David N. Beratan
Duke University
Durham, North Carolina

Research Interests

Electron transfer in macromolecules
Biological energy transduction
Energy science
Molecular chirality
Inverse molecular design
Molecular diversity and library design

Education

Ph.D., Chemistry, California Institute of Technology, Pasadena, California, 1986
B.S., Chemistry, Duke University, Durham, North Carolina, 1980

Current Positions

Duke University: R.J. Reynolds Professor of Chemistry; Professor of Biochemistry; Professor of Physics; Member of Structural Biology and Biophysics and Computational Biology and Bioinformatics Programs
University of Pittsburgh: Adjunct Professor of Chemistry

Professional Experience

•*Duke University*
Professor of Physics, Fall 2009 -
Department Chair, July 2004 – June 2007
Professor of Biochemistry, Spring 2002 –
R.J. Reynolds Professor of Chemistry, Fall 2001 –
•*University of Pittsburgh*
Adjunct Professor of Chemistry 2002 -
Professor of Chemistry 1997 - 2001
Associate Professor of Chemistry 1992 - 97
•*Jet Propulsion Laboratory*
Member of the Technical Staff 1987 - 1991
NRC/NASA Resident Research Associate 1985 - 1987

Selected Honors

Charles H. Herty Medal of the American Chemical Society Georgia Section, 2015
Feynman Prize for Nanoscience (Theory), Foresight Institute, 2013
Elected Fellow, Royal Society of Chemistry, 2013
Elected Fellow, American Chemical Society, 2013
ACS Certificate of Appreciation for contributions and service in peer review, 2011
Invited participant, 22nd Solvay Conference on Chemistry, October 2010
"Golden Goggles" Lectureship, Middle Tennessee State University, April 2009
Elected Fellow, American Association for the Advancement of Science, 2002
Elected Fellow, American Physical Society, 2001

J.S. Guggenheim Foundation Fellow, 1999-2000
Chancellor's Distinguished Research Award, University of Pittsburgh, 1998
NSF National Young Investigator (NYI) Award recipient, 1992-97
National Research Council Resident Research Associate, NASA's Jet Propulsion Laboratory, Caltech, 1985-87
Graduation with Honors and with Distinction (in Chemistry), Duke University, 1980

Selected Visiting Appointments

Visiting Scholar, Northwestern University, October-November 2008
Visiting Scholar, University of Pittsburgh, September 2008
Visiting Fellow, Institute for Nanoscale Physics and Chemistry, KU Leuven, Belgium, March 2007
Conrad E. Ronneberg Visiting Scholar, University of Chicago, April 2001
Ralph & Lucy Hirschmann Visiting Professorship (and 3 lectures), Univ. of Pennsylvania, May 2000
Visiting Fellow, All Souls College, University of Oxford, 1999 - 2000
Visiting Associate in Chemistry, Caltech, July 1989-July 1993 & June 1996
Visiting Professor, São Carlos Institute of Physics and Chemistry, University of São Paulo, São Carlos, Brazil, August 1988

Journal Editorial and Advisory Boards

Editorial Advisory Board, *Chemical & Engineering News* (2007-10)
Editorial Board, *Molecular Simulation* (2001 -)
Editorial Advisory Board, *Biopolymers* (2006 -)

Selected Professional Service

Review Panels

- NIH Study Section Member, Macromolecular Structure and Function A 2009 –13.
- Member NIH special emphasis panels: 9/13, 12/08, 12/09.
- Member of NSF proposal review panels
- *Ad hoc* Member of NIH MSFA Study section (2008)
- *Ad hoc* Member of NIH BBCA Study sections (2003, 1998, 1996) and Department of Energy Review Panels for Argonne Labs and for Basic Energy Sciences Programs (1992 & 1998)
- Site visit panels for NSF (2003-06)

Volumes Edited

- *PhysChemChemPhys* special volume on electron transfer, 2012
- *Molecular Simulation*, special volume on electron transfer theory, 2006
- *Topics in Current Chemistry*, vol. 298, 2011, "Electronic and magnetic properties of chiral molecules and supramolecular architectures"

Minicourses and Summer Schools

- Co-Director of summer school on "Bioelectronics" at the Ettore Majorana Foundation and Centre for Scientific Culture, Erice, Italy, 5/14 (one week)
- University of Cyprus, one day mini-course on "Molecular and Biomolecular Electron Transfer Concepts and Applications," 6/1/14
- Univ. Zürich Mini-Course on "Theory and modeling at the chemistry-biology interface", May 2009 (one week)

Conferences Organized

- 40 Years Later: Molecular Electronics 2015, Maa'le Hachamisha, Israel, June 2015
- Telluride Conference on Electronic and Magnetic Properties of Chiral Structures and their Assemblies, 6/14, 6/12, 6/10, 6/14
- Duke-UNC-Energy Frontier Research Conference on Energy Science, Engineering and Policy, 1/12 (250 participants)
- NIH Center for Molecular Library Design, Duke-UPitt Conference, Durham, 5/11
- ACS National Meeting, "20 years of Tunneling Pathways," Anaheim, 3/11
- Duke-Pittsburgh-Rehovot Conference on Charge transport in molecular assemblies, 3/11, Duke Marine Lab, 3/11
- Pacifichem 2010, "DNA Photonics," Honolulu, 12/10
- Southeastern Theoretical Chemistry Association, Duke University, 5/09
- Duke Workshop on Energy, Beaufort, NC, 11/08
- SERMACS Symposium on "Molecular Chirality: Theory, Synthesis, and Spectroscopy," Research Triangle Park, NC, 11/04
- SERMACS Symposium on "Electron Transfer in Nanostructures" Atlanta, GA, 11/03

Publications (H-index (ISI)= 58; ~9,900 citations; ~200 publications and one short technical film)

2015

D.N. Beratan, C. Liu, A. Migliore, N.F. Polizzi, S.S. Skourtis, P. Zhang, Y. Zhang, "Charge transfer in dynamical biosystems, or the treachery of (static) images," Acc. Chem. Res., 48, 474-481(2015).

Y. Yue, T. Grusenmeyer, Z. Ma, P. Zhang, R.H. Schmehl, D.N. Beratan, I.V. Rubtsov, "Electron Transfer Rate Modulation in a Compact Re(I) Donor-Acceptor Complex," Dalton T., in press (2015)

J. Lin, D. Balamurugan, P. Zhang, S.S. Skourtis, and D.N. Beratan, "Two electron transfer pathways," J. Phys. Chem. B., in press (2015) (Newton/Miller Festschrift).

C. Rupakheti, A.M. Virshup, W. Yang, D.N. Beratan, "A Strategy to Discover Diverse

Optimal Molecules in the Small Molecule Universe," J. Chem. Inf. Model., 55, 529-537 (2015).

P. Antoniou, Z. Ma, P. Zhang, D.N. Beratan, and S.S. Skourtis, "Vibrational control of electron transfer reactions: a feasibility study for the fast coherent transfer regime," PCCP, in press (2015).

A. Migliore, R. Naaman, D.N. Beratan, "Sensing of molecules using quantum dynamics," Proc. Natl. Acad. Sci., in press (2015).

R.M. Young, A.P.N. Singh, A.K. Thazhathveetil, V.Y. Cho, Y. Zhang, N. Renaud, F.C. Grozema, D.N. Beratan, M.A. Ratner, G.C. Schatz, Y.A. Berlin, F.D. Lewis, and M.R. Wasielewski, "Charge Transport Across DNA-based Three-Way Junctions," J. Am. Chem. Soc., in press (2015).

2014

R. Venkatramani, E. Wierzbinski, D.H. Waldeck, and D.N. Beratan, "Breaking the simple proportionality between molecular conductances and charge transfer rates," Faraday Discuss., 174, 57-78 (2014).

Y. Zhang, C. Liu, A. Balaeff, S. S. Skourtis, and D.N. Beratan, "A flickering resonance mechanism for biological charge transfer," Proc. Natl. Acad. Sci. (USA), 111, 10049-10054 (2014).

A. Migliore, N.F. Polizzi, M.J. Therien, and D.N. Beratan, "Biochemistry and theory of proton-coupled electron transfer reactions," Chem. Revs. 114, 3381-3465 (2014).

A.E. Kuznetsov and D.N. Beratan, "Structural and electronic properties of bare and capped $Cd_{33}Se_{33}$ and $Cd_{33}Te_{33}$ quantum dots," J. Phys. Chem. C, 118, 7094-7109 (2014).

Y. Yue, T.A. Grusenmeyer, Z. Ma, P. Zhang, R.H. Schmehl, D.N. Beratan and I.V. Rubtsov, "Full electron ligand-to-ligand charge transfer in a compact rhenium(I) complex," J. Phys. Chem. A 118, 10407-10415 (2014).

2013

Y. Yue, T.A. Grusenmeyer, Z. Ma, P. Zhang, T.T. Pham, J.T. Mague, J.P. Donahue, R.H. Schmehl, D.N. Beratan and I.V. Rubtsov, "Evaluating the extent of intramolecular charge transfer in the excited states of rhenium(I) donor-acceptor complexes with time-resolved vibrational spectroscopy," J. Phys. Chem. B (M.D. Fayer Festschrift), 117, 15903-15916 (2013).

B.P. Bloom, J-B. Zhao, Y. Wang, D.H. Waldeck, R. Liu, P. Zhang, and D.N. Beratan, Ligand-induced changes in the characteristic size-dependent electronic energies of CdSe nanocrystals," J. Phys Chem. C, 117, 22401-22411 (2013).

J. Lin, X. Hu, P. Zhang, A. Van Rynbach, D.N. Beratan, C. Kent, B. Mehl, J. Papanikolas, T.J. Meyer, Thomas; W. Lin, S.S. Skourtis, M. Constantinou, "Triplet excitation energy dynamics in metal-organic frameworks," J. Phys. Chem. C (R. Naaman Festschrift), 117, 22250-22259 (2013).

A. Virshup, J. Contreras-Garcia, P. Wipf, W. Yang, and D.N. Beratan, "Stochastic voyages into uncharted chemical space produce a representative library of all possible drug-like compounds," J. Am. Chem. Soc. 135, 7296-7303 (2013).

E. Wierzbinski, R. Venkatramani, K. Davis, S. Bezer, J. Kong, Y. Xing, E. Borguet, C. Achim, D.N. Beratan, D.H. Waldeck, "The single molecule conductance and electrochemical electron transfer rate are related by a power law," ACS Nano, 7, 5391-5401 (2013).

Y. Wang, J.R. King, P. Wu, D.L. Pelzman, D.N. Beratan, and E.J. Toone, "Enthalpic signature of methonium desolvation revealed in a synthetic host-guest system based on curcurbit[7]uril," J. Am. Chem. Soc., 135, 6084-6091 (2013). Erratum: 135, 17650 (2013).

D.N. Beratan and S.S. Skourtis, "Electron transfer through proteins," in *Encyclopedia of Biophysics*, G. Roberts, ed., Springer Verlag, 625-630 (2013).

N. Jiang, X. Hu, J.M. Nocek, B.M. Hoffman, B.R. Crane, and D.N. Beratan, "Distance independent charge recombination kinetics in cytochrome *c*-cytochrome *c* peroxidase complexes: compensating changes in the electronic coupling and reorganization energies," J. Phys. Chem. B, 117, 9129-9141 (2013).

2012

F. De Vleeschouwer, W. Yang, D.N. Beratan, P. Geerlings, and F. De Proft, "Inverse design of molecules with optimal reactivity properties: acidity of 2-naphthol derivatives," PCCP, 14, 16002-16013 (2012).

D.N. Beratan and J.N. Onuchic, Redox Redux, PCCP, 14, 13728 (2012).

E. Lim, A. Kuznetsov, and D.N. Beratan, "Effects of S-containing ligands on the structure and electronic properties of Cd_nSe_n/Cd_nTe_n nanoparticles (n=3, 4, 6, and 9), Chem. Phys., 407, 97-109 (2012).

S. Keinan, J.M. Nocek, D.N. Beratan and B.M. Hoffman, "Interfacial hydration, dynamics and electron transfer: multi-scale ET modeling of the transient myoglobin:cytochrome b_5 complex," PCCP, 14, 13881-13889 (2012).

E. Wierzbinski, A. de Leon, X. Yin, A.Balaeff, K.L. Davis, S. Reppireddy, R. Venkatramani, S. Keinan, D.H. Ly, M. Madrid, D.N. Beratan, C. Achim, D.H. Waldeck, "Effect of Backbone Flexibility on Charge Transfer Rates in Peptide Nucleic Acid Duplexes," J. Am. Chem. Soc., 134, 9335-9342 (2012). Erratum: 134, 13141 (2012).

N.F. Polizzi, S.S. Skourtis, and D.N. Beratan, "Physical constraints on charge transport through bacterial nanowires," Faraday Discuss., 155, 43-61 (2012).

I.A. Balabin, X. Hu, and D.N. Beratan, "Exploring biological electron transfer pathway dynamics with the Pathways plugin for VMD," J. Comput. Chem. 33, 906-910, (2012).

A.E. Kuznetsov, D. Balamurugan, S.S. Skourtis, and D.N. Beratan, "Structural and electronic properties of bare and capped Cd_nSe_n/Cd_nTe_n nanoparticles (n=6,9)," J. Phys. Chem. C, 116, 6817-6830 (2012).

N. Jiang, G. Zuber, S. Keinan, A. Nayak, W. Yang, M.J. Therein, D.N. Beratan, "Design of coupled porphyrin chromophores with unusually large hyperpolarizability," J. Phys. Chem., 116, 9724-9733 (2012).

2011

A. Balaeff, S.L. Craig, and D.N. Beratan, "B-DNA to Zip-DNA: Simulating a DNA Transition to a Novel Structure with Enhanced Charge Transport Characteristics," J. Phys. Chem. A (D.W. Pratt Festschrift), 115, 9377-9391 (2011).

K. Susumu, J.A.N. Fisher, J.R. Zheng, D.N. Beratan, A.G. Yodh, and M.J. Therien, Two-photon absorption properties of proquinoidal D-A-D and A-D-A quadrupolar chromophores, J. Phys. Chem. A 115, 5525-5539 (2011).

H. Carias, D.N. Beratan, and S.S. Skourtis, "Floquet analysis for vibronically modulated electron tunneling," J. Phys. Chem. B (S. Mukamel Festschrift), 115, 5510-5518 (2011).

J. Contreras-García, S. Keinan, D.N. Beratan, W. Yang, E.R. Johnson, R. Chaudret, "NCIPLOT: a program for plotting non-covalent interaction regions," J. Chem. Theory Comput., 7, 625-632 (2011).

R. Venkatramani, S. Keinan, A. Balaeff, and D.N. Beratan, "Electron transfer in nucleic acids: Black, white, and gray," Coord. Chem. Revs. (H.B. Gray Festschrift), 255, 635-648 (2011).

R. Venkatramani, K.L. Davis, E. Wierzbinski, S. Bezer, A. Balaeff, S. Keinan, A. Paul, L. Kocsis, D. N. Beratan, C. Achim, D.H. Waldeck, "Evidence for a near-resonant charge transport mechanism in double-stranded peptide nucleic acid (PNA)" J. Am. Chem. Soc., 133, 62-72 (2011).

V. Ben-Moshe, D.N. Beratan, A. Nitzan, S.S. Skourtis, and "Chiral control of current transfer in molecules," Top. Curr. Chem., 298, 259-278 (2011).

S. Skourtis, D.N. Beratan, and D.H. Waldeck, "Coherence in electron tunneling pathways," discussion paper for the 22nd Solvay Conference on Chemistry on 'Quantum effects in chemistry and biology', Procedia Chemistry, 61, 461-485 (2011).

M.A. Wolak, A. Balaeff, S. Gutmann, H.J. Helmrich, R. Vosloo, M.M. Beerbom, E. Wierzbinski, D.H. Waldeck, S. Bezer, C. Achim, D.N. Beratan, R. Schlaf, "Electronic structure of self-assembled peptide nucleic acid thin films," J. Phys. Chem. C, 115, 17123-17135 (2011).

2010

S. Keinan, R. Venkatramani, A. Balaeff and D.N. Beratan, "Is MD Geometry Sampling Sufficient for Nucleobase Electronic Structure Analysis of ET Reactions? Comparing Classical MD and QM/MM Methods," J. Phys. Chem. (M.A. Ratner Festschrift), 114, 20496-20502 (2010).

J.T. Hammill, J. Contreras-García, A.M. Virshup, D.N. Beratan, W. Yang, P. Wipf, "Synthesis and chemical diversity analysis of bicyclo[3.3.1]non-3-en-2-ones," Tetrahedron, 66, 5852-5862 (2010).

X. Hu, H. Hu, D.N. Beratan and W. Yang, "A gradient-directed Monte Carlo approach for protein design," J. Comp. Chem., 31, 2164-2168 (2010).

X. Hu, D. Xiao, S. Keinan, I. Asselberghs, M.J. Therien, K. Clays, W. Yang, and D.N. Beratan, "Predicting the Frequency Dispersion of Electronic Hyperpolarizabilities on the Basis of Absorption Data and Thomas-Kuhn Sum Rules," J. Phys. Chem. C, 114, 2349-2359 (2010).

Y. Xing, T-H. Park, R. Venkatramani, S. Keinan, D.N. Beratan, M.J. Therien, and E. Borguet, "Optimizing single molecule conductivity of conjugated organic oligomers with conjugated carbodithioate linkers," J. Am. Chem. Soc. 132, 7946-7956 (2010).

V. Ben-Moshe, A. Nitzan, S.S. Skourtis, and D.N. Beratan, "Steady-state theory of current transfer," J. Phys. Chem. C., 114, 8005-8013 (2010).

S.S. Skourtis, D.H. Waldeck, and D.N. Beratan, "Fluctuations in biological and bioinspired electron-transfer reactions," Annu. Rev. Phys. Chem. 61, 461-485 (2010).

2009

Z. Lin, C.M. Lawrence, D. Xiao, V.V. Kireev, S.S. Skourtis, J.L. Sessler, D.N. Beratan, and I.V. Rubtsov, "Modulating Unimolecular Charge Transfer by Exciting Bridge Vibrations," J. Am. Chem. Soc., 131, 18060-18062 (2009). [Chemical and & Engineering News Concentrate 12/7/09; Nature Chemistry Research Highlight 12/11/09].

X. Hu, D.N. Beratan, and W. Yang, "Emergent strategies for inverse molecular design," Science in China B: Chemistry, 52, 1769-1776 (2009).

X. Hu, D.N. Beratan, and W. Yang, "A gradient-directed Monte Caro method for global optimization in discrete space: Application to protein sequence design and folding," J. Chem. Phys., 131, 154117 (2009).

B.C. Rinderspacher, J. Andzelm, A. Rawlett, J. Dougherty, D.N. Beratan, W. Yang, "Discrete optimization of electronic hyperpolarizabilities in a chemical subspace," J. Chem. Theory Comput., 5, 3321-3329 (2009).

L. Yuan, J. Seo, N.S. Kang, S. Keinan, S.E. Steele, G.A. Michelotti, W.C. Wetsel, D.N. Beratan, Y-D. Gong, T.H. Lee and J. Hong, "Identification of 3-Hydroxy-2-(3-Hydroxyphenyl)-4*H*-1-Benzopyran-4-Ones as Isoform-Selective PKC-ζ Inhibitors and Potential Therapeutics for Psychostimulant Abuse," Mol. BioSyst., 5, 927-930 (2009).

D. Xiao, S.S. Skourtis, I.V. Rubtsov, and D.N. Beratan, "Turning charge transfer on and off in a molecular interferometer with vibronic pathways," Nano Lett., 9, 1818-1823 (2009).

I.A. Balabin, W. Yang, and D.N. Beratan, "Coarse-grained modeling of allosteric regulation in protein receptors," Proc. Natl. Acad. Sci. USA, 106, 14253-14258 (2009).

P. Mukhopadhyay, P. Wipf and D.N. Beratan, "Optical probes of molecular dissymmetry: combining theory and experiment to resolve stereochemical puzzles," Acc. Chem. Res. 42, 809-819 (2009).

A. Paul, S. Bezer, R. Venkatramani, L. Kocsis, E. Wierzbinski, A. Balaeff, S. Keinan, D.N. Beratan, C. Achim, D.H. Waldeck, "Role of Nucleobase Energetics in Single Stranded Peptide Nucleic Acid Charge Transfer," J. Am. Chem. Soc., 131, 6498-6507 (2009).

D.N. Beratan, S.S. Skourtis, I.A. Balabin, A. Balaeff, S. Keinan, R. Venkatramani, and D. Xiao, "Steering electrons on moving pathways," Acc. Chem. Res. 42, 1669-1678 (2009).

R. Venkatramani, D.Y. Zang, C. Oh, J. Grote, and D. Beratan, "Photoconductivity and current-voltage characteristics in thin DNA," Proceedings of SPIE-The Society of Photo-Optical Instrumentation Engineers 7403, 74030B-1 to 74030B-12 (2009).

B.C. Rinderspacher, J. Andzelm, A. Rawlett, J. Dougherty, D.N. Beratan, W. Yang, "Discrete optimization of electronic hyperpolarizabilities in a chemical subspace," Army Research Laboratory Publication ARL-TR-4833, May 2009.

2008

I.A. Balabin, D.N. Beratan, and S.S. Skourtis, "The persistence of structure over fluctuations in biological electron-transfer reactions," Phys. Rev. Lett., 101, 158102 (2008).

S. Keinan, M.J. Therien, D.N. Beratan and W. Yang, "Molecular design of porphyrin based nonlinear optical materials," J. Phys. Chem. A, 112, 12203-12207 (2008).

S.S. Skourtis, D.N. Beratan, R. Naaman, A. Nitzan, and D.H. Waldeck, "Chiral Control of electron transmission through molecules," Phys. Rev. Lett., 101, 238103 (2008).

G. Zuber, P. Wipf, D.N. Beratan, "Exploring the optical activity tensor by anisotropic Rayleigh optical activity scattering," ChemPhysChem, 9, 265-271 (2008). Corrigendum 9, 504 (2008).

J.M. Parks, R.K. Kondru, H. Hu, D.N. Beratan, and W. Yang, "Hepatitis C virus NS5B polymerase: QM/MM calculations show the important role of internal energy in ligand binding," J. Phys. Chem. B., 112, 3168-3176 (2008).

D.N. Beratan and I.A. Balabin, "Heme-copper oxidases use tunneling pathways," Proc. Natl. Acad. Sci. USA, 105, 403-404 (2008).

I.A. Balabin, D.N. Beratan, and S.S. Skourtis, "The chemical roles of water in biological electron transfer," in *Wiley Encyclopedia of Chemical Biology, Vol. 1*, T.P. Begley, ed. (published on the web at http://mrw.interscience.wiley.com/emrw/9780470048672/home/ and in print 2009).

E. Hatcher, A. Balaeff, S. Keinan, R.Venkatramani, and D.N. Beratan, "PNA versus DNA: effects of structural fluctuations on electronic structure and hole transport mechanisms," J. Am. Chem. Soc., 130, 11752-11761 (2008).

D. Balamurugan, W. Yang, and D.N. Beratan, "Exploring chemical space with discrete, gradient and hybrid optimization methods," J. Chem. Phys., 129, 174105 (2008).

D. Xiao, W. Yang and D.N. Beratan, "Inverse molecular design in a tight-binding framework," J. Chem. Phys., 129, 044106 (2008).

X. Hu, D.N. Beratan, and W. Yang, "A gradient-directed Monte Carlo approach to molecular design," J. Chem. Phys., 129, 064102 (2008).

W. He, E. Hatcher, A. Balaeff, D. Beratan, M. Madrid, R. Gil, C. Achim, "Solution structure of a peptide nucleic acid from NMR Data: features and limitations," J. Am. Chem. Soc., 130, 13264-13273 (2008).

S. Keinan, W.D. Paquette, J.J. Skoko, D.N. Beratan, W. Yang, S. Shinde, P.A. Johnston, J.S. Lazo, and P. Wipf, "Computational design, synthesis and biological evaluation of *para*-quinoid-based inhibitors for redox regulation of the dual-specificity phosphatase Cdc25B," Org. Biomol. Chem., 6, 3256-3263 (2008).

D. Xiao, F. Bulat, W. Yang, D.N. Beratan, A donor-nanotube paradigm for nonlinear optical materials, Nano Lett., 8, 2814-2818 (2008).

P. Mukhopadhyay, G. Zuber, and D.N. Beratan, "Characterizing aqueous solution conformations of a peptide backbone with theoretical analysis of the Raman optical activity spectra" Biophys. J., 95, 5574-5586 (2008).

2007

P. Mukhopadhyay, G. Zuber, P. Wipf, D.N. Beratan, "Contribution of a solute's chiral solvent imprint to optical rotation," Angew. Chemie Int. Ed., 46, 6450-6452 (2007). [See commentary in *Science*, August 10, 2007, in Chemical and Engineering News, August 6, 2007, and in Angew. Chemie Int. Ed. 46, 7738-7740 (2007)].

T.R. Prytkova, I.V. Kurnikov, D.N. Beratan, "Coupling coherence distinguishes structure sensitivity in protein electron transfer," Science, 315, 622-625 (2007).

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S. Keinan, X. Hu, D.N. Beratan, W. Yang, "Designing molecules with optimal properties using the linear combination of atomic potentials approach in an AM1 semiempirical framework," J. Phys. Chem. A, 111, 176-181 (2007).

A. Zöllner, M.A. Pasquinelli, R. Bernhardt, and D.N. Beratan, "Protein phosphorylation and intermolecular electron transfer: a Joint experimental and computational study of a hormone biosynthesis pathway," J. Am. Chem. Soc. 129, 4206-4216 (2007).

2006

J.L. Perry, M.R. Goldsmith, T.R. Williams, K.P. Radack, T. Christensen, J. Gorham, M.A. Pasquinelli, E.J. Toone, D.N. Beratan and J.D. Simon, "Binding of warfin influences the acid-base equilibrium of H242 in sudlow site I of human serum albumin" Photochem. Photobiol. 82, 1365-1369 (2006).

P. Mukhopadhyay, G. Zuber, M-Rock. Goldsmith, P. Wipf, D.N. Beratan, "Solvent effect on optical rotation: a case study of methyloxirane in water," ChemPhysChem 7, 2483-2486 (2006).

M.R. Goldsmith, C. George, G. Zuber, D.N. Beratan, D. Waldeck and R. Naaman, "Chiral image charges in metal nanoclusters," ChemPhysChem, 8, 63-67 (2006).

M. Wang, X. Hu, D.N. Beratan, and W. Yang, "Designing molecules by optimizing potentials," J. Am. Chem. Soc., 128, 3228-3232 (2006). [See commentary in *Nature*, March 16, 2006, and in *Chemical and Engineering News*, March 9, 2006; Provisional patent filed.]

S.S. Skourtis, J. Lin, and D.N. Beratan, "The effects of bridge motion on electron transfer reactions mediated by tunneling," Chapter 18 in *Modern methods for theoretical physical chemistry of biopolymers*, edited by E.B. Starikov, J.P. Lewis, and S. Tanaka, Elsevier, June 2006.

T. Kawatsu, D.N. Beratan, and T. Kakitani, "Conformationally averaged score functions for electronic propagation in proteins," J. Phys. Chem. B, 110, 5747-5757 (2006).

T. Kawatsu and D.N. Beratan, "Electron transfer between cofactors in protein domains linked by a flexible tether," Chem. Phys., 326, 259-269 (2006).

D. Kazmin, T. Prytkova, C.E. Cook, R. Wolfinger, T. Chu, D. Beratan, C. Chang, and D.P. McDonnell, "Linking ligand induced alterations in androgen receptor structure to differential gene expression; a first step in the rational design of selective androgen receptor modulators," Mol. Endocrinol., 20, 1201-1217 (2006).

2005

J. Lin, I.A. Balabin, and D.N. Beratan, "The nature of aqueous tunneling pathways between electron-transfer proteins," Science, 310, 1311-1313 (2005). [See commentary in *Chemical and Engineering News*, November 28, 2005.]

G. Zuber, M. Goldsmith, T.D. Hopkins, D.N. Beratan, and P. Wipf, "Systematic assignment of the configuration of flexible natural products by spectroscopic and computational methods: The Bistramide C Analysis, Org. Lett., 7, 5269-5272 (2005).

G. Zuber, M. Goldsmith, DN. Beratan, and P. Wipf, "Towards Raman optical activity calculations of large molecules," ChemPhysChem, 6, 595-597 (2005).

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J.R. Winkler, H.B. Gray, T.R. Prytkova, I.V. Kurnikov, and D.N. Beratan, "Electron transfer through proteins" in "*Bioelectronics*," edited by I. Willner and E. Katz, Wiley-VCH (2005), pp 15-33.

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Invited Presentations (last 5 years)

2015

Univ. of Missouri, St. Louis, 4/15
Boston University, 3/15
University of Freiburg, Germany, summer/15
Penn Theoretical Chemistry Conference, 7/15

2014

17th Foresight Conference, Palo Alto, CA, 2/14
Nanosafe Bioelectronics and Biosensing Symposium, West Virginia University, 4/14
CECAM: Investigating fine quantum effects in biological systems, Paris, 5/14
University of Paris-Sud, Orsay, France, 5/14
Interfaces between experimental and theoretical approaches to energy related enzyme catalysis, London, 6/14
University of Cyprus Information Day on vibrational control of charge transfer, Nicosia, Cyprus, 6/14
Telluride Science Center, 6/14
ACS, San Francisco, 8/14
Electron donor-acceptor interactions Gordon Research Conf., Discussion leader, 8/14

2013

Yale University, 12/13
North Carolina State University, 11/13
SERMACS, Atlanta, 11/13
PSI-K workshop on Modeling single-molecule junctions, Berlin, 10/13
University of Virginia, 9/13
Duke Fitzpatrick Institute for Photonics Annual Symposium, 3/13
MIT, 5/13

2012

UNC-Chapel Hill, 2/12
ACS, San Diego, Yang Award Symposium, 3/12
ACS, San Diego, Hoffman Award Symposium, 3/12
University of Southern California, Chemistry/Physics Colloquium, 4/12
Telluride Conference on Electronic and Magnetic Properties of Chiral Structures and their Assemblies, 6/12
ACS, Philadelphia, 2 seminars, 8/12
Materials Research Society, Boston, 11/12
CECAM Workshop, Lugano, Switzerland, 11/12

2011

University of Miami, 4/11
Institute for Pure and Applied Mathematics conference on Physical frameworks for sampling chemical compound space, UCLA, 5/11
Conference on "Designing Molecular Functionality: Challenges for Theoretical Approaches," Sursee, Switzerland, 8/11
Telluride Conference on Transport, 8/11
Faraday Discussions of Artificial Photosynthesis, 9/11
NaBi – Joint Weizmann-CNRS meeting on Nano-bioscience, Caesarea, Israel, 9/11
UPitt Science2011, Pittsburgh, PA, 10/11
VA Commonwealth University, Richmond, VA, 10/11

2010

Pacifichem, Honolulu, 12/10
University of Illinois, Urbana-Champaign, 9/10
Molecular Quantum Mechanics – 2010 Conference, UC Berkeley, 5/10
Gordon Res. Conference on Electron donor-acceptor interactions, Newport, RI, 8/10
22nd Solvay Conference on Chemistry, Hotel Métropole, Brussels, 10/10
Telluride Conference on Electronic and Magnetic Properties of Chiral Structures and their Assemblies, 6/10
Univ. of Nebraska, Lincoln, 10/10
ACS National Meeting, Electrons in Biomolecules symposium, Boston, 8/10
City University of New York, Institute for Theoretical Science, New York City, 4/10
Canadian Society of Chemistry Meeting, Toronto, 5/10

Special Teaching Initiatives at Duke

- Developing Duke "Signature Course" on biophysical chemistry; awarded Arts & Sciences Grant for the project, 2015
- Developed multi-university web-based real-time teaching approach for graduate special topics courses; awarded Duke "Collaborative Teaching Through Research Across Institutions" grant 2014-15
- Developed mini-text and *Mathematic* CDF demonstration notebooks for teaching quantum dynamics
- Developed senior level Inorganic Chemistry course, Chem 117, with emphasis on materials properties, bioinorganic chemistry, and chemical reactions
- New freshman focus course on Science Ethics (Chem 93 FCS) as part of the "Faces of Sciences" cluster
- Revised Chem 26S - Introduction to Research in Chemistry, an independent study in chemistry course for freshman, including substantive reading/guest lecture components
- Revised Chem 165, first semester Physical chemistry, using an inquiry based learning approach with electronic and computational components, and elements from the current research literature.
- Developed (with Bonk) Introduction to Modeling course, Chem 349

Special teaching and other activities at University of Pittsburgh

- Developed extensive *Mathematica* based classroom demonstrations and homework assignments for junior physical chemistry. Obtained funding for LCD device and laptop to implement these activities in the classroom, 1994.
- Developed proposal and found funding for Joint Chemistry-Physics teaching classroom, 1995 (see http://www.chem.pitt.edu/facilities/computational-resources/jcc).
- Contributed to development of a funded Hewlett Foundation Proposal to develop an integrated introductory science course sequence for non-science majors, 1997.
- Member of the Executive Committee for Academic Computing and Working Group Chair for Advanced Instructional Technology (1995-99). Ran faculty grant program, overseeing a substantial part of the University computing budget, and establishing goals for computing at the University.

Professional Associations

ACS (Fellow), APS (Fellow), AAAS (Fellow), RSC (Fellow), Biophysical Society, Phi Lambda Upsilon.

Funding

Current:

National Institutes of Health (since 1993) Tunneling pathways in proteins
National Institutes of Health: Charge Transfer Dynamics Relevant to Protein-mediated Energy Transduction (2011-15)
National Science Foundation: Collaborative Research: Directed Charge Transfer in Metal Containing Peptide Nucleic Acid Assemblies (2014-17)
National Science Foundation: Collaborative Research: Infra-red Control of Electron-Transfer Mechanisms (2010-14)
Department of Energy: Nanocrystal-based diodes for electric energy conversion (2013-16)
Office of Naval Research – MURI: Conductive DNA Systems and Molecular Devices (2011-16)
NASA: DNA Repair Under Extreme Conditions (2013-17)
Samsung: Mapping molecular materials space (2013-15)
Duke University: Collaborative Teaching Through Research Across Institutions (2014-15)

Recent past: DOE UNC-EFRC, DARPA; TeraDisc; NEDO (Japan), Keck Foundation, DOE, AFOSR, DARPA, NIH, Ben Franklin Foundation, and Pittsburgh Materials Research Center, Department of Commerce, Petroleum Research Fund, Guggenheim Foundation, Volkswagen Foundation, US-Israel Binational Science Foundation, NIH P-50.

Teaching at Duke

- Molecular Biophysics and Biophysical Chemistry (undergraduate), Spring '14
- Introduction to Modeling Complex Molecular Materials: From Energy Science to Bioscience (graduate & undergraduate, taught over the web at three universities): Fall '13, '14
- Biophysical Chemistry (undergraduate), Spring '13
- Quantum Dynamics (graduate), Spring '11, Fall '12
- Modeling Charge Transfer and Transport (graduate), Spring '10
- Inorganic Chemistry (undergraduate, Chem 117) Spring '08
- Freshman FOCUS Seminar: "Ethical Issues in Science" (Chem 93S) Fall '07 & '09
- Introduction to Molecular Modeling (graduate, Chem 349) Fall '05
- Statistical Mechanics (graduate, Chem 344) Spring '02
- Introduction to Research in Chemistry (undergraduate, Chem 26S) Spring '03 and Spring '04
- Physical Chemistry (one semester, undergraduate, Chem 165) Fall '03

Teaching at University of Pittsburgh

- Physical Chemistry (two-semesters, undergraduate)
- Atoms, Molecules and Materials (one semester, undergraduate/graduate)
- Quantum Mechanics (one semester, graduate)
- Statistical Mechanics (one semester, graduate)
- Advanced Quantum Mechanics (one semester, graduate)
- Theory of Materials (one semester, graduate)
- Special topics in Electron Transfer Chemistry (one semester minicourse, graduate/undergraduate)
- Biophysical Chemistry (one semester – team taught, graduate)

Past Group members

- 11 ACS Project SEED high school students
- 36 undergraduate researchers
- 13 graduate students
- 24 post-doctoral associates

Current research group:

- 10 graduate students
- 1 post-doctoral associates
- 2 assistant research professors