Brief 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, 198l 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.