

| KINETICS AND DYNAMICS OF HYDROGEN ADSORPTION AND DESORPTION ON SILICON SURFACES | 1 |
|---|-----|
| By Douglas J. Doren | |
| POTENTIAL ENERGY SURFACES OF TRANSITION-METAL-CATALYZED CHEMICAL REACTIONS | 61 |
| By Djamaladdin G. Musaev and Keiji Morokuma | |
| HIGH-RESOLUTION HELIUM ATOM SCATTERING AS A PROBE OF SURFACE VIBRATIONS | 129 |
| By Sanford A. Safron | |
| Ordering and Phase Transitions in Adsorbed Monolayers of Diatomic Molecules | 213 |
| By Dominik Marx and Horst Wiechert | |
| Author Index | 395 |
| Subject Index | 415 |

KINETICS AND DYNAMICS OF HYDROGEN ADSORPTION AND DESORPTION ON SILICON SURFACES

DOUGLAS J. DOREN

Department of Chemistry and Biochemistry, University of Delaware, Newark, Delaware

- I. Introduction
- II. Overview and Nomenclature
- III. Experimental Observations
 - A. Summary
 - B. Desorption Kinetics
 - 1. Early Work
 - 2. $Si(111)-7 \times 7$
 - 3. $Si(100)-2 \times 1$
 - 4. Verification of Structure-Dependent Desorption Mechanism
 - 5. Evidence for Prepairing
 - 6. Desorption After Dosing with Silanes
 - 7. Other Covalent Surfaces
 - 8. Desorption from the Dihydride Phase
 - C. Energy Distribution of Desorbing H₂
 - 1. Rotational and Vibrational Energy
 - 2. Translational Energy
 - 3. Surface Energy
 - D. Sticking Probability
 - 1. Measurements of Sticking Probability
 - 2. A Model of Adsorption and Desorption Dynamics
- IV. First Principles Theory
 - A. Evidence Against the Prepairing Mechanism
 - 1. Thermodynamics
 - 2. Activation Energies and Alternative Mechanisms
 - 3. Critique of Defect-Mediated Mechanisms

Advances in Chemical Physics, Volume XCV, Edited by I. Prigogine and Stuart A. Rice. ISBN 0-471-15430-X © 1996 John Wiley & Sons, Inc.

- B. Evidence Supporting the Prepairing Mechanism
- C. Comparison of Theoretical Results
- D. Inferences About Kinetics and Dynamics
- E. Desorption from the Dihydride
- V. Remaining Issues

Acknowledgments



POTENTIAL ENERGY SURFACES OF TRANSITION-METAL-CATALYZED CHEMICAL REACTIONS

DJAMALADDIN G. MUSAEV AND KEIJI MOROKUMA

Cherry L. Emerson Center for Scientific Computation and Department of Chemistry, Emory University, Atlanta, Georgia

CONTENTS

- I. Introduction
- II. Oxidative Addition
 - A. Oxidative Addition to d^8 Species
 - B. Oxidative Addition of H-X Bonds on the CpML Species
 - C. Oxidative Addition to d^{10} ML₂ and Related Systems
 - D. Special Topics: Dihydride-Dihydrogen Rearrangement in the Transition-Metal Polyhydride Complexes
 - E. Summary
- III. Metathesis
 - A. Summary
- IV. Olefin Insertion
 - A. Summary
- V. Full Catalytic Cycles
 - A. Olefin Hydroboration Catalytic Cycle by Rh(PR₃)₂Cl
 - B. Silastannation of Acetylene with a Palladium Catalyst
 - C. Hydroformylation Catalytic Cycle by RhH(CO)₂(PR₃)₂
 - D. Summary
- VI. Perspectives of Quantum Chemical Studies of Organometallic Reactions and Homogeneous Catalysis

HIGH-RESOLUTION HELIUM ATOM SCATTERING AS A PROBE OF SURFACE VIBRATIONS

SANFORD A. SAFRON

Department of Chemistry, Florida State University, Tallahassee, Florida

- I. Introduction
 - A. Overview
 - B. Scope
- II. Lattice Vibrations
 - A. One-Dimensional Models
 - B. Extension to Surface Dynamics
- III. Inelastic Atom-Surface Scattering
 - A. Atom-Single-Phonon Scattering
 - B. Atom-Multiphonon Scattering
- IV. Time-of-Flight Scattering Instrument
- V. Clean Crystalline Surfaces: Ionic Insulators
 - A. Alkali Halides
 - 1. LiF
 - 2. KBr and RbCl
 - 3. RbI
 - 4. NaF, KCl, and RbBr
 - 5. NaCl, NaI, and CsF
 - B. Metal Oxides
 - 1. NiO, CoO, and MgO
 - 2. KMnF₃ and High- T_C Superconductors
 - C. Multiphonon Excitations
- VI. Clean Crystalline Surfaces: Sampling of Materials
 - A. Metallic Surfaces
 - 1. Cu, Ag, and Au
 - 2. Nb, Mo, and W
 - B. Layered Materials
- VII. Epitaxially Grown Overlayers, Adsorbates, and Films
 - A. Alkali Halide/Alkali Halide Systems
 - 1. KBr/NaCl(001)

Advances in Chemical Physics, Volume XCV, Edited by I. Prigogine and Stuart A. Rice. ISBN 0-471-15430-X © 1996 John Wiley & Sons, Inc.

- 2. KBr/RbCl(001)
- 3. KCN/KBr(001)
- B. Adsorbate/Metal Systems
 - 1. Na/Cu(001)
 - 2. Ar or Kr/Ag(111) and Kr/Pt(111)
 - 3. Frustrated Translations: Benzene and CO on Rh(111)
- C. Organic Films
- VIII. Concluding Remarks

Acknowledgments





ORDERING AND PHASE TRANSITIONS IN ADSORBED MONOLAYERS OF DIATOMIC MOLECULES

DOMINIK MARX

Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

HORST WIECHERT

Institut für Physik, Johannes Gutenberg-Universität, Mainz, Germany

- I. Preliminary Remarks
 - A. Introduction
 - B. Molecular and Bulk Properties of N₂ and CO
 - C. Substrates and Coverage
- II. Orientational Ordering on a Triangular Lattice
 - A. Ground States and Mean-Field Theory
 - B. Anisotropic-Planar-Rotor Model and Some Generalizations
 - C. Symmetry Classification
- III. N₂ on Graphite
 - A. Phase Diagram
 - B. Submonolayers and Melting
 - C. Tricritical Point
 - D. Commensurate Herringbone Ordering
 - 1. Ground State and Orientational Order-Disorder Transition
 - 2. Order of the Phase Transition
 - E. Compressed Monolayers
- IV. N₂ on Boron Nitride
- V. CO on Graphite
 - A. Phase Diagram
 - B. Submonolayers and Melting
 - C. Tricritical Point
 - D. Commensurate Herringbone Ordering

Advances in Chemical Physics, Volume XCV, Edited by I. Prigogine and Stuart A. Rice. ISBN 0-471-15430-X © 1996 John Wiley & Sons, Inc.

- E. Commensurate Head-Tail Ordering
- F. Compressed Monolayers
- VI. CO on Boron Nitride
- VII. Concluding Remarks
 Acknowledgments

