

Molecular Modeling Of Corrosion Processes Scientific Development And Engineering Applications The Ecs Series Of Texts And Monographs

To protect metals or alloys from corrosion, some methods can be used such as isolating the structure from the aggressive media or compensating the loss of electrons from the corroded structure. The use of corrosion inhibitors may include organic and inorganic compounds that adsorb on the metallic structure to isolate it from its surrounding media to decrease oxidation-reduction processes. This book collects new developments about corrosion inhibitors and their recent applications.

Heterocyclic Organic Corrosion Inhibitors: Principles and Applications aims to comprehend the synthesis and application of organic heterocyclic compounds as corrosion inhibitors in various corrosive environments. Considering the high importance of corrosion inhibitor development for different industries, the book provides the fundamentals and most recent advancements in this field. The book is an indispensable reference tool for industrialists and academicians working in the field of corrosion protection. Provides a systematic overview of fundamentals and current advancements Acts as a primary reference for beginner researchers in this arena Presents a handy reference tool to different chemical industries Covers fundamentals, industrial applications and most recent advancements in this area

Metals are used at an extremely high rate in the industrial and manufacturing fields. Exemplary properties including strength and ductility have made this material highly dynamic; however, the risk of corrosion remains a vital issue. The study of corrosion prevention has attracted interest from researchers and professionals as new technologies are emerging that can assist in the prevention of material destruction. However, research is lacking on the application of these protective technologies within specific fields. *New Challenges and Industrial Applications for Corrosion Prevention and Control* provides emerging research exploring the theoretical and practical aspects of protective methods against corrosion and the implementation of these techniques within a wide span of professional disciplines. Featuring coverage on a broad range of topics such as molecular modeling, surface treatments, and biomaterials, this book is ideally designed for engineers, industrial chemists, material scientists, researchers, engineers, academicians, practitioners, and students seeking current research on the technological advancements in corrosion protection in various professional scopes. With its unique focus on specifically addressing the problems for societies and economies associated with corrosion and their solution, this book provides an up-to-date overview of the progress in corrosion chemistry and engineering. International experts actively involved in research and development place particular emphasis on how to counter the economic and environmental consequences of corrosion with the help of science and technology, making this a valuable resource for researchers as well as decision makers in industry and politics. Further major parts of the book are devoted to corrosion prevention in the naval and energy sector as well as to corrosion monitoring and waste management.

Corrosion Chemistry details the scientific background of the corrosion process and contemporary applications for dealing with corrosion for engineers and scientists,

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covering the most recent breakthroughs and trends. Corrosion is in essence a chemical process, and it is crucial to understand the dynamics from a chemical perspective before proceeding with analyses, designs and solutions from an engineering aspect. This book can be used both as a textbook and a reference book both by academics and engineers and scientists in the field. As a reference for the engineer in the field, it is both a refresher for the veteran on the causes of corrosion and the methods, processes, and technologies to deal with it, over a variety of industries. It is the most up-to-date, comprehensive treatment of corrosion available, covering the most cutting-edge new processes and theories. For the freshman engineer just entering the field, it is a tremendous introduction to corrosion. As a textbook, it can be used for a single semester technical elective course in undergraduate and postgraduate education for disciplines such as chemistry, chemical engineering, petroleum engineering, civil engineering, material engineering, mechanical engineering, metallurgical engineering, mining engineering, agricultural engineering, and other related technical fields. This book aims to provide readers with the latest and relevant trends in corrosion. Use of inhibitors is one of the most common, cheap, and globally followed methods for the protection of metals from aggressive solutions. The information contained in this book covers different corrosion inhibitors for different corrosive environments with sufficient experimental data, surface studies, and theoretical studies. These studies altogether will give readers a good view of the basic and advanced knowledge of corrosion inhibitors and will be of interest to students, academicians, and industrialists. Corrosion of nuclear materials, i.e. the interaction between these materials and their environments, is a major issue for plant safety as well as for operation and economic competitiveness. Understanding these corrosion mechanisms, the systems and materials they affect, and the methods to accurately measure their incidence is of critical importance to the nuclear industry. Combining assessment techniques and analytical models into this understanding allows operators to predict the service life of corrosion-affected nuclear plant materials, and to apply the most appropriate maintenance and mitigation options to ensure safe long term operation. This book critically reviews the fundamental corrosion mechanisms that affect nuclear power plants and facilities. Initial sections introduce the complex field of nuclear corrosion science, with detailed chapters on the different types of both aqueous and non aqueous corrosion mechanisms and the nuclear materials susceptible to attack from them. This is complemented by reviews of monitoring and control methodologies, as well as modelling and lifetime prediction approaches. Given that corrosion is an applied science, the final sections review corrosion issues across the range of current and next-generation nuclear reactors, and across such nuclear applications as fuel reprocessing facilities, radioactive waste storage and geological disposal systems. With its distinguished editor and international team of expert contributors, Nuclear corrosion science and engineering is an invaluable reference for nuclear metallurgists, materials scientists and engineers, as well as nuclear facility operators, regulators and consultants, and researchers and academics in this field. Comprehensively reviews the fundamental corrosion mechanisms that affect nuclear power plants and facilities. Chapters assess different types of both aqueous and non aqueous corrosion mechanisms and the nuclear materials susceptible to attack from them. Considers monitoring and control methodologies, as well as modelling and lifetime prediction

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As one of the results of an ambitious project, this handbook provides a well-structured directory of globally available software tools in the area of Integrated Computational Materials Engineering (ICME). The compilation covers models, software tools, and numerical methods allowing describing electronic, atomistic, and mesoscopic phenomena, which in their combination determine the microstructure and the properties of materials. It reaches out to simulations of component manufacture comprising primary shaping, forming, joining, coating, heat treatment, and machining processes. Models and tools addressing the in-service behavior like fatigue, corrosion, and eventually recycling complete the compilation. An introductory overview is provided for each of these different modelling areas highlighting the relevant phenomena and also discussing the current state for the different simulation approaches. A must-have for researchers, application engineers, and simulation software providers seeking a holistic overview about the current state of the art in a huge variety of modelling topics. This handbook equally serves as a reference manual for academic and commercial software developers and providers, for industrial users of simulation software, and for decision makers seeking to optimize their production by simulations. In view of its sound introductions into the different fields of materials physics, materials chemistry, materials engineering and materials processing it also serves as a tutorial for students in the emerging discipline of ICME, which requires a broad view on things and at least a basic education in adjacent fields.

Multiscale Modeling for Process Safety Applications is a new reference demonstrating the implementation of multiscale modeling techniques on process safety applications. It is a valuable resource for readers interested in theoretical simulations and/or computer simulations of hazardous scenarios. As multi-scale modeling is a computational technique for solving problems involving multiple scales, such as how a flammable vapor cloud might behave if ignited, this book provides information on the fundamental topics of toxic, fire, and air explosion modeling, as well as modeling jet and pool fires using computational fluid dynamics. The book goes on to cover nanomaterial toxicity, QPSR analysis on relation of chemical structure to flash point, molecular structure and burning velocity, first principle studies of reactive chemicals, water and air reactive chemicals, and dust explosions. Chemical and process safety professionals, as well as faculty and graduate researchers, will benefit from the detailed coverage provided in this book. Provides the only comprehensive source addressing the use of multiscale modeling in the context of process safety Bridges multiscale modeling with process safety, enabling the reader to understand mapping between problem detail and effective usage of resources Presents an overall picture of addressing safety problems in all levels of modeling and the latest approaches to each in the field Features worked out examples, case studies, and a question bank to aid understanding and involvement for the reader

Many of the earliest books, particularly those dating back to the 1900s and before, are now extremely scarce and increasingly expensive. We are republishing these classic works in affordable, high quality, modern editions, using the original text and artwork. The first of many important works featured in CRC Press' Metals and Alloys Encyclopedia Collection, the Encyclopedia of Iron, Steel, and Their Alloys covers all the fundamental, theoretical, and application-related aspects of the metallurgical science,

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engineering, and technology of iron, steel, and their alloys. This Five-Volume Set addresses topics such as extractive metallurgy, powder metallurgy and processing, physical metallurgy, production engineering, corrosion engineering, thermal processing, metalworking, welding, iron- and steelmaking, heat treating, rolling, casting, hot and cold forming, surface finishing and coating, crystallography, metallography, computational metallurgy, metal-matrix composites, intermetallics, nano- and micro-structured metals and alloys, nano- and micro-alloying effects, special steels, and mining. A valuable reference for materials scientists and engineers, chemists, manufacturers, miners, researchers, and students, this must-have encyclopedia: Provides extensive coverage of properties and recommended practices Includes a wealth of helpful charts, nomograms, and figures Contains cross referencing for quick and easy search Each entry is written by a subject-matter expert and reviewed by an international panel of renowned researchers from academia, government, and industry. Also Available Online This Taylor & Francis encyclopedia is also available through online subscription, offering a variety of extra benefits for researchers, students, and librarians, including: Citation tracking and alerts Active reference linking Saved searches and marked lists HTML and PDF format options Contact Taylor and Francis for more information or to inquire about subscription options and print/online combination packages. US: (Tel) 1.888.318.2367; (E-mail) e-reference@taylorandfrancis.com International: (Tel) +44 (0) 20 7017 6062; (E-mail) online.sales@tandf.co.uk

The Handbook of Environmental Degradation of Materials, Third Edition, explains how to measure, analyze and control environmental degradation for a wide range of industrial materials, including metals, polymers, ceramics, concrete, wood and textiles exposed to environmental factors, such as weather, seawater, and fire. This updated edition divides the material into four new sections, Analysis and Testing, Types of Degradation, Protective Measures and Surface Engineering, then concluding with Case Studies. New chapters include topics on Hydrogen Permeation and Hydrogen Induced Cracking, Weathering of Plastics, the Environmental Degradation of Ceramics and Advanced Materials, Antimicrobial Layers, Coatings, and the Corrosion of Pipes in Drinking Water Systems. Expert contributors to this book provide a wealth of insider knowledge and engineering expertise that complements their explanations and advice. Case Studies from areas such as pipelines, tankers, packaging and chemical processing equipment ensure that the reader understands the practical measures that can be put in place to save money, lives and the environment. Introduces the reader to the effects of environmental degradation on a wide range of materials, including metals, plastics, concrete, wood and textiles Describes the kind of degradation that effects each material and how best to protect it Includes case studies that show how organizations, from small consulting firms, to corporate giants design and manufacture products that are more resistant to environmental effects

The global economic cost from corrosion is estimated to be more than US\$2.5 trillion, or equivalent to 3.4% of the global GDP. Corrosion costs the U.S. economy close to \$300 billion per annum. About 100 billion dollars these costs could be remediated by application of corrosion-resistant materials and the use of corrosion-related technical practices such as corrosion inhibitors. A corrosion inhibitor is a chemical compound that, when added to a liquid or gas, decreases the corrosion rate of a metal, or its alloy

that comes into contact with the fluid or vapour. These chemicals are both organic and inorganic compounds, which generally form a protective layer on the metal surface. Some corrosion inhibitors contain heavy metals are harmful to human health, toxic to plants, environments, and animals. They also have adverse effect on the ecology of the receiving environment and on surface and ground water quality. This book focuses on the use of Vapro VBCI Corrosion Inhibitors which are biodegradable, less toxic, and environmentally friendly. The authors believe in creating a cleaner, greener, and better tomorrow for our children and children's children. Lead Authors Dr Benjamin Valdez Salas Dr Nelson Cheng PhD (honoris causa) Patrick Moe BSc, MSc, Grad Diploma Comprehensively covers the engineering aspects of corrosion and materials in hydrocarbon production This book captures the current understanding of corrosion processes in upstream operations and provides a brief overview of parameters and measures needed for optimum design of facilities. It focuses on internal corrosion occurring in hydrocarbon production environments and the key issues affecting its occurrence, including: the types and morphology of corrosion damage; principal metallic materials deployed; and mitigating measures to optimise its occurrence. The book also highlights important areas of progress and challenges, and looks toward the future of research and development to enable improved and economical design of facilities for oil and a gas production. Written for both those familiar and unfamiliar with the subject—and by two authors with more than 60 years combined industry experience—this book covers everything from Corrosion Resistant Alloys (CRAs) to internal metal loss corrosion threats, corrosion in injection systems to microbiologically influenced corrosion, corrosion risk analysis to corrosion and integrity management, and more, notably: Comprehensively covers the engineering aspects of corrosion and materials in hydrocarbon production Written by two, renowned experts in the field Offers practical guide to those unfamiliar with the subject whilst providing a focused roadmap to addressing the topics in a precise and methodical manner Covers all aspects of corrosion threat and remedial and mitigation measures in upstream hydrocarbon production applicable to sub-surface, surface, and transportation facilities Outlines technology challenges that need further research as a pre-cursor to moving the industry forward. Operational and Engineering Aspects of Corrosion and Materials in Hydrocarbon Production is an excellent guide for both practicing materials and corrosion engineers working in hydrocarbons production as well as those entering the area who may not be fully familiar with the subject.

Microorganisms can be both beneficial and harmful to the oil and gas industry and therefore there is an increasing need for the oil industry to characterize, quantify and monitor microbial communities in real time. Oilfield Microbiology offers a fundamental insight into how molecular microbiological methods have enabled researchers in the field to analyze and quantify in situ microbial communities and their activities in response to changing environmental conditions. Such information is fundamental to the oil industry to employ more directed, cost-effective strategies to prevent the major problems associated with deleterious microbial activities (e.g., souring and biocorrosion), as well as to encourage beneficial microbe activity (e.g. oil bioremediation). The aim of the book is to understand how the technological advances in molecular microbiological methods over the last two decades are now being utilized by the oil industry to address the key issues faced by the sector. This book contains a

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comprehensive collection of chapters written by invited experts in the field from academia and industry and provides a solid foundation of the importance of microbes to the oil and gas industry. It is aimed at microbial ecologists, molecular biologists, operators, engineers, chemists, and academics involved in the sector.

Underground pipelines transporting liquid petroleum products and natural gas are critical components of civil infrastructure, making corrosion prevention an essential part of asset-protection strategy. *Underground Pipeline Corrosion* provides a basic understanding of the problems associated with corrosion detection and mitigation, and of the state of the art in corrosion prevention. The topics covered in part one include: basic principles for corrosion in underground pipelines, AC-induced corrosion of underground pipelines, significance of corrosion in onshore oil and gas pipelines, numerical simulations for cathodic protection of pipelines, and use of corrosion inhibitors in managing corrosion in underground pipelines. The methods described in part two for detecting corrosion in underground pipelines include: magnetic flux leakage, close interval potential surveys (CIS/CIPS), Pearson surveys, in-line inspection, and use of both electrochemical and optical probes. While the emphasis is on pipelines transporting fossil fuels, the concepts apply as well to metallic pipes for delivery of water and other liquids. *Underground Pipeline Corrosion* is a comprehensive resource for corrosion, materials, chemical, petroleum, and civil engineers constructing or managing both onshore and offshore pipeline assets; professionals in steel and coating companies; and academic researchers and professors with an interest in corrosion and pipeline engineering. Reviews the causes and considers the detection and prevention of corrosion to underground pipes Addresses a lack of current, readily available information on the subject Case studies demonstrate how corrosion is managed in the underground pipeline industry

The book presents the current status of corrosion inhibitor technology. A special focus is placed on various types of green corrosion inhibitors and their applications.

Keywords: Green Corrosion Inhibitors, Sustainable Corrosion Inhibitors, Green Organic Inhibitors, Inhibitors from Biomass and Natural Sources, Polysaccharide, Applications for Concrete, Coatings, Copper and Copper Alloys, Corrosion Control in Conventional and Monolithic Metals.

Provides fundamentals needed to apply impedance spectroscopy to a broad range of applications with emphasis on obtaining physically meaningful insights from measurements. Emphasizes fundamentals applicable to a broad range of applications including corrosion, biomedical devices, semiconductors, batteries, fuel cells, coatings, analytical chemistry, electrocatalysis, materials, and sensors Provides illustrative examples throughout the text that show how the principles are applied to common impedance problems New Edition has improved pedagogy, with more than twice the number of examples New Edition has more in-depth treatment of background material needed to understand impedance spectroscopy, including electrochemistry, complex variables, and differential equations New Edition includes expanded treatment of the influence of mass transport and kinetics and reflects recent advances in understanding frequency dispersion and constant-phase elements

This book covers recent advances in the method used in testing, especially in the case of structural integrity that includes fatigue and fracture tests, vibrations test and surface engineering tests that are extremely crucial and widely used by engineers and

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industries. The book will provide you with information on how to apply the advanced formulation, advanced theory and advanced method of testing that are relevant to all engineering fields: mechanical, electrical, civil, materials and surface engineering. The topics are explained comprehensively, including the reliable test that one should perform in order to effectively investigate the strength and validation of the developed theory or model. I hope that the material is not too theoretical and that the reader finds the case study, formulation, testing method and the analysis helpful for tackling their own engineering and science based studies.

Called "a useful contribution to the current literature on corrosion science, engineering, and technology" by Corrosion Review, this book offers real-world applications and problem-solving techniques to reduce the occurrence of pits, cracks, and deterioration in industrial, automotive, marine, and electronic structures. It details the electrochemic Molecular modeling (MM) tools offer significant benefits in the design of industrial chemical plants and material processing operations. While the role of MM in biological fields is well established, in most cases MM works as an accessory in novel products/materials development rather than a tool for direct innovation. As a result, MM engineers and

With techniques bridging the gap between surface science and heterogeneous catalysis the book presents a tool-kit for anyone wishing to prepare and define solid catalysts.

State-of-the-technology tools for designing, optimizing, and manufacturing new materials Integrated computational materials engineering (ICME) uses computational materials science tools within a holistic system in order to accelerate materials development, improve design optimization, and unify design and manufacturing. Increasingly, ICME is the preferred paradigm for design, development, and manufacturing of structural products. Written by one of the world's leading ICME experts, this text delivers a comprehensive, practical introduction to the field, guiding readers through multiscale materials processing modeling and simulation with easy-to-follow explanations and examples. Following an introductory chapter exploring the core concepts and the various disciplines that have contributed to the development of ICME, the text covers the following important topics with their associated length scale bridging methodologies: Macroscale continuum internal state variable plasticity and damage theory and multistage fatigue Mesoscale analysis: continuum theory methods with discrete features and methods Discrete dislocation dynamics simulations Atomistic modeling methods Electronics structures calculations Next, the author provides three chapters dedicated to detailed case studies, including "From Atoms to Autos: A Redesign of a Cadillac Control Arm," that show how the principles and methods of ICME work in practice. The final chapter examines the future of ICME, forecasting the development of new materials and engineering structures with the help of a cyberinfrastructure that has been recently established. Integrated Computational Materials Engineering (ICME) for Metals is recommended for both students and professionals in engineering and materials science, providing them with new state-of-the-technology tools for selecting, designing, optimizing, and manufacturing new materials. Instructors who adopt this text for coursework can take advantage of PowerPoint lecture notes, a questions and solutions manual, and tutorials to guide students through the models and codes discussed in the text.

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Presents opportunities for making significant improvements in preventing harmful effects that can be caused by corrosion Describes concepts of molecular modeling in the context of materials corrosion Includes recent examples of applications of molecular modeling to corrosion phenomena throughout the text Details how molecular modeling can give insights into the multitude of interconnected and complex processes that comprise the corrosion of metals Covered applications include diffusion and electron transfer at metal/electrolyte interfaces, Monte Carlo simulations of corrosion, corrosion inhibition, interrogating surface chemistry, and properties of passive films Presents current challenges and likely developments in this field for the future

This volume maintains the series' high standards, containing chapters covering topics such as the cathodic reduction of nitrate, and including discussion of product selectivity, current efficiency, and the thermodynamics and kinetics for the reactions studied.

Molecular Modeling of Corrosion Processes Scientific Development and Engineering Applications John Wiley & Sons

A multi-disciplinary, multi-industry overview of microbiologically influenced corrosion, with strategies for diagnosis and control or prevention Microbiologically Influenced Corrosion helps engineers and scientists understand and combat the costly failures that occur due to microbiologically influenced corrosion (MIC). This book combines recent findings from diverse disciplines into one comprehensive reference. Complete with case histories from a variety of environments, it covers: Biofilm formation Causative organisms, relating bacteria and fungi to corrosion mechanisms for groups of metals Diagnosing and monitoring MIC

Electrochemical techniques, with an overview of methods for detection of MIC The impact of alloying elements, including antimicrobial metals, and design features on MIC MIC of non-metallics Strategies for control or prevention of MIC, including engineering, chemical, and biological approaches This is a valuable, all-inclusive reference for corrosion scientists, engineers, and researchers, as well as designers, managers, and operators.

Provides a comprehensive understanding of a wide range of systems and topics in electrochemistry This book offers complete coverage of electrochemical theories as they pertain to the understanding of electrochemical systems. It describes the foundations of thermodynamics, chemical kinetics, and transport phenomena—including the electrical potential and charged species. It also shows how to apply electrochemical principles to systems analysis and mathematical modeling. Using these tools, the reader will be able to model mathematically any system of interest and realize quantitative descriptions of the processes involved. This brand new edition of Electrochemical Systems updates all chapters while adding content on lithium battery electrolyte characterization and polymer electrolytes. It also includes a new chapter on impedance spectroscopy.

Presented in 4 sections, the book covers: Thermodynamics of Electrochemical Cells, Electrode Kinetics and Other Interfacial Phenomena, Transport Processes in Electrolytic Solutions, and Current Distribution and Mass Transfer in

Electrochemical Systems. It also features three appendixes containing information on: Partial Molar Volumes, Vectors and Tensors, and Numerical Solution of Coupled, Ordinary Differential Equations. Details fundamental knowledge with a thorough methodology Thoroughly updated throughout with new material on topics including lithium battery electrolyte characterization, impedance analysis, and polymer electrolytes Includes a discussion of equilibration of a charged polymer material and an electrolytic solution (the Donnan equilibrium) A peerless classic on electrochemical engineering Electrochemical Systems, Fourth Edition is an excellent resource for students, scientists, and researchers involved in electrochemical engineering.

Trends in Oil and Gas Corrosion Research and Technologies: Production and Transmission delivers the most up-to-date and highly multidisciplinary reference available to identify emerging developments, fundamental mechanisms and the technologies necessary in one unified source. Starting with a brief explanation on corrosion management that also addresses today's most challenging issues for oil and gas production and transmission operations, the book dives into the latest advances in microbiology-influenced corrosion and other corrosion threats, such as stress corrosion cracking and hydrogen damage just to name a few. In addition, it covers testing and monitoring techniques, such as molecular microbiology and online monitoring for surface and subsurface facilities, mitigation tools, including coatings, nano-packaged biocides, modeling and prediction, cathodic protection and new steels and non-metallics. Rounding out with an extensive glossary and list of abbreviations, the book equips upstream and midstream corrosion professionals in the oil and gas industry with the most advanced collection of topics and solutions to responsibly help solve today's oil and gas corrosion challenges. Covers the latest in corrosion mitigation techniques, such as corrosion inhibitors, biocides, non-metallics, coatings, and modeling and prediction Solves knowledge gaps with the most current technology and discoveries on specific corrosion mechanisms, highlighting where future research and industry efforts should be concentrated Achieves practical and balanced understanding with a full spectrum of subjects presented from multiple academic and world-renowned contributors in the industry

Consolidates the many different chemistries being employed to provide environmentally acceptable products through the upstream oil and gas industry This book discusses the development and application of green chemistry in the oil and gas exploration and production industry over the last 25 years — bringing together the various chemistries that are utilised for creating suitable environmental products. Written by a highly respected consultant to the oil and gas industry — it introduces readers to the principles and development of green chemistry in general, and the regulatory framework specific to the oil and gas sector in the North Sea area and elsewhere in the world. It also explores economic drivers pertaining to the application of green chemistry in the sector. Topics covered in Oilfield Chemistry and its Environmental Impact include

polymer chemistry, surfactants and amphiphiles, phosphorus chemistry, inorganic salts, low molecular weight organics, silicon chemistry and green solvents. It also looks at sustainability in an extractive industry, examining the approaches used and the other methodologies that could be applied in the development of better chemistries, along with discussions about where the application of green chemistry is leading in this industry sector. Provides the reader with a ready source of reference when considering what chemistries are appropriate for application to oilfield problems and looking for green chemistry solutions Brings together the pertinent regulations which workers in the field will find useful, alongside the chemistries which meet the regulatory requirements Written by a well-known specialist with a combined knowledge of chemistry, manufacturing procedures and environmental issues Oilfield Chemistry and its Environmental Impact is an excellent book for oil and gas industry professionals as well as scientists, academic researchers, students and policy makers. Corrosion is a global threat and a burning topic for new and innovative research. Corrosion causes shut downs, economic losses, delays, failures, accidents, losses of life, and losses in productivity. "Wherever metal is, there corrosion will occur" – this is a general concept as not many protection methods are available to mitigate corrosion. The available methods can only delay the process but cannot stop or protect the metal completely. So there is always a need for good research and inventions in this field. This book includes the recent research work done in the field of corrosion. The chapters are written by reputed authors in the field of corrosion and have been reviewed extensively before acceptance. The chapters focus on different aspects of corrosion to provide readers with a good idea of the overall process. The diversification of the chapters will keep the readers interested and motivated for new innovations in the field of corrosion. It will be very useful to scholars, academicians, researchers, and industrialists. Reaction Rate Theory and Rare Events bridges the historical gap between these subjects because the increasingly multidisciplinary nature of scientific research often requires an understanding of both reaction rate theory and the theory of other rare events. The book discusses collision theory, transition state theory, RRKM theory, catalysis, diffusion limited kinetics, mean first passage times, Kramers theory, Grote-Hynes theory, transition path theory, non-adiabatic reactions, electron transfer, and topics from reaction network analysis. It is an essential reference for students, professors and scientists who use reaction rate theory or the theory of rare events. In addition, the book discusses transition state search algorithms, tunneling corrections, transmission coefficients, microkinetic models, kinetic Monte Carlo, transition path sampling, and importance sampling methods. The unified treatment in this book explains why chemical reactions and other rare events, while having many common theoretical foundations, often require very different computational modeling strategies. Offers an integrated approach to all simulation theories and reaction network analysis, a unique approach not found elsewhere Gives algorithms in

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pseudocode for using molecular simulation and computational chemistry methods in studies of rare events Uses graphics and explicit examples to explain concepts Includes problem sets developed and tested in a course range from pen-and-paper theoretical problems, to computational exercises

This book is a collection of select proceedings of the FOMMS 2015 conference. FOMMS 2015 was the sixth triennial FOMMS conference showcasing applications of theory of computational quantum chemistry, molecular science, and engineering simulation. The theme of the 2015 meeting was on Molecular Modeling and the Materials Genome. This volume comprises chapters on many distinct applications of molecular modeling techniques. The content will be useful to researchers and students alike.

In ten volumes, this unique handbook covers all fundamental aspects of surface and interface science and offers a comprehensive overview of this research area for scientists working in the field, as well as an introduction for newcomers. Volume 1: Concepts and Methods Volume 2: Properties of Elemental Surfaces Volume 3: Properties of Composite Surfaces: Alloys, Compounds, Semiconductors Volume 4: Solid-Solid Interfaces and Thin Films Volume 5: Solid-Gas Interfaces I Volume 6: Solid-Gas Interfaces II Volume 7: Liquid and Biological Interfaces Volume 8: Interfacial Electrochemistry Volume 9: Applications of Surface Science I Volume 10: Applications of Surface Science II Content of Volumes 8 & 9: * Surface Analytics with X-Ray Photoelectron and Auger Electron Spectroscopy on Coated Steel Sheets * Applications of Graphene * Industrial Heterogeneous Catalysis * Automotive Catalysis * High-Throughput Heterogeneous Catalyst Research, Development, Scale-Up, and Production Support * Industrial Separation of Insulating Particles: Triboelectric Charging * Friction: Friend and Foe * Surface Science and Flotation * Application of Surface Science to Corrosion * Electrons, Electrodes, and the Transformation of Organic Molecules * Self-Cleaning Surfaces: From Fundamental Aspect to Real Technical Applications * Thin Films: Sputtering, PVD Methods and Applications * Wafer Bonding * Superconformal Deposition * Spintronics: Surface and Interface Aspects * Device Efficiency of Organic Light-Emitting Diodes * Dye-Sensitized Solar Cells * Electronic Nose: Current Status and Future Trends * Surface Science in Batteries * Surface and Interface Science in Fuel Cells Research

This book focuses on the recent research progress on the fundamental understanding of the materials degradation phenomena in PEFC, for automotive applications. On a multidisciplinary basis, through contributions of internationally recognized researchers in the field, this book provides a complete critical review on crucial scientific topics related to PEFC materials degradation, and ensures a strong balance between experimental and theoretical analysis and preparation techniques with several practical applications for both the research and the industrial communities.

Internal corrosion in pipelines is a significant issue in the upstream oil and gas industry. Corrosion engineers have developed strategies to mitigate corrosion, and among these, the use of organic corrosion inhibitors is one of the most widely used solutions. Corrosion inhibitors are substances that significantly reduce corrosion when added in small, typically ppm level, concentrations. Knowledge related to their efficiency, and associated mechanisms of inhibition, has been developed by conducting experiments in physicochemical conditions that simulate field environments during their application. Nonetheless, there is a lack of studies in the open literature that mechanistically define the effect of corrosion inhibitors on the kinetics of the electrochemical processes underlying corrosion. Consequently, the central objective of this research was to propose a mechanistic model that describes and predicts the effect of organic corrosion inhibitors on the electrochemical processes governing the carbon dioxide corrosion of mild steel. In order to develop the mechanistic model, corrosion studies included the electrochemical characterization of aqueous steel corrosion in the presence of known

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corrosion inhibitor packages (quaternary-ammonium-type and imidazoline-type) with techniques such as linear polarization resistance (LPR), electrochemical impedance spectroscopy (EIS), and potentiodynamic polarization. During these experiments, the state-of-the-art knowledge on corrosion inhibition available in the open literature related to corrosion inhibition was insufficient to explain specific experimental observations satisfactorily. This situation led to the postulation of ad hoc hypotheses to explain the effect of the organic corrosion inhibitors' molecular structure on the observed electrochemical kinetics for the corrosion process, namely, the effects of inhibitor alkyl tail length and head group.

Provides comprehensive coverage of organic corrosion inhibitors used in modern industrial platforms, including current developments in the design of promising classes of organic corrosion inhibitors Corrosion is the cause of significant economic and safety-related problems that span across industries and applications, including production and processing operations, transportation and public utilities infrastructure, and oil and gas exploration. The use of organic corrosion inhibitors is a simple and cost-effective method for protecting processes, machinery, and materials while remaining environmentally acceptable. Organic Corrosion Inhibitors: Synthesis, Characterization, Mechanism, and Applications provides up-to-date coverage of all aspects of organic corrosion inhibitors, including their fundamental characteristics, synthesis, characterization, inhibition mechanism, and industrial applications. Divided into five sections, the text first covers the basics of corrosion and prevention, experimental and computational testing, and the differences between organic and inorganic corrosion inhibitors. The next section describes various heterocyclic and non-heterocyclic corrosion inhibitors, followed by discussion of the corrosion inhibition characteristics of carbohydrates, amino acids, and other organic green corrosion inhibitors. The final two sections examine the corrosion inhibition properties of carbon nanotubes and graphene oxide, and review the application of natural and synthetic polymers as corrosion inhibitors. Featuring contributions by leading researchers and scientists from academia and industry, this authoritative volume: Discusses the latest developments and issues in the area of corrosion inhibition, including manufacturing challenges and new industrial applications Explores the development and implementation of environmentally-friendly alternatives to traditional toxic corrosion inhibitors Covers both established and emerging classes of corrosion inhibitors as well as future research directions Describes the anticorrosive mechanisms and effects of acyclic, cyclic, natural, and synthetic corrosion inhibitors Offering an interdisciplinary approach to the subject, Organic Corrosion Inhibitors: Synthesis, Characterization, Mechanism, and Applications is essential reading for chemists, chemical engineers, researchers, industry professionals, and advanced students working in fields such as corrosion inhibitors, corrosion engineering, materials science, and applied chemistry.

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