David N. Beratan, Ph.D.
Brief Biographical Sketch

Education: B.S. Chemistry, Duke University, with Honors and Distinction, 1980; Ph.D. Chemistry, California Institute of Technology, 1986; NRC Resident Research Associate, NASA's Jet Propulsion Laboratory, 1985-87

Positions: R.J. Reynolds Professor of Chemistry; Professor of Physics; Professor of Biochemistry. Adjunct Professor of Chemistry, University of Pittsburgh.

Honors: C.H. Herty Medal of the American Chemical Society Georgia Section, Feynman Prize for Nanoscience – Foresight Inst., J.S. Guggenheim Foundation Fellow, Elected Fellow - American Association for the Advancement of Science, Elected Fellow - American Physical Society, Elected Fellow – American Chemical Society, Elected Fellow – Royal Society of Chemistry, Conrad E. Ronneberg Visiting Scholar - University of Chicago, Ralph and Lucy Hirschmann Visiting Professor - University of Pennsylvania, Visiting Fellow - All Souls College (University of Oxford), Chancellor's Distinguished Research Award - University of Pittsburgh

Service: Recent editorial advisory boards: *Chemical & Engineering News*, *Molecular Simulation*, and *Biopolymers*; Advisor to Chemical Heritage Foundation, contributing to the design of museum displays and organizing Foundation activities in the Research Triangle area; Chair, Duke Department of Chemistry 2004-07, Member NIH MSFA Study Section (2009-13); Leader of Theory Team – University of North Carolina Solar Fuels Energy Frontier Research Center (2010-14).

Summary of Research Accomplishments

David has made influential contributions in theoretical bioinorganic, bioorganic, and physical-organic chemistry. Of particular note are the following:

- David developed the "standard model" for protein mediated electron-transfer reactions (with J.N. Onuchic). His tunneling pathway model was the first to link a protein's three-dimension fold to its electron transfer kinetics, making testable predictions of how secondary and tertiary structure – and of structural fluctuations - cause order of magnitude effects on reaction rates. These predictions were verified during an intensive 20 year period of experimental activity motivated by his theories, which changed the view of biological electron transfer from one of "square-barrier tunneling" to one of tunneling through structured, fluctuating molecules consisting of multiple quantum tunneling routes (determined by the covalent and noncovalent interactions in the biomacromolecule). Recent contributions have been to build predictive theories of charge transfer in bacterial nanowires and nucleic acids.
- He developed the first quantitative theoretical methods that use quantum chemically computed optical rotation data to assign the absolute stereochemistry of complex natural products containing multiple stereogenic centers (with P. Wipf). This contribution was enabled by his development of quantitative methods to compute optical rotatory dispersion spectra (a known and unsolved challenge for about 50 years), his use of extensive requisite conformational sampling, and his exploitation of essential additivity (van't Hoff) principles. More recent discoveries have defined the influence of the chiral solvent imprint and intermolecular association on optical rotations.
- David established an "inverse design" approach to enable the discovery of new structures and materials with optimal targeted properties. This line of research began with his developing theory-guided rules to optimize optical properties (of nonlinear optical materials, light-driven molecular memories, and organic light-emitting diodes). Most recently (in collaboration with W. Yang), he established a general approach to molecular property optimization. This unified scheme, known as the "linear combination of atomic potentials" approach, defines a new paradigm to mine the richness of molecular and materials space. Recent developments combine property optimization with the enumeration of maximum diversity molecular libraries to address challenges in materials science and drug discovery.