametric maps to help readers pick the right model for a particular CNT geometry (beam vs. shell vs. thin or thick shells, etc.) Presents a thorough examination of the safety issues related to CNTs, including toxicity at high aspect ratio

This open access book brings out the state of the art on how informatics-based tools are used and expected to be used in nanomaterials research. There has been great progress in the area in which “big-data” generated by experiments or computations are fully utilized to accelerate discovery of new materials, key factors, and design rules. Data-intensive approaches play indispensable roles in advanced materials characterization. "Materials informatics" is the central paradigm in the new trend. "Nanoinformatics" is its essential subset, which focuses on nanostructures of materials such as surfaces, interfaces, dopants, and point defects, playing a critical role in determining materials properties. There have been significant advances in experimental and computational techniques to characterize individual atoms in nanostructures and to gain quantitative information. The collaboration of researchers in materials science and information science is growing actively and is creating a new trend in materials science and engineering. This book is open access under a CC BY license.

Scanning transmission electron microscopy has become a mainstream technique for imaging and analysis at atomic resolution and sensitivity, and the authors of this book are widely credited with bringing the field to its present popularity. Scanning Transmission Electron Microscopy(STEM): Imaging and Analysis will provide a comprehensive explanation of the theory and practice of STEM from introductory to advanced levels, covering the instrument, image formation and scattering theory, and definition and measurement of resolution for both imaging and analysis. The authors will present examples of the use of combined imaging and spectroscopy for solving materials problems in a variety of fields, including condensed matter physics, materials science, catalysis, biology, and nanoscience. Therefore this will be a comprehensive reference for those working in applied fields wishing to use the technique, for graduate students learning microscopy for the first time, and for specialists in other fields of microscopy.

The Advanced Study Institute provided an opportunity for researchers in universities, industry and National and International Laboratories, from the disciplines ofmaterials science, physics, chemistry and engineering to meet together in an assessment of the impact of electron and scanning probe microscopy on advanced material research. Since these researchers have traditionally relied upon different approaches, due to their different scientific background, to advanced materials problem solving, presentations and discussion within the Institute sessions were initially devoted to developing a set ofmutually understood basic concepts, inherently related to different techniques ofcharacterization by microscopy and spectroscopy. Particular importance was placed on Electron Energy Loss Spectroscopy (EELS), Scanning Probe Microscopy (SPM), High Resolution Transmission and Scanning Electron Microscopy (HRTEM, HRSTEM) and Environmental Scanning Electron Microscopy (ESEM). It was recognized that the electronic structure derived directly from EELS analysis as well as from atomic positions in HRTEM or High Angle Annular Dark Field STEM can be used to understand the macroscopic behaviour of materials. The emphasis, however, was upon the analysis of the electronic band structure of grain boundaries, fundamental for the understanding of macroscopic quantities such as strength, cohesion, plasticity, etc.

Although ceramics have been known to mankind literally for millennia, research has never ceased. Apart from the classic uses as a bulk material in pottery, construction, and decoration, the latter half of the twentieth century saw an explosive growth of application fields, such as electrical and thermal insulators, wear-resistant bearings, surface coatings, lightweight armour, or aerospace materials. In addition to plain, hard solids, modern ceramics come in many new guises such as fabrics, ultrathin films, microstructures and hybrid composites. Built on the solid foundations laid down by the 20-volume series Materials Science and Technology, Ceramics Science and Technology picks out this exciting material class and illuminates it from all sides. Materials scientists, engineers, chemists, biochemists, physicists and medical researchers alike will find this work a treasure trove for a wide range of ceramics knowledge from theory and fundamentals to practical approaches and problem solutions.

This volume contains the proceedings of the third in a series of biennial NEC Symposia on Fundamental Approaches to New Material Phases sponsored by the NEC Corporation, Tokyo, Japan. The symposium was held from October 7 to 11, 1990, at the Hakone Kanko H9tel in Hakone. About 40 invited participants stayed together, became involved in intense discussions, and freely exchanged ideas both in and out of the conference room, which faced Mt. Fuji, the beautiful lake Ashinoko, and the quiet landscape in the old crater. The title of this volume, Ordering at Surfaces and Interfaces, which was also the title of the third symposium, describes the aim of the symposium: to discuss ordering properties and their underlying mechanisms at surfaces and interfaces. The topics treated include the reconstruction of surfaces of semiconductors and metals, atomic and magnetic ordering at interfaces, theoretical tools to study or dering mechanisms at surfaces and interfaces, ordering in adsorbate-surface sys tems, such as alkali-adsorbed silicon surfaces, electric current effects on semicon ductor surfaces and many related STM (scanning tunneling microscopy) results.

Volume is indexed by Thomson Reuters CPCI-S (WoS). The Industrial Revolution showed that the development and improvement of new materials and functions could bring about social change, and benefit human society. However, one can be forgiven for feeling that more recent materials research, particularly in the domain of metals, has focused only upon individual elemental characteristics and narrow specialty fields, and that the original vision of materials research has thus been lost.

The third book in a series on heterogeneous materials, this volume offers integrated approaches to the measurement and modeling of materials using approaches from materials science, physics, mechanics, biology and other disciplines. The volume contains 289 chapters presenting original research on the connections among the nano- , micro-, and mesoscale mechanical properties and behaviors of many different types of engineered and natural heterogeneous materials. The book contains a wealth of never published multiscale data on materials loading behaviors, plasticity, creep, damage, fracture and failure. A separate section is devoted to the design and functionalization of materials using multiscale data and techniques

New models for dislocation structure and motion are presented for nanocrystals, nucleation at grain boundaries, shocked crystals, interphase interfaces, quasicrystals, complex structures with non-planar dislocation cores, and colloidal crystals. A review of experimentally established main features of the magnetoplastic effect with their physical interpretation explains many diverse results of this type. The model has many potential applications for forming processes influenced by magnetic fields. • Dislocation model for the magnetoplastic effect • New mechanism for dislocation nucleation and motion in nanocrystals • New models for the dislocation structure of interfaces between crystals with differing crystallographic structure • A unified view of dislocations in quasicrystals, with a new model for dislocation motion • A general model of dislocation behavior in crystals with non-planar dislocation cores • Dislocation properties at high velocities • Dislocations in colloidal crystals

This handbook brings together, under a single cover, all aspects of the chemistry, physics, and engineering of surfaces and interfaces of materials currently studied in academic and industrial research. It covers different experimental and theoretical aspects of surfaces and interfaces, their physical properties, and spectroscopic techniques that have been applied to a wide class of inorganic, organic, polymer, and biological materials. The diversified technological areas of surface science reflect the explosion of scientific information on surfaces and interfaces of materials and their spectroscopic characterization. The large volume of experimental data on chemistry, physics, and engineering aspects of materials surfaces and interfaces remains scattered in so many different periodicals, therefore this handbook compilation is needed. The information presented in this multivolume reference draws on two decades of pioneering research on the surfaces and interfaces of materials to offer a complete perspective on the topic. These five volumes-Surface and Interface Phenomena; Surface Characterization and Properties; Nanostructures, Micelles, and Colloids; Thin Films and Layers; Biointerfaces and Applications-provide multidisciplinary review chapters and summarize the current status of the field covering important scientific and technological developments made over past decades in surfaces and interfaces of materials and spectroscopic techniques with contributions from internationally recognized experts from all over the world. Fully cross-referenced, this book has clear, precise, and wide appeal as an essential reference source long due for the scientific community. The complete reference on the topic of surfaces and interfaces of materials The information presented in this multivolume reference draws on two decades of pioneering research Provides multidisciplinary review chapters and summarizes the current status of the field Covers important scientific and technological developments made over past decades in surfaces and interfaces of materials and spectroscopic techniques Contributions from internationally recognized experts from all over the world.

Because of the intrinsic limits of the Si/SiO2 based industry, there is a great trend towards the monolithic integration of new materials into already well developed silicon technology. Having lasted for several decades now, downscaling reaches the limit, in which a critical device dimension approaches the size of one atom. At this level of the miniaturization, it is not the bulk material, but the interface between the two materials that what controls the properties of the resulting optoelectronic device. Thus, the characterization of precise atomic arrangements at different interfaces and the influence of these arrangements on the optoelectronic properties of interfaces is required. Therefore, in this study, a combination of scanning transmission electron microscopy (STEM) techniques and density functional theory calculations was used as a research tool for the characterization of interfaces. The STEM instruments used for the study were equipped with prototypes of spherical aberration correctors, enabling to achieve the highest resolution currently available both in space and energy. The combination of experimental and theoretical methods was applied to study interfaces between Si/GaAs, Si/Ge, Ge/SiO2, Si/HfO2 and Si/Al2O3. As the result of the present research, a new dislocation configuration at the Si/GaAs interface was reported for the first time. The influence of this dislocation structure on the electrical properties of the Si/GaAs interface was analyzed. Also, the transition from Si to GaAs and from Si to Ge at corresponding interfaces was described with atomic precision. For the first time, the interface between Ge and SiO2 was shown to have 'ideal' characteristics (chemical abruptness and sharpness). This indicates the potential, both for a more successful use of Ge in high-speed devices and for advances in interface engineering to enhance performance in electronic devices. The features of Si/HfO2 and Si/Al2O &

In-situ high-resolution electron microscopy is a modern and powerful technique in materials research, physics, and chemistry. In-situ techniques are hardly treated in textbooks of electron microscopy. Thus, there is a need to collect the present knowledge about the techniques and achievements of in-situ electron microscopy in one book. Since high-resolution electron microscopes are available in most modern laboratories of materials science, more and more scientists or students are starting to work on this subject.In this comprehensive volume, the most important techniques and achievements of in-situ high-resolution electron microscopy will be reviewed by renowned experts. Applications in several fields of materials science will also be demonstrated.

This book covers a broad spectrum of the silicon-based materials and their device applications. This book provides a broad coverage of the silicon-based materials including different kinds of silicon-related materials, their processing, spectroscopic characterization, physical properties, and device applications. This two-volume set offers a selection of timely topics on silicon materials namely those that have been extensively used for applications in electronic and photonic technologies. The extensive reference provides broad coverage of silicon-based materials, including different types of silicon-related materials, their processing, spectroscopic characterization, physical properties, and device applications. Fourteen chapters review the state of the art research on silicon-based materials and their applications to devices. This reference contains a subset of articles published in AP's recently released Handbook of Advanced Electronic and Photonic Materials and Devices (2000, ISBN 012-5137451, ten volumes) by Dr. Hari Nalwa. This two-volume work strives to present a highly coherent coverage of silicon-based material uses in the vastly dynamic arena of silicon chip research and technology. Key Features * Covers silicon-based materials and devices * Include types of materials, their processing, fabrication, physical properties and device applications * Role of silicon-based materials in electronic and photonic technology * A very special topic presented in a timely manner and in a format

The third International Conference on Composite Interfaces (ICCI-III) was held under the auspecies of ASM International, The Aluminum Company of America (Alcoa), The Edison Polymer Innovation Co. (EPIC), Case Western Reserve University, Nippon Glass Fiber Co., Nitto Boseki Co., Office of Naval Reserach (ONR), SAMPE Japan, Teijin Co., Mobay Co., Union Carbide Co., and Vetrotex Sain-Gobain. The underlying philosophy of the conference continues to be the promotion of fundamental understanding of the structure and role of composite interfaces. With the growth of composite interface studies, the research direction naturally changes from characterization and understanding of interfacial structure to controlling this structure. For this reason, the conference was subtitled, "Controlled Interphase Structure." The rather unfamiliar phrase "interphase" is used to emphasize the interfacial region whose properties are different from the bulk. The importance of the interphase to the mechanochemical properties has been rapidly recognized among composite researchers in recent years. The conference incorporated nine sessions. No concurrent sessions were planned because of the strong interest among panicipants and organizers to intennix researchers from different disciplines. Papers presented were redistributed in Pans I throught V. Because of this, both the conference and proceedings are not organized based on the traditional disciplines or materials, but rather around concepts.

The sixth edition of Modern Physical Metallurgy provides a comprehensive overview of the structure of matter, the physical properties of materials and their mechanical behaviour and some of the most recent advances in physical metallurgy.

This profusely illustrated text on Transmission Electron Microscopy provides the necessary instructions for successful hands-on application of this versatile materials characterization technique. The new edition also includes an extensive collection of questions for the student, providing approximately 800 self-assessment questions and over 400 questions suitable for homework assignment.

Molecular surface science has made enormous progress in the past 30 years. The development can be characterized by a revolution in fundamental knowledge obtained from simple model systems and by an explosion in the number of experimental techniques. The last 10 years has seen an equally rapid development of quantum mechanical modeling of surface processes using Density Functional Theory (DFT). Chemical Bonding at Surfaces and Interfaces focuses on phenomena and concepts rather than on experimental or theoretical techniques. The aim is to provide the common basis for describing the interaction of atoms and molecules with surfaces and this to be used very broadly in science and technology. The book begins with an overview of structural information on surface adsorbates and discusses the structure of a number of important chemisorption systems. Chapter 2 describes in detail the chemical bond between atoms or molecules and a metal surface in the observed surface structures. A detailed description of experimental information on the dynamics of bond-formation and bond-breaking at surfaces make up Chapter 3. Followed by an in-depth analysis of aspects of heterogeneous catalysis based on the d-band model. In Chapter 5 adsorption and chemistry on the enormously important Si and Ge semiconductor surfaces are covered. In the remaining two Chapters the book moves on from solid-gas interfaces and looks at solid-liquid interface processes. In the final chapter an overview is given of the environmentally important chemical processes occurring on mineral and oxide surfaces in contact with water and electrolytes. Gives examples of how modern theoretical DFT techniques can be used to design heterogeneous catalysts This book suits the rapid introduction of methods and concepts from surface science into a broad range of scientific disciplines where the interaction between a solid and the surrounding gas or liquid phase is an essential component Shows how insight into chemical bonding at surfaces can be applied to a range of scientific problems in heterogeneous catalysis, electrochemistry, environmental science and semiconductor processing Provides both the fundamental perspective and an overview of chemical bonding in terms of structure, electronic structure and dynamics of bond rearrangements at surfaces

While much progress has been made in the microscopic characterization of bulk materials, understanding the behavior, at the atomic scale, of complex materials interfaces remains a challenging problem in condensed matter physics and materials science. Development of predictive theory and modeling for interfacial systems is not only important to aid experimental interpretations but is also crucial to accelerate materials design efforts for a broad range of technological applications from the semiconductor industry to the development of new sources of energy. This dissertation presents a computational framework that combines first-principles molecular dynamics simulations for the determination of interfacial atomic structures, and advanced electronic structure methods for the description of electronic properties to understand, predict and design materials interfaces. In particular, the research presented in this thesis was carried out in two parallel directions: 1. Predictions of the interfacial atomic structure of complex materials interfaces using first-principles molecular dynamics, and validation of the predictions by relating structural models to experiments, e.g., data from X-ray, infrared spectra and sum-frequency generation spectroscopy experiments.In particular, I investigated structural and dynamical properties of the ice Ih surface and of the Al_2O_3/water interface. While the study of the ice surface is the first step towards the understanding of complex semiconductor/water interfaces, the Al_2O_3/water interface represents a suitable prototype interface for extensive comparisons between theory and experiments. 2. Development of advanced first-principles techniques to study electronic states at interfaces and application of these techniques to gain insights on the relationship between between local interface structure and electronic properties. I devised a new technique to study excited states and photoemission spectra based on many-body perturbation theory, within the so-called GW approximation, which improves both the computational efficiency and accuracy of existing methodologies, and that can be employed to study realistic systems. In addition, in the thesis I employed the new GW technique to investigate a variety of systems including molecules, nanostructures, semiconducting interfaces, liquid water and simple aqueous solutions. These studies are crucial to build a fundamental understanding of the electronic structure of semiconductor/liquid water interfaces and of, e.g., water with dissolved ions under different pH conditions, interfaced with a photoelectrode. Information provided by these two parallel research directions helped establish a structure-electronic properties-chemical reactivity paradigm, that is general and applicable to a large class of materials. An example presented in the thesis is that of functionalized Si surfaces interfaced with liquid water, in which I studied

the effect of surface functionalization on the alignment between Si band edges and water redox potentials, and I suggested a possible approach to engineer and design semiconductor surfaces for photoelectrochemical water splitting.
Derived from the highly acclaimed series Materials Science and Technology, this book provides in-depth coverage of STM, AFM, and related non-contact nanoscale probes along with detailed applications, such as the manipulation of atoms and clusters on a nanometer scale. The methods are described in terms of the physics and the technology of the methods and many high-quality images demonstrate the power of these techniques in the investigation of surfaces and the processes which occur on them. Topics include: Semiconductor Surfaces and Interfaces * Insulators * Layered Compounds * Charge Density Wave Systems * Superconductors * Electrochemisty at Liquid-Solid Interfaces * Biological Systems * Metrological Applications * Nanoscale Surface Forces * Nanotribology * Manipulation on the Nanoscale Materials scientists, surface scientists, electrochemists, as well as scientists working in catalysis and microelectronics will find this book an invaluable source of information