

VITA

ALFRED B. ANDERSON



EDUCATION AND EXPERIENCE

- 2018 Emeritus Professor of Chemistry, Case Western Reserve University
- 1985 Joint appointment as Professor of Metallurgy and Ceramics, Case Western Reserve University.
- 1979 Assistant, 1981 Associate, and 1986 Full Professor, Chemistry Department, Case Western Reserve University, Cleveland, Ohio 44106. Email aba@case.edu.
- August 1977 - January 1979 Research Associate with Arthur Hubbard, University of California, Santa Barbara.
- September 1974 - August 1977 J. W. Gibbs Instructor in Chemistry, Yale.
- September 1972 - September 1974 Research Associate with Roald Hoffmann, Cornell.
- August 1971 - September 1972 Research Associate with Harrison Shull, Indiana.
- November 1970 - Ph.D. Research under Robert G. Parr, The Johns Hopkins University.
- June 1964 - A.B. Cornell

TEACHING CONTRIBUTIONS

Freshman Chemistry, Quantum Mechanics and Molecular Orbital Theory at Yale and Case Western Reserve University. Molecular Spectroscopy, Undergraduate Physical Chemistry, Freshman Chemistry Lab, Advanced Quantum Mechanics, and Undergraduate Research at CWRU.

RESEARCH CONTRIBUTIONS

Professor Anderson developed a theory for bond stretching force constants in molecules and solids as a graduate student in the lab of Robert G. Parr at Johns Hopkins University. The electronic charge density distribution function was partitioned in rigid atomic and flexible “bond charge” components. Using the equilibrium internuclear distance, the atomic components contained information for calculating by means of a Poisson equation the bond stretching harmonic and higher order force constants to useful accuracy. During a postdoctoral year at Indiana University in Harrison Shull’s lab he extended his applications and understanding of this electron density-based theory. This effort continued into a postdoctoral stay at Cornell University in Roald Hoffmann’s lab, culminating in his atom superposition and electron delocalization theory for calculating structures of molecules, including their molecular orbitals and energy levels. The theory is based on the Hellmann-Feynman electrostatic theory for molecular forces. Anderson postulated that the total molecular energy calculated using the one-electron molecular orbital extended Hückel Hamiltonian should approximate the attractive energy due to charge redistribution accompanying bond formation. Tests were supportive. Anderson continued applications of the ASED-MO theory primarily to models of bulk and surface properties during his tenure as the J. W. Gibbs Instructor in Chemistry at Yale University. At the urging of Ernest Yeager at Case Western Reserve University he gained exposure to electrochemistry, by spending a year in the lab of Arthur Hubbard at the University of California in Santa Barbara. This was his last step before joining the Case Western Reserve University Chemistry Department faculty. In his Case lab he and his coworkers employed the ASED-MO theory to gain an understanding of structures and reactions and electronic and vibrational properties in the fields of catalysis, solid state and surface chemistry, and electrochemistry. Structures and electronic properties of dopants in diamond were explored using the ASED-MO theory. Calculations using the theory agreed that substitutional B provides a good p-type dopant behavior, as was well known, but calculations for various substitutional and interstitial defects yielded no suitable n-type dopant scenarios.

Beginning in 1998 the Anderson lab began using first-principle VASP code and *ab initio* Gaussian code methods to better quantify results of diamond modeling and also to develop the linear Gibbs energy relationship (LGER) for predicting reversible electrode potentials for electron transfer reactions. The lab also postulated a quantum approach using simple local reaction center (LRC) models for calculating electrode potential dependencies of electron transfer activation energies. From these energies reversible potentials could be deduced. These new theories extended the understanding of the thermodynamics and kinetics of electrochemical reactions.

A visitor from Toyota Central Research and Development Corporation, Dr. Ryosuke Jinnouchi arrived in the lab in April 2006 with a goal of assembling the theoretical components required for a comprehensive treatment of electrocatalysis and creating a computer program to apply it. It included a two-dimensional density functional band theory, employing atomic orbitals, for modeling electrode surfaces. The electrode potential was assigned based on the calculated Fermi level, which was

adjustable by adding charge to the multilayer atomic slab surface model. The counter charge was distributed according to a modified Poisson-Boltzmann theory and the double layer width depended on the sizes of the model ions. To model solvation of all species present, the interfacial model was also bathed in a dielectric continuum. Reacting ions with water solvation shells could be included in the calculations. The quantum mechanical and Poisson-Boltzmann distribution problems were both solved to self-consistently. This computational code implementing the model provided a means for calculating and explaining the consequences of changes in bond polarizations for adsorbed and double-layer molecules which are caused by changes in the applied potential. The computer program was called "Interface." Previous theoretical work performed throughout the world was applied at the potential of zero charge, meaning the potential was not controlled. Interface calculations could be done for electrodes at any desired potential by simply changing charge added to the transitional unit cell used in the slab-band calculations. Interface had options for 1-dimensional and 3-dimensional calculations as well. Codes similar to Interface are being advanced and applied worldwide.

Interface found many applications in the Anderson lab, most notably to hydrogen and oxygen containing molecules reacting on platinum and copper electrode surfaces.

INVITED LECTURES

2026: Applications of Quantum Theory to Understanding Diamond Properties at Case, Including Collaborations with John Angus, 249th ECS Meeting in Seattle Washington on May 26th 2026

2016: Three Levels of Theory for Determining Potentials and Mechanisms in Electrocatalysis and Sample Applications, given at EMN Electrocatalysis Conference, Orlando Florida, February 15-19, 2016.

Recently Developed Theory and Applications to Understanding Mechanisms in Electrocatalysis, Presented at 47th ACS Central Regional Meeting, Covington KY May 18-21, 2016

2015: Selective Oxidation on a Fuel Cell Anode Means Going all the way to CO₂, Alfred B. Anderson, and Haleema A. Asiri, Symposium in Honor of James Burrington, 249th National ACS Meeting, Denver, Colorado, March 22-26, 2015.

2013: Reversible Potentials for Adsorbed Intermediates During Methanol and Formic Acid Electrooxidation on Platinum. Implications for Fuel Cells and Carbon Dioxide Reduction, A. B. Anderson and Haleema Asiri, 224th Electrochemical Society Meeting, San Francisco CA October 27-November 1, 2013.

Adsorption properties of ideal fuel cell cathode electrocatalysts: can materials with these properties be made? A. B. Anderson, 246th American Chemical Society National Meeting, Indianapolis, IN September 8-12, 2013.

2011: Understanding Electrocatalysis, 43rd IUPAC World Chemistry Congress, San Juan PR, July 30-August 7, 2011.

2010: Theories for Predicting Reversible Potentials of Reactions on Electrode Surfaces from Internal and Gibbs Energies: Applications to ORR, 217th Meeting of the Electrochemical Society, Vancouver BC April 25-30, 2010.

Theoretical Study of Contributions to the Overpotential for Platinum Cathodes, 61st Annual Meeting, International Society of Electrochemistry, A. B. Anderson and Feng Tian, Nice, Fr., September 26-October 1, 2010.

Oxygen Reduction Mechanism on Platinum, A. B. Anderson and Feng Tian, Pacificchem 2010 Conference, Honolulu, December 15-20, 2010.

2009: Theories for Predicting Reversible Potentials of Reactions on Electrode Surfaces from Internal and Gibbs Energies: Applications to ORR, Pittsburgh-Cleveland Catalysis Society Meeting, October 9, 2009.

Theories for Predicting Reversible Potentials of Reactions on Electrode Surfaces from Internal and Gibbs Energies: Applications to ORR, Brookhaven National Laboratory, August 26, 2009.

Predicting Reversible Potentials of Reactions on Electrode Surfaces from Internal and Gibbs Energies, 38th Great Lakes Regional Meeting of the American Chemical Society, Lincolnshire IL May13-16, 2009.

2008: Electrocatalyst Theories Based on Local Reaction Center Models, Linear Gibbs Energy Relationships, and now the Full Gibbs Energy, 236th National Meeting of the American Chemical Society, Philadelphia Pennsylvania, August 17-21, 2008.

Will Nitrided Graphite Work as an Electrocatalyst in a Fuel Cell Oxygen Cathode? K. Kurak and A. B. Anderson, 236th National Meeting of the American Chemical Society, Philadelphia Pennsylvania, August 17-21, 2008.

2007: Chemical Approach to Electrocatalysis: When Should Complexity be Introduced? 233rd American Chemical National Meeting, Chicago Illinois, March 25-29, 2007.

Predicting Mechanisms from Adsorption Bond Strengths and Activation Energies from Electron Affinities or Ionization Potentials of the Reaction Center. Presented at the 234th American Chemical Society National Meeting, Boston, Mass., August 19-23, 2007

2006: The Origin of Shallow n-type Conductivity in Boron Doped Diamond with H or S Co-Doping: a Density Functional Study, 11th International Conference on New Diamond Science and Technology and 9th Applied Diamond Conference, lecture by A. B. Anderson (Y. Cai, T. Zhang, J. C. Angus, L. N. Kostadinov co authors) May 15-18, 2006 Research Triangle Park, North Carolina, sponsored by the MRS.

2005: Why is there such a Small Overpotential for O₂ Electro Reduction by Copper Laccase?, 207th Meeting of the Electrochemical Society, Quebec City, Canada, May 15-20, 2005.

The Heyrovsky Step in Hydrogen Reactions on Diamond, Platinum, and Gold Electrodes, 38th Heyrovsky Discussion, Castle Trest, Czech Republic, June 12-16, 2005

Toward the Understanding and Prediction of Mechanisms in Electrocatalysis, Ernest B. Yeager Frontiers in Electrochemical Sciences and Electrochemical Technology, Case Western Reserve University, October 12-14, 2005.

2004: Pt₃Cr Alloy Effect on the Overpotential of O₂ Reduction on Acid Fuel Cell Cathodes: Theoretical Approach, J. Roques and A. B. Anderson, First International Conference on Fuel Cell Development and Deployment, Storrs, March 7-12, 2004.

Predicting Tafel Plots for Hydrogen Oxidation on Pt(100) Electrodes, A. B. Anderson and Y. Cai, First International Conference on Fuel Cell Development and Deployment, Storrs, March 7-12, 2004.

Theoretical Model for Predicting Potentials for upd H and OH(ads) Formation on Platinum in Base, Y. Cai and A. B. Anderson, 2004 Joint International Meeting of the Electrochemical Society, Honolulu, October 3-8, 2004.

Hydrogen Evolution on Diamond Electrodes and its Dependence on Surface C-H Bond Strengths Y. Cai, A. B. Anderson, J. C. Angus and L. Kostadinov, 2004 Joint International Meeting of the Electrochemical Society, Honolulu, October 3-8, 2004.

Electron Transfer Theory and Fuel Cell Chemistry, Stanford University, Nov. 10, 2004.

2003: Theoretical Calculation of Activation Energies for $\text{Pt} + \text{H}^+(\text{aq}) + \text{e}^-(U) \leftrightarrow \text{Pt-H}$: Activation Energy-Based Symmetry Factors in the Marcus Normal and Inverted Regions, Electrochemistry and Surface Science Symposium in Memory of Mike Weaver held at the 225th National Meeting of the American Chemical Society, New Orleans, March 23-27, 2003.

Constrained Variation Calculations of Electron-Transfer Transition States Using the Lagrange Method, A. B. Anderson, Computational Chemistry Symposium held at the 203rd Meeting of the Electrochemical Society, Paris, France April 27-May 2, 2003.

Roles of Interstitial Hydrogen and Substitutional Boron During H₂ Evolution on Diamond Electrodes. Model DFT Calculations, A. B. Anderson, Eighth International Symposium on Diamond Materials held at the 203rd Meeting of the Electrochemical Society, Paris, France, April 27-May 2, 2003.

Pt₃Cr Alloy Effect on the Reversible Potential of OH(ads) Formation from H₂O(ads): Comparison with Pure Pt(111) Surface, poster by J. Roques and A. B. Anderson, Pittsburgh-Cleveland Catalysis Society Spring 2003 Meeting, Carnegie Mellon University, June 24, 2003.

Pt₃Cr and Pt₃Co Alloy Effect on the Reversible Potential of OH(ads) Formation from H₂O(ads): Comparison with Pure Pt(111) Surface, poster by J. Roques and A. B. Anderson, 10th International Congress on the Application of Density Functional Theory, Brussels, Belgium, September 7-12, 2003.

Electrode Potential-Dependent Stages in OH(ads) Formation on the Pt₃Cr Alloy (111) Surface, Fundamental Understanding of Electrode Processes Symposium in Memory of Professor Ernest B. Yeager held at the 204th Meeting of the Electrochemical Society, Orlando, October 12-16, 2003.

The Reversible Hydrogen Electrode: Potential-Dependent Activation Energies over Platinum from Quantum Theory, Electrochemistry Symposium in Honor of Mike Weaver held at the 204th Meeting of the Electrochemical Society, Orlando, October 12-16, 2003.

Pt₃Cr Alloy Effect on the Reversible Potential of OH(ads) Formation from H₂O(ads): Comparison with Pure Pt(111) Surface, poster by J. Roques and A. B. Anderson, Fundamental Understanding of Electrode Processes Symposium in Memory of Professor Ernest B. Yeager held at the 204th Meeting of the Electrochemical Society, Orlando, October 12-16, 2003.

2002: O₂ Reduction and CO Oxidation at the Pt-electrolyte Interface. The Role of H₂O and OH adsorption Bond Strengths, 223rd National Meeting of the American Chemical Society, Orlando, Florida, April 7-11, 2002.

Cause of the CO Oxidation Prewave on Polycrystalline Pt in Acid Electrolyte. Insight from Density Functional Calculation, poster by J. Narayanasamy and A. B. Anderson, 223rd National Meeting of the American Chemical Society, Orlando, Florida, April 7-11, 2002.

Quantum Mechanical Calculation of the Symmetry Factors for the Underpotential Deposition of Hydrogen and its Oxidation on Pt, poster by R. A. Sidik, J. Narayanasamy, A. B. Anderson, and P. Shiller, 223rd National Meeting of the American Chemical Society, Orlando, Florida, April 7-11, 2002.

Density Functional Study of O₂ Electroreduction when Bonded to a Pt Dual Site, R. A. Sidik and A. B. Anderson, 223rd National Meeting of the American Chemical Society, Orlando, Florida, April 7-11, 2002.

Your Fundamental Dream Catalyst for Oxygen Reduction, Biofuel Cell Workshop, Washington, DC June 30-July 2, 2002.

Mechanisms in Fuel Cell Electrocatalysis: A Quantum Viewpoint, A. B. Anderson, Fuel Cell Gordon Conference, Roger Williams University, July 28-August 2, 2002

Theory at the Electrochemical Interface: Reversible Potentials and Potential-Dependent Activation Energies, 4th International Symposium on Electrocatalysis. From theory to Industrial Application (ECS'02), Como Italy, September 22-25, 2002.

Understanding of the O₂ Reduction Overpotential at the Pt Cathode and Probing of Alternative Catalysts via Computational Chemistry, R. A. Sidik and A. B. Anderson, AIChE National Meeting, Indianapolis, Indiana, November 3-8, 2002.

Theory at the Electrochemical Interface: Reversible Potentials and Potential-Dependent Activation Energies, University of New Mexico, November 21, 2002.

Theory at the Electrochemical Interface: Reversible Potentials and Potential-Dependent Activation Energies, Pittsburgh-Cleveland Catalysis Society Fall 2002 Meeting, Carnegie Mellon University, December 16, 2002.

2001: Electron Transfer Reactions and Electrocatalysis, Plenary Lecture, Workshop on the Application of First-Principles-Based Computational Methods to the Design of Electrochemical Power Systems, Berkeley, California, August 30 – September 1, 2001.

Dopants in Diamond Nanoparticles and Bulk: Density Functional Study of Substitutional B, N, P, SB, S, PN, O, NN, and Interstitial H, A. B. Anderson, T. V. Albu and J. C. Angus, 2001 Joint International Meeting of the Electrochemical Society and the International Society of Electrochemistry, San Francisco, California, September 2-7, 2001.

DFT Study of O₂ Reduction on Platinum, R. A. Sidik and A. B. Anderson, 2001 Joint International Meeting of the Electrochemical Society and the International Society of Electrochemistry, San Francisco, California, September 2-7, 2001.

Mechanism of the Electrooxidation of Water on Platinum: Quantum Chemical Theory, A. B. Anderson and N. M. Neshev, R. A. Sidik, and P. Shiller, 2001 Joint International Meeting of the Electrochemical Society and the International Society of Electrochemistry, San Francisco, California, September 2-7, 2001.

Theory of the Electrochemical Interface, Poster, NSF Workshop on Low Temperature PEM Fuel Cells, Arlington, Virginia, November 11-15, 2001.

2000: Quantum Chemical Modeling of Potential Dependencies at the Electrochemical Interface, International Conference on Elementary Processes in Molecular-Metal Surface Interactions, San Juan, Puerto Rico, November 11-15, 2000

1999: Plenary Lecture “Overcoming the Hurdles in Applying Quantum Chemistry to Understanding Electrocatalysis in Fuel Cells”, Workshop on Designed Catalysts for Fuel Processor/Fuel Cell Systems sponsored by the Army Research Office and DARPA, Chicago, IL, April 18-21, 1999.

Keynote Lecture “Using Quantum Chemistry to Determine Electrochemical Potential Dependence of Adsorbate Properties and Redox Activation Energies”, Tutorials in Electrochemical Engineering - Mathematical Modeling, Electrochemical Society Meeting, Seattle, WA, May 2-6, 1999.

1997: NSF-DOE Workshop on “Future Directions for Theoretical Catalysis: Homogeneous, Heterogeneous, and Surface Reactivity”, San Francisco, CA, April 18, 1997, presentation entitled “Theoretical Electrocatalysis.”

Duquesne University, Pittsburgh, PA, October 10, 1997, “Hydrogen Evolution from Diamond Film Electrodes: *Ab initio* Theory for Mechanism and Potential Dependence.”

1996: ACS National Meeting, Orlando, FL, Aug. 25. “Quantum Chemical Modeling of Electrocatalytic Reactions Including Potential Dependence. Beginning Stages.”

Chemistry Department, Case Western Reserve University, Cleveland, OH, Feb. 1, 1996. “Mechanisms in Methanol Electrocatalysis.”

1995: Lawrence Berkeley Laboratory, Berkeley, CA, March 7, “Theory of CO Oxidation on Pt Alloy Surfaces.”

Electrochemical Society Meeting, Chicago, IL, October 9, “Quantum Chemical Modeling of H₂O(ads) Decomposition to OH(ads) on Pt Alloy Surfaces.”

1991: Central Midwest ACS Meeting, Indianapolis, May 31, “Methoxy Mobility and Methane Formation on the Alumina Support.”

ACS National Meeting, New York, Aug. 28, "Hydrogen Binding and Diffusion in Diamond."

Workshop on Structural Effects in Electrocatalysis and Oxygen Electrochemistry, Case Western Reserve University, Cleveland, Oct. 29 - Nov. 1, "Molecular Orbital Approach to the Study of Electrochemical Interfaces."

Workshop on Structural Effects in Electrocatalysis and Oxygen Electrochemistry, Case Western Reserve University, Cleveland, Oct. 29 - Nov. 1, "A New Model for Predicting Oxygen Evolution and Reduction Mechanisms. Application to Strontium Ferrate."

1990: Purdue University, Jan. 26, "Electron Transfer in Surface Science and Electrochemistry, Molecular Orbital Approach."

Workshop on the Science and Technology of Diamond Thin Films, Quail Hollow, May 20-24, "Adoption and Bonding of C_1H_x and C_2H_4 on Unreconstructed Diamond(111): Dependence on Coverage and Coadsorbed Hydrogen." (Poster)

1989: CWRU/NASA/DuPont Workshop on Alumina, Cleveland, January 26, " Al_2O_3 /Metal Interface Theory."

Eleventh North American Meeting of the Catalysis Society, Dearborn, May 7-11, "The Influence of Electrochemical Potential on Chemistry at Electrode Surfaces Modeled by MO Theory."

Eleventh North American Meeting of the Catalysis Society, Dearborn, May 7-11, "CO-Al Interactions on Ni(111): Elucidation of Electronic Factors."

Liquid Lubricants Workshop, NASA-Lewis, Cleveland, Sept. 26, "Computational Chemistry at Case Western Reserve University."

Distinguished Visitor, Ford Motor Co., Dearborn, Sept. 28, "Catalyst Surfaces as Sources and Sinks of Electrons - Molecular Orbital Approach."

Symposium Honoring Harrison Shull, Bloomington, Oct. 27-28, "The Catalyst Surface as a Source and Sink of Electrons: A Concept Materialized Through MO Theory."

1989 Annual Conference of the Case Center for Electrochemical Sciences, Cleveland, Oct. 30-31, "Electron Transfer in Surface Science and Electrochemistry: Molecular Orbital Approach."

1989 International Chemical Conference of Pacific Basin Societies, Honolulu, Dec. 17-22, "Methane Conversion and Fischer-Tropsch Catalysis Over MoS_2 . Predictions and Interpretations from MO Theory."

1988: Lehigh University, Department of Chemistry, “Applications of Molecular Orbital Theory to Real Problems.”

Pittsburgh-Cleveland Catalysis Society Spring Symposium, Cleveland, April 8, “Methyl Group Coupling on MoS₂: Theoretical Predictions.”

196th ACS National Meeting, Los Angeles, Sept. 25-30, “Methane Activation and Subsequent Reactions on MoS₂. Predictions from Molecular Orbital Theory.”

196th ACS National Meeting, Los Angeles, Sept. 25-30, “Oxygen Evolution on a SrFeO₄ Anode. Mechanistic Considerations from Molecular Orbital Theory.”

II International Symposium Mechanism of Heterogeneous Catalysis - Quantum Chemical Approach, Zakopane, Poland, Oct. 2-9, “Quantum Theory of Chemisorption.”

1987: Lord Corporation, Jan. 5, “Surface Theory.”

Spring Symposium of the Catalysis Club of Philadelphia, May 13, “Methane on Oxide and Metal Surfaces: Hydrogen Abstraction and Metal Insertion into CH. Mechanisms from Molecular Orbital Theory.”

Gordon Research Conference on Catalysis, Colby-Sawyer College, June 23, “Activation of Hydrogen on Molybdenum Disulfide Catalysts.”

ACS Symposium on Molecular Processes at Solid Surfaces: The Structure of Molecules Adsorbed on Metal Surfaces, New Orleans, September, “Structure and Electronic Factors that Influence the Structures of Molecules Adsorbed on Transition Metal Surfaces.”

1986: Standard Oil, Cleveland, Jan. 31, “Principles of CH Bond Activation.”

Spring Symposium of the Catalysis Club of Chicago, I.I.T., May 12, “Structures and Orientations of Molecules on Surfaces, with an Emphasis on CO and CH Activation.”

Twenty-Fifth Annual Symposium of the Pittsburgh-Cleveland Catalysis Society, Cleveland, May 14-16, “Principles of Heterogeneous and Homogeneous CH Bond Activation from the Perspective of Molecular Orbital Theory.”

General Motors Research Laboratories, Dec. 17, “Theory in Electrocatalysis”.

1985: Methane Activation Chemistry Workshop, Sponsored by the Gas Research Institute, Houston, Feb. 4-6, “CH Activation by Metals and Metal Oxides.”

Dalhousie University: "Structural and Electronic Factors Influencing the Orientation and Reactivity of Carbon Monoxide and Acetylene on Transition Metal Surfaces."

Texas A&M University, "Surface Theory."

Chemistry Department, University of Wisconsin, Milwaukee. "Sulfate Formation."

Physics Department, University of Wisconsin, Milwaukee. "Surface Theory."

University of California, Berkeley, "Surface Theory."

Stanford Research Institute. "Surface Theory."

University of California, Los Angeles, "Surface Theory."

Symposium on Chemistry of Phthalocyanines, Central Regional ACS Meeting, Akron, June 6, "Electronic and Redox Properties of Stacked-Ring Silicon Phthalocyanines from Molecular Orbital Theory."

Symposium on Transition Metal Catalysis, Central Regional ACS Meeting, Akron, June 5, "CH Activation by Metals and Metal Oxides."

1984: General Electric, Nela Park, "Oxides: Predicting Some Solid State and Surface Properties."

B. F. Goodrich. "Applications of Molecular Orbital Theory."

University of Akron, "Applications of MO Theory."

188th ACS National Meeting, Philadelphia: Propylene Oxidation on Bismuth Molybdates Symposium, invited talk. 3rd International Conference on Transport in Non-stoichiometric Compounds, "Defect Structures in Transition Metal Oxides."

1983: Oxidation, Deposition and Hot Corrosion Conference at NASA Lewis, "Surface Reaction at NaCl and Sodium Pyrosulfate Formation."

1982: Chapman Conference on Point Defects in Minerals, "Electronic Properties of Crystals."

Ohio State, "Surface Electrochemistry Theory."

Southern Illinois, "Surface Electrochemistry Theory."

Purdue (Indianapolis), "Surface Electrochemistry Theory."

- 1981: Wayne State, "Surface Theory."
- NASA Lewis, "Sodium Sulfate Formation."
- 1980: Argonne, Visiting Scientist Lectures in Surface Science and Catalysis, "Surface and Catalysis Theory."
- Sohio, "Theory."
- 1979: Battelle, "Surface and Molecular Theory."
- CWRU: Oxygen Electrochemistry Workshop: Surface Theory MAIF Annual Meeting. "Surface Theory."
- 1978: Gordon Conference on Catalysis, "Surface Catalysis Theory."
- MIT, "Surface Theory."
- University of Toronto, "Molecular Theory."
- Honeywell, "Theory."
- Ames Research Center, Moffett Field, "Molecular Theory."
- 1977: IBM Yorktown Heights, "Surface Theory."
- UCLA, "Transition Metal Coordination Theory."
- New England Society of Inorganic Chemistry, "Theory Organometallic Complexes."
- 1976: DuPont, Wilmington, "Theory."
- 1975: Cornell, "Theory."
- Upstate New York American Vacuum Society Meeting, "Coal Gassification Catalysis."
- 1974: Electron Factor in Catalysis Meeting, NBS. "Surface Theory."
- 1971: Argonne, "Force Constant Theory."
- University of Minnesota. "Force Constant Theory."

CONTRIBUTED LECTURES

Many lectures at American Chemical Society, American Vacuum Society, and American Physical Society, Electrochemical Society and other Society meetings throughout the period 1971-present. Additional recruiting lectures at various colleges and universities and local lectures at CWRU.

PROFESSIONAL HONORS AND SOCIETY MEMBERSHIPS

American Chemical Society, American Physical Society, Electrochemical Society. Member of Case Center for Electrochemical Sciences.

PROFESSIONAL DUTIES

Chemistry Undergraduate and Graduate Committees, including Chairmanship of the latter; Chairman, Case Curriculum Committee; Case Academic Standing Committee; Case Assembly; Editor, Chemistry Graduate Brochure; Chairmanship of a Faculty Search Committee; Graduate Recruiting Committee.

BOOKS

Past and Current Models in Electrochemistry, A. B. Anderson, [*Past and Current Models in Electrochemistry*](#) (Springer Nature Switzerland, published October 2025, ISBN 978-3-031-97790-9).

BOOK CHAPTERS

Point Defects in Crystals: A Quantum Chemical Methodology and its Applications, A. B. Anderson, *American Geophysical Union Monograph 31, Mineral Physics* (American Geophysical Union, Washington, D. C., 1985) p. 18-25.

Molecular Orbital Theory of Surfaces, A. B. Anderson in *Surface Imaging and Visualization*, A. T. Hubbard, Ed. (CRC Press, Boca Raton, 1995) 465-472.

Quantum Chemical Modeling of Electrocatalytic Reactions, Including Potential Dependencies: Beginning Steps, A. B. Anderson in *Interfacial Electrochemistry, Theory, Experiment, and Applications*, A. Wieckowski, Ed. (Marcel Dekker, New York, 1999) 83-96.

BOOK REVIEWS

Book review for J. Am. Chem. Soc. 97, 943 (1975), [*Essays in Chemistry*](#), Vol. V by J. N. Bradley, R. D. Gillard, and R. F. Hudson.

Book review for J. Am. Chem. Soc. 104, 1157 (1982), [*Chemistry, Quantum Mechanics and Reductionism*](#), H. Primas (Springer-Verlag, NY, 1981).

Book review for American Scientist 71, no. 4 (1983), The Force Concept in Chemistry, B. M. Deb (Van Nostrand Reinhold, New York, 1981).

Review of Orbital Interactions in Chemistry by Albright, Burdett and Whangbo, American Scientist, 74, 81 (1986).

Review of The Structure of Surfaces, Ed. M. A. Van Hove and S. Y. Tong, American Scientist, 75, 79 (1987).

List of Publications

1. A. B. Anderson **Applications of Quantum Theory to Understanding Diamond Properties at Case, Including Collaborations with John Angus**, ECS Meeting Abstracts, Volume MA2026-01, H01: Wide-Bandgap Semiconductor Materials and Devices 27: In Memory of John C. Angus (2026) 10.1149/MA2026-01331501mtgabs.
2. A. B. Anderson **Classical Theories for Electrochemical Measurements and Electrocatalysis**, Chapter 1 in Past and Current Models in Electrochemistry, Springer Nature (2025) 10.1007/978-3-031-97791-6_1.
3. A. B. Anderson **Born Model for Ion Solvation Energies**, Chapter 2 in Past and Current Models in Electrochemistry, Springer Nature (2025) 10.1007/978-3-031-97791-6_2.
4. A. B. Anderson **Models of the 1950s and 60s**, Chapter 3 in Past and Current Models in Electrochemistry, Springer Nature (2025). 10.1007/978-3-031-97791-6_3.
5. A. B. Anderson **Further Explorations on the Gurney-Butler and Marcus-Hush Themes**, Chapter 4 in Past and Current Models in Electrochemistry, Springer Nature (2025). 10.1007/978-3-031-97791-6_4.
6. A. B. Anderson **Interplay of New Spectroscopies and Semiempirical Quantum Theory Applied to Electrochemistry: 1970s–1980s. The Chemical Bond is Robust Under Perturbation**, Chapter 5 in Past and Current Models in Electrochemistry, Springer Nature (2025). 10.1007/978-3-031-97791-6_5.
7. A. B. Anderson **Electronic Structure Picture of Anode, Cathode: Equilibrium with No Current and Conditions at Steady State with Current**, Chapter 6 in Past and Current Models in Electrochemistry, Springer Nature (2025). 10.1007/978-3-031-97791-6_6.
8. A. B. Anderson **Double Layer Formation on Insulators**, Chapter 7 in Past and Current Models in Electrochemistry, Springer Nature (2025). 10.1007/978-3-031-97791-6_7.
9. A. B. Anderson **Quantum Theories for Predicting Reversible Potentials and Activation Energies for Electron Transfer Reactions, But Still Omitting Surface Charging and Double Layer Polarization: 1980s to Present Time**, Chapter 8 in Past and Current Models in Electrochemistry, Springer Nature (2025). 10.1007/978-3-031-97791-6_8.
10. A. B. Anderson **Advanced First Principles Methods**, Chapter 9 in Past and Current Models in Electrochemistry, Springer Nature (2025). 10.1007/978-3-031-97791-6_9.

11. A. B. Anderson **Advanced First Principles Studies Involving Hydrogen Adsorption**, Chapter 10 in Past and Current Models in Electrochemistry, Springer Nature (2025). 10.1007/978-3-031-97791-6_10.
12. A. B. Anderson **First Principles Modeling at the pzc Including Polarizable Electrolyte: Oxygen Reactions on the Pt Cathode and Electroless Copper Deposition**, Chapter 11 in Past and Current Models in Electrochemistry, Springer Nature (2025). 10.1007/978-3-031-97791-6_11.
13. A. B. Anderson **Recent Theoretical Studies of pH Dependence of Several Surface Reactions**, Chapter 12 in Past and Current Models in Electrochemistry, Springer Nature (2025). 10.1007/978-3-031-97791-6_12.
14. A. B. Anderson **Concluding Comments and the View Ahead**, Chapter 13 in Past and Current Models in Electrochemistry, Springer Nature (2025). 10.1007/978-3-031-97791-6_13.
15. A. B. Anderson **How Computational Theorists Deal with Electrode Potential**, J. Electrochem. Soc. 172, 036501(2025).
16. A. B. Anderson **Perspective on Theories for Reversible Potentials for Reactions Taking Place on Electrode Surfaces**, J. Electroanal. Chem. 898, 115926 (2021).
17. A. B. Anderson and E. F. Holby **Pathways for O₂ Electroreduction over Substitutional FeN₄, HOFen₄, and OFen₄ in Graphene Bulk Sites: Critical Evaluation of Overpotential Predictions Using LGER and CHE Models**, J. Phys. Chem. C 123, 18398-18409 (2019).
18. A. B. Anderson **Pourbaix Diagrams for H₂O Oxidation to Adsorbed OH on Pt(111) and Why They Differ from Those for Bulk Solids**, J. Phys. Chem. C 122, 9958–9964 (2018).
19. M. Zhao and A. B. Anderson **Predicting the Double Layer Width on Pt(111) in Acid and Base with Theory and Extracting It from Experimental Voltammograms**, J. Phys Chem. C 121, 28051-28064 (2017).
20. M. Zhao and A. B. Anderson **Theory of Hydrogen Deposition and Evolution on Cu(111) Electrodes**, Journal of The Electrochemical Society, 164 (9) H691-H695 (2017).
21. A. B. Anderson, **Concepts and Computational Methods for the Electrochemical Interface and Applications: Past, Present, and Future**, Current Opinion in Electrochemistry 1, 27-33 (2017).
22. M. Zhao, L. Yu, R. Akolkar and A. B. Anderson **Mechanism of Electroless Copper Deposition from [Cu^{II}EDTA]¹⁻ Complexes Using Aldehyde-Based Reductants**, J. Phys. Chem. C 120, 24789-24793 (2016).

23. M. Zhao and A. B. Anderson **Prediction pH Dependencies of Electrode Surface Reactions in Electrocatalysis**, *Electrochem. Communications* 69, 64-67, (2016).
24. M. Zhao and A. B. Anderson **Predicting Reversible Potentials in Acid and Base from Self-Consistent Quantum Theory: H(ads) and OH(ads) Deposition on the Pt(111) Electrode**, *J. Phys Chem. Lett.* 7, 711-714 (2016).
25. Alfred B. Anderson and Meng Zhao **Reaction Energy for an Electrode Surface Atom Inserting into an R-H Bond and its Dependence on Electrode Potential: Application to Pt(111)**, *J. Electrochem. Soc.*, 162, H583-H589 (2015).
26. A. Asiri and A. B. Anderson **Mechanisms for Ethanol Electrooxidation on Pt(111) and Adsorption Bond Strengths Defining the Ideal Catalyst**, *J. Electrochem. Soc.*, 162 (1) F115-F122 (2015).
27. A. B. Anderson and H. A. Asiri **Reversible Potentials for Steps in Methanol and Formic Acid Oxidation to CO₂; Adsorption Energies of Intermediates on the Ideal Electrocatalyst for Methanol Oxidation and CO₂ Reduction**, *Phys. Chem. Chem. Phys.* 16, 10587-10599 (2014).
28. J. Uddin and A. B. Anderson **Trends with coverage and pH in Stark tuning rates for CO on Pt(111) Electrodes**, *Electrochim. Acta* 108, 398-403 (2013).
29. H. A. Asiri and A. B. Anderson **Using Gibbs Energies to Calculate the Pt(111) Hupd Cyclic Voltammogram**, *J. Phys. Chem. C*, 2013, 117, 17509-17513.
30. A. B. Anderson, R. Jinnouchi, and J. Uddin **Effective Reversible Potentials and Onset Potentials for O₂ Electroreduction on Transition Metal Electrodes: Theoretical Analysis**, *J. Phys. Chem. C* 117, 41-48 (2013).
31. A. B. Anderson, **Insights into Electrocatalysis** *Phys. Chem. Chem. Phys.* 14, 1330-1338 (2012).
32. A. B. Anderson **Volcano Plots and Effective Reversible Potentials for Oxygen Electroreduction** *Electrocatalysis* 3, 176-182 (2012).
33. F. Tian and A. B. Anderson **Effective Reversible Potentials, Energy Loss, and Overpotential on Platinum Fuel Cell Cathodes**, *J. Phys. Chem. C* 115, 7076-7088 (2011).
34. K. A. Kurak and A. B. Anderson **Selenium: a Nonprecious Metal Cathode Catalyst for Oxygen Electroreduction**, *J. Electrochem. Soc.* 157, B173-B179 (2010).

35. A. B. Anderson **Theories for Predicting Reversible Potentials of Reactions on Electrode Surfaces from Internal and Gibbs Energies: Applications to ORR**, ECS Transactions 28, 1-17 (2010).
36. A. B. Anderson, J. Uddin, and R. Jinnouchi **Solvation and Zero-Point-Energy Effects on OH(ads) Reduction on Pt(111) Electrodes**, J. Phys. Chem. C 114, 14946-14952 (2010).
37. K. A. Kurak and A. B. Anderson **Nitrogen-Treated Graphite and Oxygen Electroreduction on Pyridine Edge Sites**, J. Phys. Chem. C 113, 6730-6734 (2009).
38. F. Tian, R. Jinnouchi, and A. B. Anderson **How Potentials of Zero Charge and Potentials for Water Oxidation to OH(ads) on Pt(111) Electrodes Vary With Coverage**, J. Phys. Chem. C 113, 17484-17492 (2009).
39. T. Zhang and A. B. Anderson **Parameter Dependence in the Local Reaction Center Model for the Electrochemical Interface**, J. Phys. Chem. C 113, 3197-3202 (2009).
40. F. Tian and A. B. Anderson **Theoretical Study of Early Steps in Corrosion of Pt and Pt/Co Alloy Electrodes**, J. Phys. Chem. C, 112, 18566-18571 (2008).
41. R. Jinnouchi and A. B. Anderson **Aqueous and Surface Redox Potentials from Self-Consistently Determined Gibbs Energies**, J. Phys Chem. C, 112, 8747-8750 (2008).
42. V. Chakrapani, C. Pendyala, K. Kash, A. B. Anderson, M. K. Sunkara, and J. C. Angus **Electrochemical Pinning of the Fermi Level: Mediation of Photoluminescence from Gallium Nitride and Zinc Oxide**, J. Am. Chem. Soc. 130, 12944–12952 (2008).
43. R. Jinnouchi and A. B. Anderson **Electronic Structure Calculations of Liquid-Solid Interfaces: a Combination of Density Functional Theory and Modified Poisson-Boltzmann Theory**, Phys. Rev. B77, 2454170-24541718 (2008).
44. T. Zhang and A. B. Anderson **Oxygen Reduction on Platinum Electrodes in Base: Theoretical Study**, Electrochim. Acta 52, 982-989 (2007).
45. E. Vayner, R. A. Sidik, A. B. Anderson, B. N. Popov **Experimental and Theoretical Study of Cobalt Selenide as a Catalyst for O₂ Electroreduction**, J. Phys. Chem. C, 2007, 111, 10508-10513.

46. E. Vayner and A. B. Anderson **Theoretical Predictions Concerning Oxygen Reduction on Nitrated Graphite Edges and a Cobalt Center Bonded to Them**, J. Phys. Chem. C, 111, 9330-9336 (2007).
47. T. Zhang and A. B. Anderson **Hydrogen Oxidation and Evolution on Platinum Electrodes in Base: Theoretical Study**, J. Phys. Chem. C, 111, 8644-8648 (2007).
48. E. Vayner, H. Schweiger, and A. B. Anderson **Four-Electron Reduction of O₂ Over Multiple Cu^I Centers” Quantum Theory**, J. Electroanal. Chem. 607, 90-100 (2007).
49. V. Chakrapani, J. C. Angus, A. B. Anderson, S. D. Wolter, B. R. Stoner, and G. U. Sumanasekera **Charge Transfer Equilibria Between Diamond and an Aqueous Oxygen Electrochemical Redox Couple**, Science, 318, 1424-1430 (2007).
50. Y. Cai, A. B. Anderson, J. C. Angus, and L. N. Kostadinov **Hydrogen Evolution on Diamond Electrodes by the Volmer Heyrovsky Mechanism: Prediction of Reversible Potentials and Activation Energies**, J. Electro. Chem. Soc. 154, F36-F43 (2007).
51. Y. Cai, T. Zhang, A. B. Anderson, J. C. Angus, L. N. Kostadinov, T. V. Albu **The Origin of Shallow n-type Conductivity in Boron-doped Diamond with H or S Co-doping: Density Functional Theory Study**, Diamond and Related Materials, 15, 1868-1877 (2006).
52. A. B. Anderson and E. Vayner **Hydrogen Oxidation and Proton Transport at the Ni-Zirconia Interface in Solid Oxide Fuel Cells: Quantum Chemical Predictions**, Solid State Ionics, 177, 1355-1359 (2006).
53. R. A. Sidik and A. B. Anderson, **Co₉S₈ as a Catalyst for Electroreduction of O₂: Quantum Chemistry Predictions**, J. Phys. Chem. B, 110, 936-931 (2006).
54. R. A. Sidik, A. B. Anderson, N. P. Subramanian, S. P. Kumaraguru, and B. N. Popov **O₂ Reduction on Graphite and Nitrogen-doped Graphite: Experiment and Theory**, J. Phys. Chem. B, 110, 1787-1793 (2006).
55. H. Schweiger, E. Vayner, and A. B. Anderson **Why is there such a Small Overpotential for O₂ Electroreduction by Copper Laccase?**, Electrochem. Sol. St. Lett., 8, A585-A587 (2005).
56. V. Chakrapani, A. B. Anderson, and J. C. Angus **Surface Conductivity of Undoped, Hydrogen-Terminated Diamond**, AlChE Annu. Meet. Conf. Proc., 395c/1-395c/10 (2005).

57. J. Roques and A.B. Anderson **Pt₃Cr(111) Alloy Effect on the Reversible Potential of OOH(ads) formation from O₂(ads) Relative to Pt(111)**, J Fuel Sci. Technol. 2, 86-93 (2005).
58. V. Chakrapani, S. C. Eaton, A. B. Anderson, M. Tabib-Azar, and J. C. Angus **Studies of Adsorbate-Induced Conductance of Diamond Surfaces**, Electrochem. Sol. St. Lett., 8, E4-E8 (2005).
59. A. B. Anderson, J. Roques, S. Mukerjee, V. S. Murthi, N. M. Markovic, and V. Stamenkovic **Activation Energies for Oxygen Reduction on Platinum Alloys: Theory and Experiment**, J. Phys. Chem. B, 109, 1198-1203 (2005).
60. A. B. Anderson, Y. Cai, R. Sidik, and D. B. Kang **Advancements in the Local Reaction Center Electron Transfer Theory and the Transition State Structure in the First Step of Oxygen Reduction over Platinum**, J. Electroanal. Chem., 580, 17-22 (2005).
61. Y.Cai and A.B. Anderson **Calculating Reversible Potentials for Pt-H and Pt-OH Bond Formation in Basic Solution**, J. Phys. Chem. B, 2005, 109, 7557-7563 (2005).
62. Y. Cai, A. B. Anderson, J. C. Angus, and Lubomir N. Kostadinov **Hydrogen Evolution on Diamond Electrodes and Its Dependence on Surface C-H Bond Strengths**, Electrochem. Solid State Lett., 8, E62-E65 (2005).
63. J. Roques and A. B. Anderson **Cobalt Concentration Effect in Pt_{1-x}Co_x on the Reversible Potential for Forming OH_{ads} from H₂O_{ads} in Acid Solution**, Surface Sci., 581, 105-117 (2005).
64. J. Roques, A. B. Anderson, V. S. Murthi, and S. Mukerjee **Potential Shift for OH(ads) Formation on the Pt Skin on Pt₃Co(111) in Acid. Theory and Experiment**, J. Electrochem. Soc., 152, E193-E199 (2005).
65. A. B. Anderson and Y. Cai **Calculation of the Tafel Plot for H₂ Oxidation on Pt(100) from Potential-Dependent Activation Energies**, J. Phys. Chem. B, 108, 19917-19920 (2004).
66. J. Roques and A. B. Anderson **Theory for the Potential Shift for OH_{ads} Formation on the Pt-Skin on Pt₃Cr(111) in Acid**, J. Electrochem. Soc. A, 151, E85-E91 (2004).
67. Y. Cai and A. B. Anderson **The Reversible Hydrogen Electrode: Potential-Dependent Activation Energies over Platinum from Quantum Theory**, J. Phys. Chem. B, 108, 9829-9833 (2004).

68. J. Roques and A. B. Anderson **Electrode Potential-Dependent Stages in OH(ads) Formation on the Pt₃Cr Alloy (111) Surface**, J. Electrochem Soc., 151, E340-E347 (2004).
69. A. B. Anderson and R. A. Sidik **Oxygen Electroreduction on Fe^{II} and Fe^{III} Coordinated to N₄ Chelates. Reversible Potentials for the Intermediate Steps from Quantum Theory**, J. Phys. Chem. B, 108, 5031-5035 (2004).
70. J. Narayanasamy and A. B. Anderson **Calculating Reversible Potentials for Elementary Reactions in Acid and Base from Model Reaction Energies**, J. Phys. Chem. B 107 (2003) 6898-6901.
71. A. B. Anderson **Theory at the Electrochemical Interface: Reversible Potentials and Potential-Dependent Activation Energies**, Electrochim. Acta 48 (2003) 3743-3749.
72. A. B. Anderson, R. A. Sidik, J. Narayanasamy, and P. Shiller **Theoretical Calculation of Activation Energies for Pt + H⁺(aq) + e⁻(U) ↔ Pt-H: Activation Energy-Based Symmetry Factors in the Marcus Normal and Inverted Regions**, J. Phys Chem. B 107 (2003) 4618-4623.
73. A. B. Anderson, L. N. Kostadinov, and J. C. Angus **Hydrogen Atom Pairs in Diamond Bulk and at the Surface: Hybrid Density Functional Theory and Cluster Models**, Phys. Rev. B 67 (2003) 233402-1-233402-4.
74. J. Narayanasamy and A. B. Anderson **Mechanism for the Electrooxidation of Carbon Monoxide on Platinum by H₂O. Density Functional Theory Calculation**, J. Electroanal. Chem. 554-555 (2003) 35-40.
75. L. N. Kostadinov and A. B. Anderson **Constrained Variation Calculations of Electron-Transfer Transition States Using the Lagrange Method**, Electrochem. and Solid State Lett. 6 (2003) E30-E33.
76. Anderson, A. B.; Neshev, N. M.; Sidik, R. A.; Shiller P. **Mechanism for the Electrooxidation of Water to OH and O bonded to Platinum: Quantum Chemical Theory**, Electrochim. Acta 47 (2002) 2999-3008.
77. Anderson, A. B. **O₂ Reduction and CO Oxidation at the Pt-Electrolyte Interface. The Role of H₂O and OH Adsorption Bond Strengths**, Electrochim. Acta 47 (2002) 3759-3763.
78. S. C. Eaton; Yu. E. Evstefeeva; J. C. Angus; A. B. Anderson; Yu. V. Pleskov **Sulfur-Doped n-Type diamond: Preparation and Electrochemical Properties**. Russian J. Electrochem. 39, 154-159 (2003).
79. S. C. Eaton; Yu. E. Evstefeeva; J. C. Angus; A. B. Anderson; Yu. V. Pleskov

- Diamond growth in the presence of boron and sulfur.** Diamond and Related Materials **12** (2003) 1627-1632.
80. S. C. Eaton, A. B. Anderson, J. C. Angus, Y. E. Evstefeeva, and Y. Pleshkov **Co-doping of Diamond with Boron and Sulfur.** Electrochem. Sol. St. Lett. **5** (2003) G65-G68.
 81. Sidik, R. A.; Anderson, A. B. **Density Functional Theory Study of O₂ Electroreduction When Bonded to a Pt Dual Site.** J. Electroanal. Chem. 528 (2002) 69-76.
 82. Anderson, A. B.; Neshev, N. M. **Mechanism for the Electro-oxidation of Carbon Monoxide on Platinum, Including Electrode Potential Dependence.** J. Electrochem. Soc. 149 (2002) E383-E388.
 83. Albu, T. V.; Anderson, A. B.; Angus, J. C. **Dopants in Diamond Nanoparticles and Bulk: Density Functional Study of Substitutional B, N, P, SB, S, PN, O, NN, and Interstitial H.** J. Electrochem. Soc., (2002) 149, E143-E147.
 84. Albu, T. V.; Anderson, A. B. **Studies of model dependence in an ab initio approach to uncatalyzed oxygen reduction and the calculation of transfer coefficients.** Electrochim. Acta (2001), 46(19), 3001-3013.
 85. Anderson, A. B. **Shallow n-type dopants in diamond: Theory.** EMIS Datarev. Ser. (2000), 26(Properties, Growth and Applications of Diamond), 232-235.
 86. Anderson, Alfred B.; Albu, Titus V. **Catalytic effect of platinum on oxygen reduction. An ab initio model including electrode potential dependence.** J. Electrochem. Soc. (2000), 147(11), 4229-4238.
 87. Anderson, Alfred B.; Albu, Titus V. **Ab Initio Determination of Reversible Potentials and Activation Energies for Outer-Sphere Oxygen Reduction to Water and the Reverse Oxidation Reaction.** J. Am. Chem. Soc. (1999), 121(50), 11855-11863.
 88. Anderson, Alfred B. **Using quantum chemistry to determine electrochemical potential dependencies of adsorbate properties and redox activation energies.** Proc. - Electrochem. Soc. (1999), 99-14(Tutorials in Electrochemical Engineering--Mathematical Modeling), 1-7.
 89. Grantscharova-Anderson, E.; Anderson, Alfred B. **The prewave in CO oxidation over roughened and Sn alloyed Pt surfaces: possible structure and**

- electronic causes.** *Electrochim. Acta* (1999), 44(25), 4543-4550.
90. Anderson, Alfred B.; Albu, Titus V. **Ab initio approach to calculating activation energies as functions of electrode potential. Trial application to four-electron reduction of oxygen.** *Electrochem. Commun.* (1999), 1(6), 203-206.
 91. Martin, Heidi B.; Smith, Bridget A.; Angus, John C.; Landau, Uziel; Anderson, Alfred B.. **Boron-doped diamond films for electrochemical applications.** *Mater. Res. Soc. Symp. Proc.* (1999), 555 (Properties and Processing of Vapor-Deposited Coatings), 217-226.
 92. Swain, Greg M.; Anderson, Alfred B.; Angus, John C. **Applications of diamond thin films in electrochemistry.** *MRS Bull.* (1998), 23(9), 56-60.
 93. Anderson, Alfred B.; Kang, Dae Bok. **Quantum Chemical Approach to Redox Reactions Including Potential Dependence: Application to a Model for Hydrogen Evolution from Diamond.** *J. Phys. Chem. A* (1998), 102(29), 5993-5996.
 94. Anderson, Alfred B.; Shiller, Paul. **Mechanism for Oxidative Dissolution of a Cr Atom from a Pt Surface: Molecular Orbital Theory.** *J. Phys. Chem. B* (1998), 102(15), 2696-2698.
 95. Anderson, Alfred B.; Kostadinov, Lubomir N. **P and N compensation in diamond molecular orbital theory.** *J. Appl. Phys.* (1997), 81(1), 264-271.
 96. Anderson, Alfred B.; Grantscharova, Emilia J.; Angus, John C. **Molecular-orbital theory of monatomic and diatomic substitutional defects as shallow n-type dopants in diamond.** *Phys. Rev. B: Condens. Matter* (1996), 54(20), 14341-14348.
 97. Anderson, Alfred B.; Seong, Seeyearl; Grantscharova, E. **Molecular orbital investigation of water reactions with tin hydroxide complexes in association with platinum electrodes.** *J. Phys. Chem.* (1996), 100(44), 17535-17538.
 98. Anderson, A. B. **Quantum chemical modeling of electrocatalytic reactions, including potential dependence. Beginning stages.** Book of Abstracts, 212th ACS National Meeting, Orlando, FL, August 25-29 (1996), COLL-001.
 99. Anderson, Alfred B.; Grantscharova, E.; Seong, Seeyearl. **Systematic**

- theoretical study of alloys of platinum for enhanced methanol fuel cell performance.** J. Electrochem. Soc. (1996), 143(6), 2075-2082.
100. Martin, Heidi B.; Argoitia, Alberto; Landau, Uziel; Anderson, Alfred B.; Angus, John C. **Hydrogen and oxygen evolution on boron-doped diamond electrodes.** J. Electrochem. Soc. (1996), 143(6), L133-L136.
 101. Seong, Seeyearl; Anderson, Alfred B. **Water Dissociation on Pt(111) and (100) Anodes: Molecular Orbital Theory.** J. Phys. Chem. (1996), 100(28), 11744-11747.
 102. Anderson, Alfred B.; Grantscharova, Emilia; Seong, Seeyearl. **Quantum chemical modeling of H₂O(ads) decomposition to OH(ads) on Pt alloy surfaces.** Proc. - Electrochem. Soc. (1996), 95-26(Oxygen Electrochemistry), 1-12.
 103. Anderson, Alfred B.; Shiller, Paul. **Dehydrogenation of methoxy adsorbed on Pt(111) and Cr(110):. the stabilizing effect of the more electropositive surface.** Surf. Sci. (1996), 345(3), 274-80.
 104. Anderson, Alfred B. **Molecular orbital theory of surfaces.** Handb. Surf. Imaging Visualization (1995), Ed. Hubbard, Arthur CRC Press, 465-72.
 105. Anderson, Alfred B.; Grantscharova, E.; Shiller, Paul. **On the lack of activity of substitutional Sn atoms toward the electro-oxidation of CO on Pt anodes. Molecular orbital theory.** J. Electrochem. Soc. (1995), 142(6), 1880-4.
 106. Anderson, Alfred B.; Grantscharova, E. **Catalytic Effect of Ruthenium in Ruthenium-Platinum Alloys on the Electrooxidation of Methanol. Molecular Orbital Theory.** J. Phys. Chem. (1995), 99(22), 9149-54.
 107. Anderson, Alfred B.; Grantscharova, E. **Potential Dependence of CO(ads) Oxidation by OH(ads) on Platinum Anodes. Molecular Orbital Theory.** J. Phys. Chem. (1995), 99(22), 9143-8.
 108. Mehendru, S. P.; Anderson, Alfred B. **The migration of interstitial H in diamond and its pairing with substitutional B and N: molecular orbital theory.** J. Mater. Res. (1994), 9(2), 383-95.
 109. Anderson, Alfred B. **Electron density distribution functions and the ASED-MO theory.** Int. J. Quantum Chem. (1994), 49(5), 581-9.

110. Anderson, Alfred B.; Mehandru, S. P. **N-type dopants and conduction-band electrons in diamond: cluster molecular-orbital theory.** Phys. Rev. B: Condens. Matter (1993), 48(7), 4423-7.
111. Lundeen, Munime; Anderson, Alfred B. **An ASED-MO calculation of a side-on bound dimer model of oxyhaemocyanin.** Polyhedron (1993), 12(7), 739-743.
112. Shiller, Paul; Anderson, Alfred B. **Dehydrogenation of adsorbed methoxy on clean and oxidized metals: an electronic effect and its implications.** J. Phys. Chem. (1993), 97(1), 189-92.
113. Shiller, Paul; Anderson, Alfred B. **Potential dependence of carbon monoxide oxidation by water on a platinum anode. A molecular orbital theory.** J. Electroanal. Chem. (1992), 339(1-2), 201-10.
114. Mehandru, S. P.; Anderson, Alfred B.; Angus, John C. **Hydrogenation of the {10.hivin.10} graphite edge: structural considerations from band calculations.** J. Phys. Chem. (1992), 96(26), 10978-82.
115. Jen, S. F.; Anderson, Alfred B.. **Why the addition of carbon monoxide leads to acyl decarbonylation in a supported rhodium dimer complex.** Inorg. Chem. (1992), 31(12), 2651-4.
116. Jen, S. F.; Anderson, Alfred B.; Hill, Craig L. **Alkane reactions with photoactivated decatungstate in neutral and acid solution: molecular orbital theory.** J. Phys. Chem. (1992), 96(13), 5658-62.
117. Anderson, Alfred B. **Molecular orbital approach to the study of electrochemical interfaces.** Proc. - Electrochem. Soc. (1992), 92-11(Proc. Workshop Struct. Eff. Electrocatal. Oxygen Electrochem., 1992), 1-16.
118. Anderson, Alfred B. **A new model for predicting oxygen evolution and reduction mechanisms. Application to strontium ferrate.** Proc. - Electrochem. Soc. (1992), 92-11(Proc. Workshop Struct. Eff. Electrocatal. Oxygen Electrochem., 1992), 434-9.
119. Mehandru, S. P.; Anderson, Alfred B.; Angus, John C. **Hydrogen binding and diffusion in diamond.** J. Mater. Res. (1992), 7(3), 689-95.
120. Angus, John C.; Li, Zhidan; Sunkara, Mahendra; Gat, Roy; Anderson, Alfred

- B.; Mehandru, Satya P.; Geis, Michael W. **Nucleation and growth processes in chemical vapor deposition of diamond.** Proc. - Electrochem. Soc. (1991), 91-8 (Proc. Int. Symp. Diamond Mater., 2nd, 1991), 125-41.
121. Mehandru, S. P.; Anderson, Alfred B.; Angus, John C. **Hydrogen binding and diffusion in diamond.** Prepr. Pap. - Am. Chem. Soc., Div. Fuel Chem. (1991), 36(3), 1053-8.
122. Anderson, Alfred B.; Jen, Shu Fen. **Methoxy mobility and methane formation on the alumina support.** J. Phys. Chem. (1991), 95(20), 7792-5.
123. Yu, Jenwei; Anderson, Alfred B. **Adsorption of hydrogen, carbon monoxide, methylene, methyl, and ethene on molybdenum carbide (MoC). Molecular orbital theory.** Surf. Sci. (1991), 254(1-3), 320-8.
124. Mehandru, S. P.; Anderson, Alfred B. **Adsorption of atomic hydrogen, methyl, methylene, and acetylene on 2×1 restructured diamond (100). Theoretical study of structures, bonding, and migration.** Surf. Sci. (1991), 248(3), 369-81.
125. Mehandru, S. P.; Anderson, Alfred B. **Adhesion and bonding of polar and non-polar silicon carbide surfaces to titanium(0001).** Surf. Sci. (1991), 245(3), 333-44.
126. Shiller, Paul; Anderson, Alfred B. **Thermal generation of methyl radical from methanol adsorbed on oxygen-covered molybdenum (110): carbon-oxygen bond strength considerations from molecular orbital theory.** J. Phys. Chem. (1991), 95(3), 1396-9.
127. Yu, Jenwei; Anderson, Alfred B. **Binding of ethylene and acetylene to sulfur (S_2^-) in $C_5H_5MoS_4MOC_5H_5$ and on crystalline molybdenum disulfide: molecular orbital theory.** J. Mol. Catal. (1990), 62(2), 223-32.
128. Mehandru, S. P.; Anderson, Alfred B. **Structures and energetics for polar and nonpolar silicon carbide surface relaxations.** Phys. Rev. B: Condens. Matter (1990), 42(14), 9040-9.
129. Mehandru, S. P.; Anderson, Alfred B. **Adsorption and bonding of C_1H_x and C_2H_y on unreconstructed diamond(111). Dependence on coverage and coadsorbed hydrogen.** J. Mater. Res. (1990), 5(11), 2286-95.
130. Anderson, Alfred B. **Structure and electronic factors in heterogeneous catalysis: C.tplbond.C, C.tplbond.O, and C-H activation processes on metals**

- and oxides.** Theor. Aspects Heterog. Catal. (1990), 431-57.
131. Shiller, Paul; Anderson, Alfred B. **Effects of chemisorbed and substitutional O, I, and II germanium, tin, and lead on carbon monoxide adsorption on platinum(111): molecular orbital theory.** Surf. Sci. (1990), 236(3), 225-32.
 132. Yu, Jenwei; Anderson, Alfred B. **Carbon-hydrogen bond activation in methane and tert-butoxide(ads) by oxygen chemisorbed on Ag(110). Molecular orbital theory.** J. Am. Chem. Soc. (1990), 112(20), 7218-21.
 133. Hong, S. Y.; Anderson, Alfred B.; Smialek, James L. **Sulfur at nickel-alumina interfaces. Molecular orbital theory.** Surf. Sci. (1990), 230(1-3), 175-183.
 134. Mehandru, S. P.; Anderson, A. B. **Adsorption and Bonding of C_1H_x and C_2H_y on Unreconstructed Diamond(111): Dependence on Coverage and Coadsorbed Hydrogen.** Carbon, (1990), 28, 797
 135. Nath, K.; Anderson, Alfred B. **Adhesion and bonding of polar and nonpolar silicon monocarbide and aluminum nitride surfaces: tight-binding band theory.** Phys. Rev. B: Condens. Matter (1989), 40(11), 7916-23.
 136. Anderson, Alfred B. **The influence of electrochemical potential on chemistry at electrode surfaces modeled by MO theory.** J. Electroanal. Chem. Interfacial Electrochem. (1990), 280(1), 37-48.
 137. Schioett, Birgit; Hoffmann, Roald; Awad, Mohamed K.; Anderson, Alfred B. **Ethynidyne on the rhodium(100) surface: a theoretical investigation.** Langmuir (1990), 6(4), 806-16.
 138. Jen, S. F.; Anderson, Alfred B. **Carbon monoxide oxidation mechanisms over zinc oxide: molecular orbital theory.** Surf. Sci. (1989), 223(1-2), 119-30.
 139. Anderson, Alfred B.; Jen, S. F. **Activation of carbon monoxide on nickel-aluminum alloy surfaces and by interstitial trapping in a nickel matrix. Structure and electronic factors from molecular orbital theory.** J. Phys. Chem. (1990), 94(4), 1607-11.
 140. Awad, Mohamed K.; Anderson, Alfred B. **Photodimerization of cyclohexene and methane by decatungstate anions: molecular orbital theory.** J. Am. Chem. Soc. (1990), 112(4), 1603-6.

141. Anderson, Alfred B. **Quantum theory of chemisorption.** J. Mol. Catal. (1989), 54(3), 281-7.
142. Hong, Sung Y.; Anderson, Alfred B. **Diffusion and surface segregation of carbon in α -iron: molecular-orbital theory.** Phys. Rev. B: Condens. Matter (1989), 40(11), 7508-12.
143. Awad, Mohamed K.; Anderson, Alfred B. **Methane activation by hole sites on aluminum mononitride: a molecular orbital study.** Surf. Sci. (1989), 218(2-3), 543-52.
144. Mehandru, S. P.; Anderson, Alfred B. **Formate adsorption and azimuthal orientation on copper (100) from molecular orbital theory.** Surf. Sci. (1989), 219(1-2), 68-76.
145. Anderson, Alfred B.; Yu, Jenwei. **Methane conversion and Fischer-Tropsch catalysis over molybdenum disulfide: predictions and interpretations from molecular orbital theory.** J. Catal. (1989), 119(1), 135-45.
146. Mehandru, S. P.; Anderson, Alfred B. **Binding and orientations of oxygen on silver(100) and lead/silver(100). Relationships to oxygen reduction by UPD lead on a silver electrode.** Surf. Sci. (1989), 216(1-2), 105-24.
147. Anderson, Alfred B.; Shiller, Paul; Zarate, Eugene A.; Tessier-Youngs, Claire A.; Youngs, Wiley J. **Bonding in transition-metal-silyl dimers. Molecular orbital theory.** Organometallics (1989), 8(10), 2320-2.
148. Anderson, Alfred B.; Choe, S. J. **Ethylene hydrogenation mechanism on the platinum(111) surface: theoretical determination.** J. Phys. Chem. (1989), 93(16), 6145-6149.
149. Mehandru, S. P.; Anderson, Alfred B. **Oxygen evolution on a strontium iron oxide (SrFeO₃) anode. Mechanistic considerations from molecular orbital theory.** J. Electrochem. Soc. (1989), 136(1), 158-66.
150. Nath, K.; Anderson, Alfred B. **Oxidative bonding of (0001) α -alumina to close-packed surfaces of the first transition-metal series, scandium through copper.** Phys. Rev. B: Condens. Matter (1989), 39(2), 1013-19.
151. Mehandru, S. P.; Anderson, A. B. **Potential-induced variations in properties for carbon monoxide adsorbed on a platinum electrode.** J. Phys. Chem.

- (1989), 93(5), 2044-7.
152. Anderson, Alfred B.; Maloney, John J.; Yu, Jenwei. **Methane activation over molybdenum disulfide and CH_n stabilities: molecular orbital theory.** J. Catal. (1988), 112(2), 392-400.
 153. Nath, K.; Anderson, Alfred B. **Bonding at the calcium fluoride/silicon(111) interface from tight-binding cluster and band theory.** Phys. Rev. B: Condens. Matter (1988), 38(12), 8264-8.
 154. Hong, Sung Y.; Anderson, Alfred B. **Segregation of substitutional bulk sulfur to the iron(100) surface and the iron-iron oxide interface: molecular-orbital theory.** Phys. Rev. B: Condens. Matter (1988), 38(14), 9417-24.
 155. Awad, Mohamed K.; Anderson, Alfred B. **Photoactivation of water by p-benzoquinone and the role of manganese(III) complexes in oxygen evolution: molecular orbital theory.** J. Am. Chem. Soc. (1989), 111(3), 802-6.
 156. Grimes, Robin W.; Anderson, Alfred B.; Heuer, Arthur H. **Predictions of cation distributions in AB₂O₄ spinels from normalized ion energies.** J. Am. Chem. Soc. (1989), 111(1), 1-7.
 157. Fierro, C.; Anderson, A. B.; Scherson, D. A. **Electron donor-acceptor properties of porphyrins, phthalocyanines, and related ring chelates: a molecular orbital approach.** J. Phys. Chem. (1988), 92(24), 6902-7.
 158. Anderson, Alfred B.; Hong, S. Y. **Sulfur and iron binding to the iron(100) surface and in the bulk: molecular orbital theory for surface segregation of sulfur.** Surf. Sci. (1988), 204(1-2), L708-L712.
 159. Anderson, Alfred B.; Ravimohan, C. **Bonding of α -silicon carbide basal planes to close-packed titanium, copper, and platinum surfaces: molecular-orbital theory.** Phys. Rev. B: Condens. Matter (1988), 38(2), 974-7.
 160. Nath, K.; Anderson, Alfred B. **An ASED band theory: lattice constants, atomization energies, and bulk moduli for graphite, diamond, silicon and α - and β -silicon carbide.** Solid State Commun. (1988), 66(3), 277-80.
 161. Mehandru, S. P.; Anderson, Alfred B. **Binding and orientations of carbon monoxide on iron(110), (100), and (111): a surface structure effect from molecular orbital theory.** Surf. Sci. (1988), 201(1-2), 345-60.

162. Chu, San Yan; Anderson, Alfred B. **Acetylene adsorption on silicon(111): molecular orbital theory.** Surf. Sci. (1988), 194(1-2), 55-62.
163. Mehendru, S. P.; Anderson, Alfred B. **H_xMoO₃ bronzes: structures, stabilities, and electronic properties.** J. Am. Chem. Soc. (1988), 110(7), 2061-5.
164. Mehendru, S. P.; Anderson, Alfred B.; Brazdil, James F. **Methyl radical formation over lithium-doped magnesium oxide. Molecular orbital theory.** J. Am. Chem. Soc. (1988), 110(6), 1715-19.
165. Anderson, Alfred B.; Maloney, John J. **Activation of methane on iron, nickel, and platinum surfaces: a molecular orbital study.** J. Phys. Chem. (1988), 92(3), 809-12.
166. Anderson, Alfred B.; Al-Saigh, Zeki Y.; Hall, W. Keith. **Hydrogen on molybdenum disulfide: theory of its heterolytic and homolytic chemisorption.** J. Phys. Chem. (1988), 92(3), 803-809.
167. Anderson, Alfred B.; Maloney, John J. **Activation of methane on iron, nickel, and platinum surfaces. A molecular orbital study.** Prepr. Pap. - Am. Chem. Soc., Div. Fuel Chem. (1987), 32(3), 291-8.
168. Ward, Michael D.; Brazdil, James F.; Mehendru, S. P.; Anderson, Alfred B. **Methane photoactivation on copper molybdate: an experimental and theoretical study.** J. Phys. Chem. (1987), 91(26), 6515-21.
169. Anderson, Alfred B.; Baldwin, Shawn. **Ground and excited-state iron atom interactions with methane and ethylene. Molecular orbital theory for coordination and carbon-hydrogen activation.** Organometallics (1987), 6(8), 1621-1625.
170. Anderson, Alfred B.; Hong, Sung Y.; Smialek, J. L. **Comparison of bonding in first transition-metal series: diatomic and bulk sulfides and oxides.** J. Phys. Chem. (1987), 91(16), 4250-4.
171. Anderson, Alfred B.; Grimes, Robin W.; Hong, Sung Y. **Toward a better understanding of the atom superposition and electron delocalization molecular orbital theory and a systematic test: diatomic oxides of the first transition-metal series, bonding and trends.** J. Phys. Chem. (1987), 91(16), 4245-50.

172. Anderson, Alfred B.; Ravimohan, C.; Mehandru, S. P. **Bonding at the α -alumina(001)/platinum(111) interface: molecular orbital theory.** Surf. Sci. (1987), 183(3), 438-48.
173. Anderson, Alfred B.; Awad, Mohamed K. **Binding of ruthenium, oxygen, and ruthenium oxide RuO_n (n = 1-4) to the ruthenium(001) surface: structures, stabilities, and diffusion barriers.** Surf. Sci. (1987), 183(1-2), 289-301.
174. Mehandru, S. P.; Anderson, Alfred B.; Brazdil, James F.; Grasselli, Robert K. **Role of oxide surface radicals for methane carbon-hydrogen bond activation and subsequent reactions on molybdena: molecular orbital theory.** J. Phys. Chem. (1987), 91(11), 2930-4.
175. Grimes, Robin W.; Anderson, Alfred B.; Heuer, Arthur H. **Interaction of dopant cations with 4:1 defect clusters in nonstoichiometric 3d transition metal monoxides: a theoretical study.** J. Phys. Chem. Solids (1987), 48(1), 45-50.
176. Anderson, Alfred B.; Dowd, Donald Q. **Carbon monoxide adsorption on platinum(111) doped with titanium oxide (TiO), iron oxide (FeO), zinc oxide, and iron and platinum ad-atoms. Molecular orbital study of carbon monoxide-dopant interactions.** J. Phys. Chem. (1987), 91(4), 869-873.
177. Mehandru, Satya P.; Anderson, Alfred B.; Brazdil, James F. **Carbon-hydrogen bond activation and radical-surface reactions for propylene and methane over bismuth oxide (α -Bi₂O₃).** J. Chem. Soc., Faraday Trans. 1 (1987), 83(2), 463-75.
178. Nath, K.; Kreuzer, H. J.; Anderson, Alfred B. **Field adsorption of rare gases.** Surf. Sci. (1986), 176(1-2), 261-83.
179. Grimes, Robin W.; Anderson, Alfred B.; Heuer, Arthur H. **Defect clusters in nonstoichiometric 3d transition-metal monoxides.** J. Am. Ceram. Soc. (1986), 69(8), 619-23.
180. Mehandru, S. P.; Anderson, Alfred B.; Ross, P. N. **Carbon monoxide adsorption on (111) and (100) surfaces of the platinum-titanium (Pt₃Ti) alloy: evidence for parallel binding and strong activation of carbon monoxide.** J. Catal. (1986), 100(1), 210-18.

181. Anderson, Alfred B.; Nichols, Jeffrey A. **Hydrogen on zinc oxide. Theory of its heterolytic adsorption.** J. Am. Chem. Soc. (1986), 108(16), 4742-4746.
182. Anderson, Alfred B.; Grimes, Robin W.; Heuer, Arthur H. **A predictive molecular orbital theory applied to defects and structures of transition metal oxides.** NATO ASI Ser., Ser. B (1985), 129(Transp. Nonstoichiom. Compd.), 527-37.
183. Mehandru, S. P.; Anderson, Alfred B. **Why carbon monoxide bonds side-on at low coverage and both side-on and upright at high coverage on the chromium(110) surface.** Surf. Sci. (1986), 169(2-3), L281-L288.
184. Mehandru, S. P.; Anderson, Alfred B. **Adsorption of oxygen, sulfur dioxide and sulfur trioxide, on nickel oxide.** J. Electrochem. Soc. (1986), 133(4), 828-32.
185. Anderson, Alfred B.; Ewing, David W.; Kim, Yunsoo; Grasselli, Robert K.; Burrington, James D.; Brazdil, James F. **Mechanism for propylene oxidation to acrolein on bismuth molybdate (Bi₂Mo₃O₁₂): a quantum chemical study.** J. Catal. (1985), 96(1), 222-233.
186. Anderson, Alfred B.; Nichols, Jeffrey A. **Relaxation in zinc oxide (1010), (0001), and (1000) surfaces and the adsorption of carbon monoxide.** J. Am. Chem. Soc. (1986), 108(7), 1385-8.
187. Kang, Dae Bok; Anderson, Alfred B. **Adsorption and decomposition of acetylene on vanadium (100), (110), and (111) surfaces; the effect of large d orbitals.** Surf. Sci. (1986), 165(1), 221-33.
188. Anderson, Alfred B. **Molecular orbital studies in oxidation: sulfate formation and metal-metal oxide adhesion.** NASA Contract. Rep. (1985), (NASA-CR-176070, NAS1.26:176070), 5 pp.
189. Kang, Dae Bok; Anderson, Alfred B. **Theoretical interpretation of the cyclohexane → benzene reaction on the platinum(III) surface.** J. Am. Chem. Soc. (1985), 107(26), 7858-61. CODEN: JACSAT ISSN:0002-7863. CAN 104:19266 AN 1986:19266 CAPLUS (Copyright 2001 ACS)
190. Anderson, Alfred B.; Awad, M. K. **Factors determining carbon monoxide adsorption sites on palladium and platinum (100) and (111) surfaces: theoretical study.** J. Am. Chem. Soc. (1985), 107(26), 7854-7857.

191. Mehandru, S. P.; Anderson, Alfred B. **Adsorption of oxygen, sulfur dioxide, sulfur trioxide on nickel oxide. Mechanism for sulfate formation.** NASA Contract. Rep. (1985), (NASA-CR-176072, NAS1.26:176072), 28 pp.
192. Mehandru, S. P.; Anderson, Alfred B. **Why carbon monoxide bonds side-on at low coverage and both side-on and upright at high coverage on the chromium(110) surface.** NASA Contract. Rep. (1985), (NASA-CR-176071, NAS1.26:176071), 16 pp.
193. Kang, Dae Bok; Anderson, Alfred B. **Adsorption and structural rearrangements of acetylene and ethylene on platinum(111); theoretical study.** Surf. Sci. (1985), 155(2-3), 639-52.
194. Mehandru, S. P.; Anderson, Alfred B. **Mechanism for chelated sulfate formation from sulfur dioxide and bis(triphenylphosphine)platinum.** Inorg. Chem. (1985), 24(16), 2570-3.
195. Anderson, Alfred B.; Mehandru, S. P.; Smialek, J. L. **Dopant effect of yttrium and the growth and adherence of alumina on nickel-aluminum alloys.** J. Electrochem. Soc. (1985), 132(7), 1695-701.
196. Anderson, Alfred B.; Onwood, David P. **Why carbon monoxide is stable lying down on a negatively charged ruthenium(001) surface but not on platinum(111).** Surf. Sci. (1985), 154(2-3), L261-L267.
197. Anderson, A. B.; Gordon, T. L.; Kenny, M. E. **Electronic and redox properties of stacked-ring silicon phthalocyanines from molecular orbital theory.** Report (1984), (CWRU/DC/TR15; Order No. AD-A147161/4/GAR), 28 pp.
198. Mehandru, S. P.; Anderson, Alfred B. **Dependence of carbon-carbon and carbon-hydrogen bond activation on d band position: acetylene on platinum(111) and iron(100). An electrochemical model.** J. Am. Chem. Soc. (1985), 107(4), 844-9.
199. Anderson, Alfred B.; Gordon, Teresa L.; Kenney, Malcolm E. **Electronic and redox properties of stacked-ring silicon phthalocyanines from molecular orbital theory.** J. Am. Chem. Soc. (1985), 107(1), 192-5.
200. Mehandru, S. P.; Anderson, Alfred B. **Acetylene adsorption on platinum(111) and unreconstructed (110) and (100) surfaces.** Appl. Surf. Sci. (1984), 19(1-

- 4), 116-34.
201. Anderson, Alfred B.; Ray, N. K. **Photon-assisted carbon-hydrogen bond activation in a coordinated methoxy. A molecular orbital explanation.** J. Am. Chem. Soc. (1985), 107(1), 253-4.
202. Fang, Howard L.; Swofford, Robert L.; McDevitt, Michael; Anderson, Alfred B. **Carbon-hydrogen stretching overtone spectrum of propylene. Molecular-orbital analysis in the local-mode model.** J. Phys. Chem. (1985), 89(2), 225-9.
203. Anderson, Alfred B.; Grimes, Robin W.; Heuer, Arthur H. **Defect clusters in wustite, Fe_{1-x}O.** J. Solid State Chem. (1984), 55(3), 353-61.
204. Anderson, Alfred B.; McDevitt, Michael R.; Urbach, F. L. **Structure and electronic factors in benzene coordination to chromium tricarbonyl (Cr(CO)₃) and to cluster models of nickel, platinum, and silver (111) surfaces.** Surf. Sci. (1984), 146(1), 80-92.
205. Anderson, Alfred B.; Kang, D. B.; Kim, Y. **Propylene adsorption and α -hydrogen abstraction on platinum(III). Mechanism for 1,3-sigmatropic shifts.** J. Am. Chem. Soc. (1984), 106(22), 6597-600.
206. Anderson, Alfred B. **Mechanism for forming hydrogen chloride and sodium sulfate from sulfur trioxide, water, and sodium chloride.** J. Am. Chem. Soc. (1984), 106(21), 6262-5.
207. Anderson, Alfred B.; Kang, Dae Bok. **Structure of the iron pentacarbonyl anion.** Inorg. Chem. (1984), 23(8), 1170-2
208. Anderson, Alfred B.; Mehandru, S. P. **Acetylene adsorption to iron(100), (110), and (111) surfaces; structures and reactions.** Surf. Sci. (1984), 136(2-3), 398-418.
209. Trzcinska, Barbara M.; Fackler, John P., Jr.; Anderson, Alfred B. **Olefin oligomerization on nickel. A theoretical study of the barrier to olefin rotation and insertion.** Organometallics (1984), 3(2), 319-23.
210. Anderson, Alfred B.; Kim, Yunsoo; Ewing, David W.; Grasselli, Robert K.; Tenhover, M. **Electronic properties of bismuth oxide (Bi₂O₃) and molybdenum trioxide and relationships to oxidation catalysis.** Surf. Sci. (1983), 134(1), 237-56.

211. Anderson, Alfred B.; Hung, S. C. **Mechanism for forming sodium pyrosulfate from sodium chloride, sulfur dioxide, and oxygen.** J. Am. Chem. Soc. (1983), 105(26), 7541-7543.
212. Nickles, David E.; Anderson, Alfred B.; Urbach, F. L. **A molecular orbital study of thio ether coordination to copper ions.** Copper Coord. Chem.: Biochem. Inorg. Perspect. (eds. Karlin, K. D. and Zubieta, J.), pp. 203-222. Adenine Press, New York, 1983.
213. Debnath, N. C.; Anderson, Alfred B. **Water adsorption on an iron oxide surface.** Surf. Sci. (1983), 128(1), 61-9.
214. Ray, Naba K.; Anderson, Alfred B. **Molecular orbital study of carbon monoxide chemisorption on a platinum(111) surface in the presence of potassium.** Surf. Sci. (1983), 125(3), 803-12.
215. Anderson, Alfred B.; Debnath, N. C. **Reactions of sodium chloride(s) with sulfur dioxide(g) and molecular oxygen(g) to form sodium sulfate(s). A charge-transfer reaction.** J. Phys. Chem. (1983), 87(11), 1938-41.
216. Anderson, Alfred B. **Structures of sulfur tetroxide (SO₄) and sodium sulfate.** Chem. Phys. Lett. (1982), 93(6), 538-539.
217. Anderson, Alfred B.; Debnath, N. C. **Mechanism of dissolution and passivation of iron in an aqueous medium: active and transition ranges.** J. Am. Chem. Soc. (1983), 105(1), 18-22.
218. Debnath, N. C.; Anderson, Alfred B. **Chlorine and hydrogen chloride on clean and oxygen-covered iron(100): Bonding and reactions.** J. Vac. Sci. Technol. (1982), 21(4), 945-51.
219. Ray, Naba K.; Anderson, Alfred B.. **Variations in carbon-oxygen and platinum-carbon frequencies for carbon monoxide on a platinum electrode.** J. Phys. Chem. (1982), 86(25), 4851-2.
220. Debnath, N. C.; Anderson, A. B. **Optical spectra of ferrous and ferric oxides and the passive film: a molecular orbital study.** J. Electrochem. Soc. (1982), 129(10), 2169-74.
221. Ray, Naba K.; Anderson, Alfred B. **Molecular orbital study of carbon**

- monoxide chemisorption and oxidation on a platinum(111) surface.** Surf. Sci. (1982), 119(1), 35-45.
222. Anderson, Alfred B.; Ray, N. K. **Structures and reactions of hydronium, water, and hydroxyl on an iron electrode. Potential dependence.** J. Phys. Chem. (1982), 86(4), 488-94.
223. Anderson, Alfred B.; Koetz, Ruediger; Yeager, Ernest. **Theory for carbon-nitrogen(1-) ion and silver-carbon vibrational frequency dependence on potential: cyanide on a silver electrode.** Chem. Phys. Lett. (1981), 82(1), 130-4.
224. Anderson, Alfred B.; Fitzgerald, George. **Structure and bonding in (cyclobutadiene)iron tricarbonyl.** Inorg. Chem. (1981), 20(10), 3288-91.
225. Donn, B.; Hecht, J.; Khanna, R.; Nuth, J.; Stranz, D.; Anderson, A. B. **The formation of cosmic grains: an experimental and theoretical study.** Surf. Sci. (1981), 106(1-3), 576-581.
226. Anderson, Alfred B. **Reactions and structures of water on clean and oxygen covered platinum (111) and iron (100).** Surf. Sci. (1981), 105(1), 159-176.
227. Anderson, Alfred B. **Atom superposition and electron delocalization (ASED) theory for catalysis. Dissociative properties of acetylene on iron and nickel(100) with coadsorbed oxygen, sulfur, selenium and implications for tellurium.** J. Catal. (1981), 67(1), 129-44.
228. Anderson, Alfred B.; Hubbard, Arthur T. **Theoretical determination of the structure of acetylene on platinum (111).** Surf. Sci. (1980), 99(2), 384-91.
229. Anderson, Alfred B. **Structure and electronic properties of α -quartz from silicon tetroxide and silicon oxide (Si₅O₄) models.** Chem. Phys. Lett. (1980), 76(1), 155-8.
230. Anderson, Alfred B.; Ohwada, Ken. **Comments on Ohwada's pairwise interaction model for polyatomic force fields.** J. Chem. Phys. (1980), 73(4), 2016.
231. Anderson, Alfred B. **Nickel(II) oxide bulk properties: initial-state molecular orbital nickel oxide (Ni₄O₄) and nickel oxide (Ni₁₃O₁₄) cluster studies.** Chem. Phys. Lett. (1980), 72(3), 514-17.

232. Anderson, Alfred B. **Lattice constants and force constants for iron, nickel, and copper from orbital energies added to pairwise atomic repulsions in cluster models.** Chem. Phys. Lett. (1979), 61(2), 388-90.
233. Anderson, Alfred B. **Nickel (100) with chalcogen overlayers: theory for structures, force constants, binding energies, photoemission spectra; importance of final-state multiplet splittings.** J. Vac. Sci. Technol. (1978), 15(2), 616-18.
234. Anderson, A. B. **Structures and electronic properties of copper clusters and bulk.** Conf. Ser. - Inst. Phys. (1978), 39(Transition Met., 1977), 379-83.
235. Muetterties, E. L.; Pretzer, W. R.; Thomas, M. G.; Beier, B. F.; Thorn, D. L.; Day, V. W.; Anderson, A. B. **Metal clusters in catalysis. 14. The chemistry of dinuclear metal-acetylene complexes.** J. Am. Chem. Soc. (1978), 100(7), 2090-7.
236. Anderson, Alfred B. **Structures and electronic properties of copper clusters and bulk; comments on Mulliken-Walsh diagrams and on criticisms of the extended Hueckel procedure.** J. Chem. Phys. (1978), 68(4), 744-51.
237. Rhodin, Thor N.; Brucker, Charles F.; Anderson, Alfred B. **Structure and bonding of acetylene and ethylene on α -iron surfaces at low temperatures.** J. Phys. Chem. (1978), 82(8), 894-8.
238. Anderson, Alfred B., **Molecular orbital theory for catalysis. Structures, energy levels, and reactions of acetylene with Ni₂(COD)₂(RC.tplbond.CR), Ni₂(C₅H₅)₂(RC.tplbond.CR), and the nickel(111) surface.** J. Am. Chem. Soc. (1978), 100(4), 1153-9.
239. Anderson, Alfred B. **Molecular orbital theory of bonding of nitrogen atoms to copper(100).** Chem. Phys. Lett. (1977), 49(3), 550-4.
240. Anderson, Alfred B. **Molecular-orbital theory of bonding in iron monoxide and chemisorbed oxygen on iron(100).** Phys. Rev. B (1977), 16(2), 900-5.
241. Anderson, Alfred B. **Comment on the local mode approximation for molecular vibrations.** J. Chem. Phys. (1977), 66(10), 4709-10.
242. Anderson, Alfred B. **Theory of ultraviolet spectra for diatomic nickel and triatomic nickel and hypothesis for argon matrix frequency shifts for nickel**

- atoms.** J. Chem. Phys. (1977), 66(11), 5108-11.
243. Anderson, Alfred B. **Theory for chemisorption and catalysis.** NBS Spec. Publ. (U. S.) (1977), 475, 166-70.
244. Anderson, Alfred B., **Determination of chalcogen structures on nickel surfaces from orbital energies added to pairwise atomic repulsions.** J. Chem. Phys. (1977), 66(5), 2173-5.
245. Anderson, Alfred B.; Hastings, Jerome B. **Calculation of harmonic and cubic Einstein force constants in diamond-like crystals.** Phys. Rev. B (1977), 15(4), 2422-5.
246. Anderson, Alfred B. **Molecular orbital study of the interaction of carbon monoxide and carbon dioxide with copper (100).** Surf. Sci. (1977), 62(1), 119-32.
247. Anderson, Alfred B. **Interaction of hydrogen, carbon, ethylene, acetylene, and alkyl fragments with iron surfaces. Catalytic hydrogenation, dehydrogenation, carbon bond breakage, and hydrogen mobility.** J. Am. Chem. Soc. (1977), 99(3), 696-707.
248. Anderson, Alfred B. **Theoretical study of structures and binding properties of nickel tetracarbonyl, iron pentacarbonyl, and diiron and dicobalt hexacarbonyl acetylenes.** Inorg. Chem. (1976), 15(11), 2598-602.
249. Anderson, Alfred B. **Structural and orbital analysis of ethylene and acetylene on nickel(111) surfaces.** J. Chem. Phys. (1976), 65(5), 1729-34.
250. Anderson, A. B.; Rhodin, T.N.; Brucker, C. F. **Decomposition of Acetylene and Ethylene on Clean Iron at Low Temperature.** Physical Electronics Conference, Bull. Am. Phys. Soc. (1976), 21, (7) 940.
251. Anderson, Alfred B. **Structures, binding energies, and charge distributions for two to six atom titanium, chromium, iron, and nickel clusters and their relation to nucleation and cluster catalysis.** J. Chem. Phys. (1976), 64(10), 4046-55.
252. Anderson, Alfred B. **Molecular orbitals and bonding in diatomic argon, diatomic krypton, argon krypton (ArKr), dimeric diatomic chlorine, triatomic argon hydrogen chlorine (ArHCl), and solid chlorine.** J. Chem. Phys. (1976),

- 64(5), 2266-7.
253. Anderson, Alfred B. **Vibrational potentials and structures in molecular and solid carbon, silicon, germanium, and tin.** J. Chem. Phys. (1975), 63(10), 4430-6.
254. Anderson, Alfred B. **Transition metal catalysis of olefin isomerizations.** Chem. Phys. Lett. (1975), 35(4), 498-9.
255. Anderson, Alfred B. **Derivation of the extended Hueckel method with corrections. One electron molecular orbital theory for energy level and structure determinations.** J. Chem. Phys. (1975), 62(3), 1187-8.
256. Anderson, Alfred B.; Hoffmann, Roald. **Molecular orbital studies of dissociative chemisorption of first period diatomic molecules and ethylene on (100) tungsten and nickel surfaces.** J. Chem. Phys. (1974), 61(11), 4545-59.
257. Anderson, Alfred B.; Hoffmann, Roald. **Description of diatomic molecules using one-electron configuration energies with two-body interactions.** J. Chem. Phys. (1974), 60(11), 4271-3.
258. Anderson, Alfred B. **Derivation of and comments on Bonaccorsi-Scrocco-Tomasi potentials for electrophilic additions.** J. Chem. Phys. (1974), 60(6), 2477-9. CODEN: JCPSA6 CAN 81:16843 AN 1974:416843 CAPLUS (Copyright 2001 ACS)
259. Anderson, Alfred B. **Valence-force-field potentials for diamondlike crystals.** Phys. Rev. B (1973), 8(8), 3824-7
260. Anderson, Alfred B. **Analytical energy surfaces for the collinear atomic hydrogen + molecular hydrogen and lithium + molecular hydrogen exchange reactions.** Chem. Phys. Lett. (1973), 18(2), 303-5.
261. Anderson, Alfred B. **Evaluating force constants from LCAO-MO-SCF electronic charge densities for diatomic molecules.** J. Chem. Phys. (1973), 58(1), 381-3.
262. Anderson, Alfred B. **On Effective molecular electronic charge densities and vibrational potential energy functions.** J. Mol. Spectrosc. (1972), 44(3), 411-24.

263. Anderson, Alfred B. **Theoretical approach to potential energy functions for linear AB₂ and ABC and bent AB₂ triatomic molecules.** J. Chem. Phys. (1972), 57(10), 4143-52.
264. Anderson, Alfred B.; Parr, Robert G. **Poisson equation for vibrational potentials of diatomic molecules.** Theor. Chim. Acta (1972), 26(4), 301-10. CODEN: TCHAAM CAN 77:143995 AN 1972:543995 CAPLUS (Copyright 2001 ACS)
265. Anderson, Alfred B. **Simple potential energy function for carbon dioxide.** J. Chem. Phys. (1972), 56(8), 4228-9.
266. Anderson, Alfred Bennett. **Electrostatic theory for molecular vibrational potential functions near equilibrium and comments on the single-center method for calculation of molecular wavefunctions.** PhD Thesis, The Johns Hopkins University (1970), 127 pp.
267. Anderson, Alfred B.; Parr, Robert G. **Diatomic vibrational potential functions from integration of a Poisson equation.** J. Chem. Phys. (1971), 55(12), 5490-3.
268. Anderson, A. B.; Parr, R. G. **Universal force constant relations and a definition of atomic radius.** Chem. Phys. Lett. (1971), 10(3), 293-6.
269. Anderson, Alfred B. **Single-center method.** J. Chem. Phys. (1971), 54(2), 806-9.
270. Anderson, Alfred B.; Parr, Robert G. **Single-center variational calculations with basis functions depending on the lesser and greater [electronic coordinates] r_1 and r_2 .** J. Chem. Phys. (1970), 53(10), 4098-100.
271. Anderson, Alfred B.; Parr, Robert G. **Vibrational force constants from electron densities.** J. Chem. Phys. (1970), 53(8), 3375-6.
272. Anderson, Alfred B.; Handy, Nicholas C.; Parr, Robert G. **Relationships between vibrational force constants and quadrupole coupling constants for molecules and solids.** J. Chem. Phys. (1969), 50(8), 3634-5.
273. Rulfs, Charles L.; Pacer, Richard A.; Anderson, Alfred. **The polarography of aqueous pertechnetate ion.** J. Electroanal. Chem. Interfacial Electrochem. (1967), 15(1), 61-6.

