# VITA

## ALFRED B. ANDERSON

EDUCATION AND EXPERIENCE

1985 Joint appointment as Professor of Metallurgy and Ceramics, Case Western Reserve University.

1979 Assistant, 198l Associate, and 1986 Full Professor, Chemistry Department, Case Western Reserve University, Cleveland, Ohio 44106. Telephone Nos. 216-368-5044, 216-368-2608. Chemistry Department No. 216-368-3622.

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| 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 under R. G. Parr. During his postdoctoral year with H. Shull he extended his applications and understanding of this electron density-based theory. This effort continued into his postdoctoral stays with Harrison Shull and Roald Hoffmann, culminating in his atom superposition and electron delocalization

theory for bonding (based on the Hellmann-Feynman electrostatic theory for molecular forces). He discovered that a one-electron molecular orbital energy as given by extended Huckel-type hamiltonians approximated well the attractive energy due to charge redistribution accompanying bond formation. The repulsive component, due to the first step of superimposing rigid atoms, contains the information used in his theory for force constants. Professor Anderson and his coworkers at Case have used 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. The properties of doped diamond were also studied using the ASED-MO theory.

Beginning in 1998 the Anderson lab began using *ab initio* methods and has developed two quantum theoretic methods and models for predicting reversible electrode potentials for forming intermediates in electrocatalytic reactions. It has also developed a quantum approach using simple reaction center models for calculating electrode potential dependencies of electron transfer activation energies. These new theories have significantly extended our fundamental understanding of the thermodynamics and kinetics of electrochemical reactions and in helping with the discovery of new electrocatalysts for applications in fuel cell and other technologies.

A visitor from Toyota Central Research and Development Corporation, Dr. Ryosuke Jinnouchi arrived in the lab in April 2006 to develop a theory and computer program for the comprehensive treatment of electrocatalysis. It is a two-dimensional density functional band theory, employing atomic orbitals, in which the electrode potential is exactly identified with the Fermi level, which is adjustable. This is a significant advancement over three-dimensional band theory models for electrocatalysis studies. It includes treatment of solvation of the reaction center using a dielectric continuum model. The Poisson-Boltzmann distribution for the electrolyte and counter charge is used and the whole hamiltonian is solved self-consistently. The computations proceed rapidly, and, for translational cells used so far, they are significantly faster than plane wave density functional calculations. Initial applications are yielding excellent predictions. The plan is to carry out wide-ranging studies in electrocatalysis with this theory, beginning with a reevaluation of the past studies that used the molecular local reaction center model and the linear Gibbs energy relationship. Extensions will be made to new catalyst analysis and predictions. Major advancements are expected from this critical and timely research.

The properties of doped diamond were also studied by Professor Anderson using the ASED-MO theory. In 1998 he began using *ab initio* methods to study dopants in diamond and their interactions and relationships to charge transport in electrochemistry over diamond surface.

## INVITED LECTURES

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

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

Predicting Reversible Potentials of Reactions on Electrode Surfaces from Internal and Gibbs Energies, A. B. Anderson, 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.

K. Kurak and A. B. Anderson, Will Nitrided Graphite Work as an Electrocatalyst in a Fuel Cell Oxygen Cathode? 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 $O_2$ 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 Electocatalysis, Ernest B. Yeager Frontiers in Electrochemical Sciences and Electrochemical Technology, Case Western Reserve University, October 12-14, 2005.

2004: $Pt_3Cr$ Alloy Effect on the Overpotential of $O_2$ Reduction on Acid Fuel Cell Cathodes: Theoretical Approach, J. Roques (A. B. Anderson, co author) at the 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 (Y. Cai co-author) at the 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, co-author) 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, co-author) A. B. Anderson (J. C. Angus and L. Kostadinov, co-authors), 2004 Joint International Meeting of the Electrochemical Society, Honolulu, October 3-8, 2004.

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

2003: Theoretical Calculation of Activation Energies for $Pt + H^+(aq) + e^-(U) \leftrightarrow Pt\text{-}H$: Activation Energy-Based Symmetry Factors in the Marcus Normal and Inverted Regions, lecture given by A. B. Anderson at the Electrochemistry and Surface Science Symposium in Memory of Mike Weaver held at the 225$^{th}$ 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, lecture by A. B. Anderson given in the Computational Chemistry Symposium held at the 203$^{rd}$ Meeting of the Electrochemical Society, Paris, France April 27- May 2, 2003.

Roles of Interstitial Hydrogen and Substitutional Boron Durong $H_2$ Evolution on Diamond Electrodes. Model DFT Calculations, Lecture by A. B. Anderson in the Eighth International Symposium on Diamond Materials held at the 203$^{rd}$ Meeting of the Electrochemical Society, Paris, France, April 27-May 2, 2003.

$Pt_3Cr$ Alloy Effect on the Reversible Potential of OH(ads) Formation from $H_2O$(ads): Comparison with Pure Pt(111) Surface, poster by J. Roques (A. B.

Anderson, co-author) at the Pittsburgh-Cleveland Catalysis Society Spring 2003 Meeting, Carnegie Mellon University, June 24, 2003.

$Pt_3Cr$ and $Pt_3Co$ Alloy Effect on the Reversible Potential of OH(ads) Formation from $H_2O$(ads): Comparison with Pure Pt(111) Surface, poster by J. Roques (A. B. Anderson, co-author) at the 10th International Congress on the Application of Density Functional Theory, Brussels, Belgium, September 7-12, 2003.

Electrode Potential-Dependent Stages in OH(ads) Formation the $Pt_3Cr$ Alloy (111) Surface, lecture by A. B. Anderson at the 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, lecture given by A. B. Anderson at the Electrochemistry Symposium in Honor of Mike Weaver held at the 204$^{th}$ Meeting of the Electrochemical Society, Orlando, October 12-16, 2003.

$Pt_3Cr$ Alloy Effect on the Reversible Potential of OH(ads) Formation from $H_2O$(ads): Comparison with Pure Pt(111) Surface, poster by J. Roques (A. B. Anderson, co-author) at the Fundamental Understanding of Electrode Processes Symposium in Memory of Professor Ernest B. Yeager held at the 204$^{th}$ Meeting of the Electrochemical Society, Orlando, October 12-16, 2003.

2002: $O_2$ Reduction and CO Oxidation at the Pt-electrolyte Interface. The Role of $H_2O$ and OH adsorption Bond Strengths, lecture by A. B. Anderson at the 223$^{rd}$ 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 (A. B. Anderson, co-author) at the 223$^{rd}$ 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, P. Shiller, co-authors) at the 223$^{rd}$ National Meeting of the American Chemical Society, Orlando, Florida, April 7-11, 2002.

Density Functional Study of $O_2$ Electroreduction when Bonded to a Pt Dual Site, lecture by R. A. Sidik (A. B. Anderson, co-author) at the 223$^{rd}$ National Meeting of the American Chemical Society, Orlando, Florida, April 7-11, 2002.

Your Fundamental Dream Catalyst for Oxygen Reduction, lecture by A. B. Anderson at the Biofuel Cells Workshop, Washington, DC June 30-July 2, 2002.

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

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

Understanding of the $O_2$ Reduction Overpotential at the Pt Cathode and Probing of Alternative Catalysts via Computational Chemistry, lecture by R. A. Sidik (A. B. Anderson, co-author) at the AIChE National Meeting, Indianapolis, Indiana, November 3-8, 2002.

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

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

2001: Electron Transfer Reactions and Electrocatalysis, Plenary Lecture by A. B. Anderson at the 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, lecture by A. B. Anderson (T. V. Albu and J. C. Angus, co-authors) at the 2001 Joint International Meeting of the Electrochemical Society and the International Society of Electrochemistry, San Francisco, California, September 2-7, 2001.

DFT Study of $O_2$ Reduction on Platinum, lecture by R. A. Sidik (A. B. Anderson, co-author) at the 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, lecture by A. B. Anderson (N. M. Neshev, R. A. Sidik, and P. Shiller, co authors) at the 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 by A. B. Anderson at the 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, Lecture by A. B. Anderson at the 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, Seatle, WA, May 2-6, 1999.

1997: NSF-DOE Workshop on "Future Directions for Theoretical Catalysis: Homogeneous, Heterogeneous, and Surface Reactivity", San Franciso, 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 $H_2O$(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, MolecularOrbital 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 $MoS_2$: Theoretical Predictions."

196th ACS National Meeting, Los Angeles, Sept. 25-30, "Methane Activation and Subsequent Reactions on $MoS_2$. Predictions from Molecular Orbital Theory."

196th ACS National Meeting, Los Angeles, Sept. 25-30, "Oxygen Evolution on a $SrFeO_4$ 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 Phtholocyanines, 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 Sociey. 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.

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. K. A. Kurak and A. B. Anderson, **Selenium: a Nonprecious Metal Cathode Catalyst fort Oxygen Electroreduction**, J. Electrochem. Soc. 157, B173-B179 (2010).

2. 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).

3. 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).

4. 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).

5. 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).

6. 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).

7. 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).

8. 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).

9. 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).

10. T. Zhang and A. B. Anderson, **Oxygen Reduction on Platinum Electrodes in Base: Theoretical Study**, Electrochim. Acta 52, 982-989 (2007).

11. E. Vayner, R. A. Sidik, A. B. Anderson, B. N. Popov, **Experimental and Theoretical Study of Cobalt Selenide as a Catalyst for $O_2$ Electroreduction**, *J. Phys. Chem. C*, **2007**, 111, 10508-10513.

12. E. Vayner and A. B. Anderson, **Theoretical Predictions Concerning Oxygen Reduction on Nitrided Graphite Edges and a Cobalt Center Bonded to Them,** J. Phys. Chem. C, 111, 9330-0336 (2007).

13. 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).

14. E. Vayner, H. Schweiger, and A. B. Anderson, **Four-Electron Reduction of $O_2$ Over Multiple $Cu^I$ Centers" Quantum Theory**, J. Electroanal. Chem. 607, 90-100 (2007).

15. 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).

16. 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).

17. 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).

18. 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).

19. R. A. Sidik and A. B. Anderson, **$Co_9S_8$ as a Catalyst for Electroreduction of $O_2$: Quantum Chemistry Predictions**, J. Phys. Chem. B, 110, 936-931 (2006).

20. R. A. Sidik, A. B. Anderson, N. P. Subramanian, S. P. Kumaraguru, and B. N. Popov, **$O_2$ Reduction on Graphite and Nitrogen-doped Graphite: Experiment and Theory**, J. Phys. Chem. B, 110, 1787-1793 (2006).

21. H. Schweiger, E. Vayner, and A. B. Anderson, **Why is there such a Small Overpotential for $O_2$ Electroreduction by Copper Laccase?,** Electrochem. Sol. St. Lett., 8, A585-A587 (2005).

22. 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).

23. J. Roques and A.B. Anderson, **$Pt_3Cr(111)$ Alloy Effect on the Reversible Potential of OOH(ads) formation from $O_2$(ads) Relative to Pt(111),** J Fuel Sci. Technol. 2, 86-93 (2005).

24. 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. E4-E8 (2005).

25. 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).

26. 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).

27. 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).

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