

**David N. Beratan**  
Duke University  
Durham, North Carolina  
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## **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

## **Professional Experience**

### • *Duke University*

Director, NSF Center for Chemical Innovation - Center for  
Synthesizing Quantum Coherence, 2019 -  
Professor of Physics, Fall 2009 -  
Chair, Department of Chemistry, 2004 - 07  
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 - 91  
NRC/NASA Resident Research Associate 1985 - 87

## **Honors**

### • **Awards and Fellowships**

Bourke Award of the Royal Society of Chemistry, 2019  
Murray S. Goodman Memorial Prize, American Chemical Society, Division of  
Biological Chemistry and *Biopolymers*, 2018  
Florida Award, American Chemical Society, Florida Section, 2017  
Charles H. Herty Medal, 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  
Elected Fellow, American Association for the Advancement of Science, 2002  
Elected Fellow, American Physical Society, 2001  
Conrad E. Ronneberg Visiting Scholar, University of Chicago, April 2001  
J.S. Guggenheim Foundation Fellow, 1999-2000  
Ralph & Lucy Hirschmann Visiting Professorship, Univ. of Pennsylvania, May 2000  
Visiting Fellow, All Souls College, University of Oxford, 1999 - 2000  
Burroughs-Wellcome Travel Fellow, University of Oxford, 1999-2000

NSF National Young Investigator (NYI) Award recipient, 1992-97  
Chancellor's Distinguished Research Award, University of Pittsburgh, 1998  
National Research Council Resident Research Associate, NASA's Jet Propulsion  
Laboratory, Caltech, 1985-87  
American Institute of Chemists Award, 1980  
Graduation with Honors and with Distinction, Duke University, 1980

- **Lectureships and Directorships**

RSC Bourke Lecture Tour (2019)  
Director, Duke Summer Research Experience for Undergraduates in Theoretical  
Chemistry (2019- )  
Tiangong Forum Distinguished Lecturer, Tianjin Institute of Industrial  
Biotechnology, Chinese Academy of Sciences," Tianjin, China, May 2017  
Director of Theory Team, University of North Carolina-Chapel Hill, Energy Frontier  
Research Center, 2011-13  
22<sup>nd</sup> Solvay Conference on Chemistry, October 2010  
"Golden Goggles" Lectureship, Middle Tennessee State University, April 2009  
Hirschmann Lectures, Univ. of Pennsylvania, May 2000

- **Editorial and Advisory Boards**

Editorial Advisory Board, *Chemical & Engineering News* (2007-10)  
Editorial Board, *Molecular Simulation* (2001 - 2019)  
Editorial Advisory Board, *Biopolymers* (2006 - 2019 )

### **Mini-courses and Summer Schools**

- 4<sup>th</sup> Bioinorganic Workshop (Penn State University), June 2016
- Co-Director, summer school on "Bioelectronics" at the Ettore Majorana Foundation and Centre for Scientific Culture, Erice, Italy, May 2014
- University of Cyprus, one day mini-course on Electron Transfer Concepts and Applications, June 2014
- University of Zürich mini-course on "Theory and Modeling at the Chemistry-Biology Interface," May 2009

### **Meetings & Symposia Organized**

- Elected Vice-Chair (2020) and Chair (2023) American Conference on Theoretical Chemistry
- Elected Co-Vice Chair (2016) and Co-Chair (2018), Gordon Conference on Electron Donor-Acceptor Interactions
- Co-organizer, 40 Years Later: Molecular Electronics 2015, Ma'ale Hachamisha, Israel, June 2015
- Co-organizer, Telluride Conference on Electronic and Magnetic Properties of Chiral Structures and their Assemblies, 2020, 2018, 2016, 2014, 2012, 2010
- Co-organizer, Duke-UNC-Energy Frontier Research Conference on Energy Science, Engineering and Policy, 1/12
- Co-organizer, NIH Center for Molecular Library Design, Duke-UPitt Conference, Durham, 5/11

- Co-organizer, ACS National Meeting – Physical Division: 20 years of Tunneling Pathways, Anaheim, 3/11
- Co-organizer, Duke-Pittsburgh-Rehovot Conference on Charge transport in molecular assemblies, Duke Marine Lab, 3/11
- Co-organizer, Pacificchem 2010: DNA Photonics, Honolulu, 12/10
- Co-organizer, Southeastern Theoretical Chemistry Association, Duke University, 5/09
- Co-organizer, Duke Workshop on Energy, Duke Marine Lab, 11/08
- Co-organizer, SERMACS Symposium on “Molecular Chirality: Theory, Synthesis, and Spectroscopy,” Research Triangle Park, NC, 11/04
- Co-organizer, SERMACS Symposium on “Electron Transfer in Nanostructures” Atlanta, GA, 11/03

### **Research Interests**

Electron transfer in macromolecules

Free energy transduction

Molecular chirality

Inverse design of molecules and materials with optimal properties

Molecular diversity and “molecular space” exploration

### **Publications**

#### **2020**

J. Tong, P. Zhang, L. Zhang, D. Zhang, D.N. Beratan, H. Song, Y. Wang, T. Li, “A robust bioderived wavelength-specific photosensor based on BLUF proteins,” *Sensor. Actuat. B – Chem.*, 310, 127838 (2020).

X. Li, J. Valdiviezo, S.D. Banziger, P. Zhang, T. Ren, D.N. Beratan, and I.V. Rubtsov, Symmetry controlled photo-selection and charge separation in butadiyne-bridged donor-bridge-acceptor compounds, submitted (2020).

J. Yuly, P. Zhang and D.N. Beratan, “Universal free energy landscape produces efficient and reversible electron bifurcation,” submitted (2020).

L. Xiang, P. Zhang, C. Liu, X. He, H.B. Li, Y. Li, Z. Wang, J. Hihath, S.H. Kim, D.N. Beratan, and N-J. Tao, “The conductance and configuration of molecular gold-water-gold junctions under electric fields,” submitted (2020).

Y. Jin, X. Ru, N.Q. Su, Y. Mei, D.N. Beratan, P. Zhang, W. Yang, “Revisiting the hole size in double helical DNA with localized orbital scaling correction,” submitted (2020).

#### **2019**

Y.K. Kang, P. Zhang, I.V. Rubtsov, J. Zheng, G. Bullard, D.N. Beratan, and M.J. Therien, “Orientational dependence of cofacial porphyrin-quinone electronic interactions within the strong coupling regime,” *J. Phys. Chem. B*, 123, 10456-10462 (2019).

R.D. Teo, B.J.G. Rousseau, E.R. Smithwick, R. Di Felice, D.N. Beratan, and A. Migliore, "Charge transfer between [4Fe4S] proteins and DNA is unidirectional. Implications for biomolecular signaling," *Chem.*, 5, 122-137 (2019).

R.D. Teo, E.R. Smithwick, A. Migliore, and D.N. Beratan, "A single AT-GC exchange can modulate charge transfer-induced p53-DNA dissociation," *Chem. Commun.*, 55, 206-209 (2019).

K. Michaeli, D.N. Beratan, D.H. Waldeck and R. Naaman, "Voltage induced long-range coherent electron transfer through organic molecules," *Proc. Natl. Acad. Sci. (USA)*, 116, 5931-5936 (2019).

D.N. Beratan, "Why are protein and DNA electron transfer so different?" *Annu. Rev. Phys. Chem.*, 70, 71-97 (2019).

S. Bai, P. Zhang, P. Antoniou, S. Skourtis, and D.N. Beratan, "Quantum interferences among Dexter coupling pathways," *Faraday Discuss.*, 216, 301-318 (2019).

N.F. Polizzi, T. Jiang, D.N. Beratan, and M.J. Therien, "Engineering opposite electronic polarization of singlet and triplet states increases the yield of high-energy photoproducts," *Proc. Natl. Acad. Sci. (USA)*, 116, 14465-14470 (2019).

X. Ru, P. Zhang, and D.N. Beratan, "Assessing possible mechanisms of micrometer scale electron transfer in heme free *Geobacter sulfurreducens* pili," *J. Phys. Chem. B*, 123, 5035-5047 (2019).

R.D. Teo, R. Wang, E.R. Smithwick, A. Migliore, M.J. Therien, D.N. Beratan, "Mapping hole hopping escape routes in proteins," *Proc. Natl. Acad. Sci. (USA)*, 116, 15811-15816 (2019).

J.L. Yuly, C.E. Lubner, P. Zhang, D.N. Beratan, J.W. Peters, "Electron bifurcation: progress and grand challenges," *Chem. Commun.*, 55, 11823-11832 (2019).

S. Banziger, X. Li, J. Valdiviezo, M. Zeller, P. Zhang, D.N. Beratan, I.V. Rubtsov, T. Ren, "Unsymmetrical bis-alkynyl complexes based on Co(III)(cyclam): Synthesis, ultrafast charge separation, and analysis," *Inorg. Chem.*, 58, 15487-15497 (2019).

## **2018**

R.D. Teo, K. Terai, A. Migliore, and D.N. Beratan, "Electron transfer characteristics of 2'-deoxy-2'-fluoro-arabinonucleic acid, a nucleic acid with enhanced chemical stability," *PCCP* 20, 26063-26067 (2018).

B.P. Bloom, R. Liu, P. Zhang, S. Ghosh, R. Naaman, D.N. Beratan, and D.H. Waldeck, "Directing charge transfer in quantum dot assemblies," *Acc. Chem. Res.*, 51, 2565-2573 (2018).

S.S. Skourtis and D.N. Beratan, "Editorial Overview: Biological pathways for electrons, protons, and photo-excitations," *Curr. Op. Chem. Biol.*, 47, A1-A3 (2018).

L.C. Seefeldt, J.W. Peters, D.N. Beratan, B. Bothner, S. D. Minteer, S. Raugei, B.M. Hoffman, "Control of electron transfer in nitrogenase," *Curr. Op. Chem. Biol.*, 47, 54-59 (2018).

L.C. Seefeldt, B.M. Hoffman, J.W. Peters, S. Raugei, D.N. Beratan, E. Antony, and D.R. Dean, "Energy transduction in nitrogenase," *Acc. Chem. Res.*, 51, 2179-2186 (2018).

J.W. Peters, D.N. Beratan, B. Bothner, C.S. Harwood, Z.M. Heiden, R. Hille, A.K. Jones, P.W. King, Y. Lu, C.E. Lubner, S.D. Minteer, S. Raugei, L.C. Seefeldt, M.W.W. Adams, "A new era for electron bifurcation," *Curr. Op. Chem. Biol.*, 47, 32-38 (2018)

Z. Ma, P. Antoniou, P. Zhang, S.S. Skourtis, D.N. Beratan "A non-equilibrium molecular dynamics study of infra-red perturbed electron transfer," *JCTC*, 14, 4818-4832 (2018).

Z. Ma, Z. Lin, C. M. Lawrence, I. V. Rubtsov, P. Antoniou, S.S. Skourtis, P. Zhang, D.N. Beratan, "How can infra-red excitation both accelerate and slow charge transfer in the same molecule?" *Chem. Sci.*, 9, 6395-6405 (2018).

R. Sha, L. Xiang, C. Liu, A. Balaeff, Y. Zhang, P. Zhang, Y. Li, D.N. Beratan, N-J. Tao, and N.C. Seeman, "Charge splitters and charge transport junctions based on guanine quadruplexes," *Nature Nanotechnol.*, 13, 316-321 (2018).

B.J.G. Rousseau, S. Shafei, A. Migliore, R.J. Stanley, D.N. Beratan, "Determinants of Photolyase's DNA repair mechanism in mesophiles and extremophiles," *J. Am. Chem. Soc.*, 140, 2853-2861 (2018).

R. Liu, B.P. Bloom, D.H. Waldeck, P. Zhang, and D.N. Beratan, "Improving solar cell performance using quantum dot triad charge-separation engines," *J. Phys. Chem. C*, 122, 5924-5934 (2018).

J. W. Peters, D.N. Beratan, G.J. Schut, and M.W.W. Adams, "On the nature of organic and inorganic redox cofactors that bifurcate electrons, coupling exergonic and endergonic redox reactions," *Chem. Comm.*, 54, 4091-4099 (2018).

## **2017**

D.N. Beratan, R. Naaman, and D.H. Waldeck, "Charge and spin transport through nucleic acids," *Curr. Opin. Electrochem.*, 4, 175-181 (2017).

N.F. Polizzi, Y. Wu, T. Lemmin, S-Q. Zhang, J. Rawson, D.N. Beratan, M.J. Therien, W.F. DeGrado, "Strategy for designing hyperstable, non-natural protein-cofactor complexes with sub-Å accuracy," *Nature Chem.*, 9, 1157-1164 (2017).

P. Zhang, J. Yuly, C.E. Lubner, D.W. Mulder, P.W. King, J.W. Peters, and D.N. Beratan, "Electron bifurcation: Thermodynamics and kinetics of multi-electron brokering in biological redox chemistry," *Acc. Chem. Res.*, 50, 2410-2417 (2017).

Y. Bai, J. Rawson, S.A. Roget, J-H. Olivier, J. Lin, P. Zhang, D.N. Beratan and M.J. Therien, "Controlling the excited-state dynamics of low band gap, near-infrared absorbers via proquinoidal unit electronic structural modulation," *Chem. Sci.*, 8, 5889-5901 (2017).

B.P. Bloom, B.M. Graff, S. Ghosh, D.N. Beratan and D.H. Waldeck, Chirality control of electron transfer in quantum dot assemblies, *J. Am. Chem. Soc.*, 139, 9038-9043 (2017).

R. Liu, B.P. Bloom, D.H. Waldeck, P. Zhang, and D.N. Beratan, Controlling electron-transfer kinetics of quantum-dot assemblies, *J. Phys. Chem. C*, 121, 14401-14412 (2017).

E. Beall, S. Ulku, C. Liu, E. Wierzbinski, Y. Zhang, Y. Bae, P. Zhang, C. Achim, D.N. Beratan, and D.H. Waldeck, "Effects of the backbone and chemical linker on the molecular conductance of nucleic acid duplexes," *J. Am. Chem. Soc.*, 139, 6726-6735 (2017).

## **2016**

A. Nayak, J. Park, K. De Mey, X. Hu, T.V. Duncan, D.N. Beratan, K. Clays, M.J. Therien, "Large hyperpolarizabilities at telecommunication-relevant wavelengths in donor-acceptor-donor nonlinear optical chromophores," *ACS Cent. Sci.*, 2, 954-966 (2016).

N.F. Polizzi, M.J. Therien, D.N. Beratan, Mean first passage times in biology, *Isr. J. Chem.*, 56, 816-824 (2016).

D.N. Beratan and D.H. Waldeck, "DNA Charge transfer: hot holes break the speed limit," *Nature Chem.*, 8, 992-993 (2016).

S.S. Skourtis, C. Liu, P. Antoniou, A.M. Virshup, and D.N. Beratan, "Dexter energy transfer pathways," *Proc. Natl. Acad. Sci. (USA)*, 113, 8115-8120 (2016).

C. Liu, L. Xiang, Y. Zhang, P. Zhang, D.N. Beratan, Y. Li, and N-J. Tao, Engineering nanometer-scale coherence in soft matter," *Nature Chem.*, 8, 941-945 (2016).

Y. Zhang, W.B. Zhang, C. Liu, P. Zhang, A. Balaeff, and D.N. Beratan, "DNA charge transport: moving beyond 1D," *Surf. Sci.*, 652, 33-38 (2016).

C. Liu, D.N. Beratan, and P. Zhang, and "Coarse-grained theory of biological charge transfer with spatially and temporally correlated noise," *J. Phys. Chem. B*, 120, 3624-3633 (2016).

C. Rupakheti, R. Al-Saadon, P. Zhang, A.M. Virshup, W. Yang, D.N. Beratan, "Diverse optimal molecular libraries for organic light emitting diodes," *J. Chem. Theory Comp.*, 12, 1942-1952 (2016).

N.F. Polizzi, M.J. Eibling, J.M. Perez-Aguilar, J. Rawson, C.J. Lanci, H. C. Fry, D.N. Beratan, J.G. Saven, M. J. Therien, "Photoinduced electron transfer elicits a change in the static dielectric constant of a *de novo* designed protein," *J. Am. Chem. Soc.*, 138, 2130-2133 (2016).

L. Zheng, A.R. Dave, N.F. Polizzi, A. Migliore, D.N. Beratan, "Where is the electronic oscillator strength? Mapping oscillator strength across molecular absorption spectra," *J. Phys. Chem. A*, 120, 1933-1943 (2016).

## **2015**

N.F. Polizzi and D.N. Beratan, "Open-access, interactive exploration for teaching and learning quantum dynamics," *J. Chem. Ed.*, 92, 2161-2164 (2015).

N.F. Polizzi, A. Migliore, M.J. Therien, and D.N. Beratan, "Defusing redox bombs?" *Proc. Natl. Acad. Sci.*, 112, 10821-10822 (2015).

Y. Zhang, R. Young, A.K. Thazhathveetil, A. Singh, C. Liu, Y.A. Berlin, F.C. Grozema, F.D. Lewis, M.A. Ratner, N. Renaud, K. Siriwong, A. Voityuk, M.R. Wasielewski, D.N. Beratan, "Conformationally gated charge transfer in DNA three-way junctions," *J. Chem. Phys. Lett.*, 6, 2434-2438 (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 Trans.*, 44, 8609-8616 (2015).

J. Lin, D. Balamurugan, P. Zhang, S.S. Skourtis, and D.N. Beratan, "Two-electron transfer pathways," *J. Phys. Chem. B.*, 119, 7589-7597 (2015).

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*, 17, 30854-30866 (2015).

A. Migliore, R. Naaman, D.N. Beratan, "Sensing of molecules using quantum dynamics," *Proc. Natl. Acad. Sci.*, 112, E2419-E2428 (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.

Wasielowski, "Charge Transport Across DNA-based Three-Way Junctions," *J. Am. Chem. Soc.*, 137, 5113-5122 (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).

## **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, "Biological charge transfer via flickering resonance," *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," *Chem. Revs.*, 114, 3381-3465 (2014).

A.E. Kuznetsov and D.N. Beratan, "Structural and electronic properties of bare and capped Cd<sub>33</sub>Se<sub>33</sub> and Cd<sub>33</sub>Te<sub>33</sub> 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*, 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.A. Kent, B.P. Mehl, J.M. Papanikolas, T.J. Meyer, Thomas; W. Lin, S.S. Skourtis, M. Constantinou, "Triplet excitation energy dynamics in metal-organic frameworks," *J. Phys. Chem. C*, 117, 22250-22259 (2013).

A. Virshup, J. Contreras-García, 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). 200

E. Wierzbinski, R. Venkatramani, K.L. 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, A. Kuznetsov, J.M. Nocek, B.M. Hoffman, B.R. Crane, X. Hu, 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<sub>n</sub>Se<sub>n</sub>/Cd<sub>n</sub>Te<sub>n</sub> 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*<sub>5</sub>] 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<sub>n</sub>Se<sub>n</sub>/Cd<sub>n</sub>Te<sub>n</sub> nanoparticles (n=6,9)," *J. Phys. Chem. C*, 116, 6817-6830 (2012).

N. Jiang, G. Zuber, S. Keinan, A. Nayak, W. Yang, M.J. Thierien, D.N. Beratan, "Design of coupled porphyrin chromophores with unusually large hyperpolarizability," *J. Phys. Chem. C*, 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*, 115, 9377-9391 (2011).

K. Susumu, J.A.N. Fisher, J. Zheng, D.N. Beratan, A.G. Yodh, and M.J. Thierien, 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*, 115, 5510-5518 (2011).

J. Contreras-García, E.R. Johnson, S. Keinan, R. Chaudret, J-P. Piquemal, D.N. Beratan, W. Yang, R. Chaudret, "NCIPLLOT: 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, "Nucleic acid charge transfer: Black, white, and gray," *Coord. Chem. Revs.*, 255, 635-648 (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 transfer pathways," discussion paper for the 22<sup>nd</sup> Solvay Conference on Chemistry on 'Quantum effects in chemistry and biology', *Procedia Chemistry*, 3, 99-104 (2011).

M.A. Wolak, A. Balaeff, S. Gutmann, H.J. Helmrach, 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**

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 (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.*, 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).

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 Carlo 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)-4H-1-Benzopyran-4-Ones as Isoform-Selective PKC- $\zeta$  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 with experiment to address 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, “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, R.R. Gil, M. Madrid, C. Achim, "Solution structure of a peptide nucleic acid duplex 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 Raman optical activity computations," *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).

S.S. Skourtis, T.R. Prytkova, D.N. Beratan, "Flavin charge transfer transitions assist DNA photolyase charge transfer," AIP Conf. Proc., 963, 674-677 (2007).

S.S. Skourtis, D.N. Beratan, "A molecular double slit paradigm," AIP Conf. Proc., 963, 809-812 (2007).

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

S.S. Skourtis and D.N. Beratan, "Photosynthesis from the protein's perspective," Science, 316, 703-704 (2007).

T.R. Prytkova, S.S. Skourtis, D.N. Beratan, "Photoselected electron transfer pathways in DNA photolyase," Proc. Natl. Acad. Sci. (USA), 104, 802-807 (2007).

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.B. George, G. Zuber, R. Naaman, D.H. Waldeck, P. Wipf, D.N. Beratan, and, "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).

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, 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).

S.S. Skourtis and D.N. Beratan, "Guest Editorial: Electron Transfer," *Mol. Sim.*, 32, 675-676 (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).

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).

M. Galperin and D.N. Beratan, "Simulation of STM images of 1,3 cyclohexadiene bound to a silicon surface," *J. Phys. Chem. B*, 109, 1473-1480 (2005).

T. Prytkova, I.V. Kurnikov, and D.N. Beratan, "Ab initio based calculations of electron transfer rates in metalloproteins," *J. Phys. Chem. B*, 109, 1618-1625 (2005).

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

S. S. Skourtis, I.A. Balabin, T. Kawatsu, and D.N. Beratan, "Protein dynamics and electron transfer: electronic decoherence and non-Condon effects," *Proc. Natl. Acad. Sci. (USA)*, 102, 3552-3557 (2005).

J. Lin and D.N. Beratan, "Simulation of electron transfer between cytochrome  $c_2$  and the bacterial photosynthetic reaction center: Brownian dynamics analysis of the native protein and double mutants," *J. Phys. Chem. B*, 109, 7529-7534 (2005).

J. Lee, I. Balabin, D.N. Beratan, J-G. Lee, and J.T. Yates, Jr., "Charge transfer through chemisorbed organic molecules – neutralization of ionization processes at local sites in the molecule," *Chem. Phys. Lett.*, 412, 171-175 (2005).

J. Zheng, Y.K. Kang, M.J. Therien, and D.N. Beratan, "Generalized Mulliken-Hush analysis of electronic coupling interactions in compressed  $\pi$ -stacked porphyrin-bridge-quinone systems" *J. Am. Chem. Soc.*, 127, 11303-11310 (2005).

G. Zuber, M.R. Goldsmith, D.N. Beratan, and P. Wipf, "Assignment of the Absolute Configuration of  $[n]$ -Ladderanes by TD-DFT Optical Rotation Calculations," *Chirality*, 17, 507-510 (2005).

## **2004**

Z-X. Liang, I.V. Kurnikov, J.M. Nocek, A.G. Mauk, D.N. Beratan, and B.M. Hoffman, "Dynamic docking and electron transfer between cytochrome  $b_5$  and a suite of myoglobin surface-charge mutants. Introduction of a functional-docking algorithm for protein-protein complexes," *J. Am. Chem. Soc.*, 126, 2785-2798 (2004).

I.V. Rubtsov, Y.K. Kang, N.P. Redmore, R.M. Allen, J. Zheng, D.N. Beratan, and M.J. Therien, "The degree of charge transfer in ground and charge-separated states revealed by ultrafast visible pump/mid-IR probe spectroscopy," *J. Am. Chem. Soc.*, 126, 5022-5023 (2004).

Y.A. Berlin, I.V. Kurnikov, M.A. Ratner, and A.L. Burin, and D.N. Beratan, "DNA electron transfer processes: some theoretical notions," *Top. Curr. Chem.*, 237, 1-36 (2004).

J. Lin and D.N. Beratan, "Tunneling while pulling: the dependence of tunneling current on end-to-end distance in a flexible molecule," *J. Phys. Chem. B*, 108, 5655-5661 (2004).

J-L. Liao and D.N. Beratan, "How does protein architecture facilitate the transduction of ATP chemical-bond energy into mechanical work? The cases of nitrogenase and ATP binding cassette proteins," *Biophys. J.*, 87, 1369-1377 (2004).

J.L. Perry, M.R. Goldsmith, M. Peterson, D.N. Beratan, G. Wozniak, F. Rüker, M. Dockal, J.D. Simon, "Structure of the ochratoxin A binding site within human serum albumin," *J. Phys. Chem. B*, 108, 16960-16964 (2004).

S.S. Skourtis, D.H. Waldeck, and D.N. Beratan, "Inelastic electron tunneling erases coupling-pathway interferences," *J. Phys. Chem. B*, 108, 15511-15518 (2004).

## **2003**

D.N. Beratan, "Molecular control of electron transfer events within and between biomolecules," in *Molecular electronics: biosensors and biocomputers*, L. Barsanti, V.

Evangelista, P. Gualtieri, V. Passarelli, and S. Vestri, eds., Kluwer Academic Publishers, 2003, pp 227-236.

J.L. Perry, T. Christensen, M.R. Goldsmith, E.J. Toone, D.N. Beratan, and J.D. Simon, "Binding of Ochratoxin A to human serum albumin stabilized by a protein-ligand ion pair," *J. Phys. Chem. B*, 107, 7884-7888 (2003).

M.R. Goldsmith, P. Wipf, and D.N. Beratan, "Optical rotation of non-covalent aggregates," *J. Am. Chem. Soc.*, 125, 15696-15697 (2003).

## **2002**

D.N. Beratan, R.K. Kondru, and P. Wipf, "Optical activity: from structure-function to structure prediction," in ACS Symposium Series, *Physical Chemistry of Chirality*, J. Hicks, editor, 2002, 104-118.

I.V. Kurnikov, G.S.M. Tong, M. Madrid, and D.N. Beratan, "Hole size and energetics in oxidized double helical DNA: competition between quantum delocalization and solvation localization," *J. Phys. Chem. B*, 106, 7-10 (2002).

Z-X. Liang, J.M. Nocek, K.H. Huang, R.T. Hayes, I.V. Kurnikov, and D.N. Beratan, and B.M. Hoffman, "Dynamic docking and electron transfer between Zn-myoglobin and cytochrome *b<sub>5</sub>*," *J. Am. Chem. Soc.*, 124, 6849-6859 (2002).

G.S.M. Tong, I.V. Kurnikov, and D.N. Beratan, "Tunneling energy effects on GC oxidation in DNA," *J. Phys. Chem. B*, 106, 2381-2392 (2002).

M.L. Jones, I.V. Kurnikov, and D.N. Beratan, "The nature of tunneling pathway and average packing density models for protein-mediated electron transfer," *J. Phys. Chem. A*, 106, 2002-2006 (2002).

F.D. Lewis, J. Liu, W. Weigel, W. Rettig, I.V. Kurnikov, and D.N. Beratan, "Donor-bridge-acceptor energetics determine the distance dependence of electron tunneling in DNA," *Proc. Natl. Acad. Sci. (USA)*, 99, 12536-12541 (2002).

## **2001**

K.M. Specht, J. Nam, D.M. Ho, N. Berova, R.K. Kondru, D.N. Beratan, P. Wipf, R.A. Pascal Jr., D. Kahne, "Determining absolute configuration in flexible molecules: a case study," *J. Am. Chem. Soc.*, 123, 8961-8966 (2001).

I.V. Kurnikov, A.K. Charnley, and D.N. Beratan, "From ATP to electron transfer: electrostatics and free energy transduction in nitrogenase," *J. Phys. Chem. B*, 105, 5359-5367 (2001).

T.L. Perry, A. Dickerson, A.A. Khan, M. Kelley, R.K. Kondru, D.N. Beratan, R.K. Kondru, P. Wipf, M.T. Hamann, "New peroxy lactones from a Jamaican marine sponge

of the genus *Plakortis onkodes*, with inhibitory activity against the AIDS opportunistic infection *Toxoplasma gondii*," *Tetrahedron*, 57, 1483-1487 (2001).

S.S. Skourtis and D.N. Beratan, "Chapter 3: Single and multi-electron transfer processes," in *Electron Transfer Reactions: Theory & Principles*, Wiley-VCH (Weinheim), V. Balzani editor, 2001. pp 109-125.

G.C. Walker and D.N. Beratan, "Electron Transfer Reactions," in *Encyclopedia of Chemical Physics and Physical Chemistry*, Institute of Physics Publishing, editors: J. Moore and N. Spencer, Institute of Physics Press, 2001.

## **2000**

R.K. Kondru, D.N. Beratan, G.K. Friestad, A.B. Smith III, and P. Wipf and, "Chiral action at a distance: remote substituent effects on the optical activity of Calyculins A and B," *Org. Lett.*, 2, 1509-1512 (2000).

S. Ribe, R.K. Kondru, D.N. Beratan, and P. Wipf, "Optical rotation computation, total synthesis, and stereochemistry assignment of the marine natural product Pitiamide A," *J. Am. Chem. Soc.*, 122, 4608-4617 (2000).

M. Lee, M.J. Shephard, S.M. Risser, S. Priyadarshy, M.N. Paddon-Row, and D.N. Beratan, "The nature of tunnel splitting mediated by stacked aromatics," *J. Phys. Chem. A*, 104, 7593-7599 (2000).

Z-X. Liang, J.M. Nocek, I.V. Kurnikov, D.N. Beratan and B.M. Hoffman, Electrostatic control of electron transfer between myoglobin and cytochrome *b*<sub>5</sub>: effect of methylating the heme propionates of Zn-myoglobin, *J. Am. Chem. Soc.*, 122, 3552-3553 (2000).

E. Babini, I. Bertini, M. Borsari, F. Capozzi, C. Luchinat, X.-Y. Zhang, G.L.C. Moura, I.V. Kurnikov, D.N. Beratan, A. Ponce, A.J. DiBilio, J.R. Winkler, and H.B. Gray "Bond-mediated electron tunneling in ruthenium-modified high-potential iron-sulfur protein," *J. Am. Chem. Soc.*, 122, 4532-4533 (2000).

## **1999**

R.K. Kondru, C.H.-T. Chen, D.P. Curran, P. Wipf and D.N. Beratan, "Determination of the absolute configuration of 1,3,5,7-tetramethyl-1,3-dihydroindol-2-one by optical rotation computation," *Tetrahedron: Asymmetry*, 10, 4143-4150 (1999).

R.K. Kondru, P. Wipf, and D.N. Beratan, "Structural and conformational dependence of optical rotation angles," *J. Phys. Chem. A*, 103, 6603-6611 (1999).

L.D. Zusman and D.N. Beratan, "Electron transfer in three-state systems" *J. Chem. Phys.*, 110, 10468-10481 (1999).

S.S. Skourtis and D.N. Beratan, "Theories of structure-function relationships for bridge-mediated electron transfer," *Adv. Chem. Phys.*, 106, 1999, 377-452 (1999).

### **1998**

R.K. Kondru, P. Wipf, and D.N. Beratan, "Atomic contributions to the optical rotation angle as a quantitative probe of molecular chirality," *Science*, 282, 2247-2250 (1998).

D.N. Beratan and S.S. Skourtis, "Protein-mediated electron transfer: pathways, orbital interactions and contact maps." In *Biological electron-transfer chains: Genetics, Composition and Mode of Operation*, G.W. Canters and E. Vijgenboom, eds., Kluwer Academic Publishers, Dordrecht, The Netherlands, 1998, pp 9-27.

S. Priyadarshy, S.M. Risser, and D.N. Beratan, "DNA-mediated electron transfer," *J. Bioinorg. Chem.*, 3, 196-200 (1998).

D.N. Beratan and S.S. Skourtis, "Electron transfer mechanisms," *Curr. Opin. Chem. Biol.*, 2, 235-243 (1998).

R.K. Kondru, P. Wipf, and D.N. Beratan, "Theory assisted determination of absolute stereochemistry for complex natural products via computation of molar rotation angles." *J. Am. Chem. Soc.*, 120, 2204-2205 (1998).

K. Kumar, I.V. Kurnikov, D.N. Beratan, D.H. Waldeck, and M.B. Zimmt, "Use of modern theories to determine electronic coupling matrix elements in intramolecular systems," *J. Phys. Chem. A*, 102, 5529-5541 (1998).

L.D. Zusman and D.N. Beratan, "Electron transfer in the photosynthetic reaction center: mechanistic implications of mutagenesis studies," *Spectrochim. Acta A*, 54A, 1211-1218 (1998).

A. Roitberg, M. Holden, M. Mayhew, I.V. Kurnikov, D.N. Beratan, and V. Vilker, "Binding and electron transfer between putidaredoxin and cytochrome P-450cam. Theory and experiments," *J. Am. Chem. Soc.*, 120, 8927-8932 (1998).

### **1997**

I.V. Kurnikov, L.D. Zusman, M. Kurnikova, R.S. Farid, and D.N. Beratan, "Structural fluctuations, spin, reorganization energy, and tunneling energy control of intramolecular electron transfer: the surprising case of electron transfer in a d<sup>8</sup>-d<sup>8</sup> bimetallic system," *J. Am. Chem. Soc.*, 119, 5690-5700 (1997).

L.D. Zusman and D.N. Beratan, "Structure of the electrical double layer in high-temperature superconductors. Origin of the dip in the double layer capacitance near the superconducting transition," *J. Phys. Chem. B*, 101, 7095-7099 (1997).

L.D. Zusman and D.N. Beratan, "Three-state model for two-electron transfer reactions," *J. Phys. Chem. A*, 101, 4136-4141 (1997).

S.S. Skourtis and D.N. Beratan, "High and low resolution theories of protein electron transfer," *J. Bioinorg. Chem.*, 2, 378-386 (1997).

D.N. Beratan, S. Priyadarshy, and S.M. Risser, "DNA: wire or insulator?" *Chemistry and Biology*, 4, 3-8 (1997).

R.K. Kondru, S. Lim, P. Wipf, and D.N. Beratan, "Synthetic and model computational studies of optical angle additivity for interacting chiral centers. A reinvestigation of van't Hoff's principle," *Chirality*, 9, 469-477 (1997).

J. Wolfgang, S.M. Risser, S. Priyadarshy and, D.N. Beratan, "Secondary structure conformations and long range electronic interactions in oligopeptides," *J. Phys. Chem. B*, 101, 2987-2991 (1997).

S.S. Skourtis and D.N. Beratan, "Electron transfer contact maps," *J. Phys. Chem. B*, 101, 1215-1234 (1997).

J.N. Onuchic, S.M. Risser, S.S. Skourtis, D.N. Beratan, "The design of starburst dendrimer electron transfer systems," in *Molecular Electronics*, M. Ratner and J. Jortner, editors, Chemistry for the 21st Century Series, Blackwell Science, Oxford, 1997. Chapter 12, pp 369-379.

D.N. Beratan, "Molecular control of electron tunneling processes," Chapter 3.2 in *IBC Molecular Nanotechnology Conference Proceedings*, 1997, IBC Press.

### **1996**

I.V. Kurnikov and D.N. Beratan, "Ab initio based effective Hamiltonians for long-range electron transfer: Hartree-Fock analysis," *J. Chem. Phys.*, 105, 9561-9573 (1996).

J.M. Nocek, J. Zhou, S. DeForest, S. Priyadarshy, D. N. Beratan, J.N. Onuchic, B. M. Hoffman, "Theory and practice of electron transfer within protein-protein complexes: Application to the multi-domain binding of cytochrome *c* by cytochrome *c* peroxidase," *Chem. Rev.*, 96, 2459-2489 (1996).

S. Priyadarshy, S.M. Risser, and, D.N. Beratan, "DNA is not a molecular wire: protein-like electron-transfer predicted in an extended pi-electron system," *J. Phys. Chem.*, 100, 17678-17682 (1996).

S. Priyadarshy, S.M. Risser, and, D.N. Beratan, "DNA double helix mediated long range electron transfer," *Int. J. Quantum Chem. Quantum Biol. Symp.*, 60, 1789 -1795 (1996).

S. Priyadarshy, M.J. Therien, and D.N. Beratan, "Acetylenyl-linked, porphyrin-bridged, donor-acceptor molecules: a theoretical analysis of the molecular first hyperpolarizability in highly conjugated push-pull chromophore structures," *J. Am. Chem. Soc.*, 118, 1504-1510 (1996).

S. Priyadarshy, S.S. Skourtis, S.M. Risser, and D.N. Beratan, "Bridge mediated electronic interactions: differences between Hamiltonian and Green function partitioning in a non-orthogonal basis," *J. Chem. Phys.*, 104, 9473-9481 (1996).

C. Kuhn and D.N. Beratan, "Inverse strategies for molecular design," *J. Phys. Chem.*, 100, 10595-10599 (1996).

D.N. Beratan and J.N. Onuchic, "Chapter 2: The protein bridge between redox centers," in *Protein Electron Transfer*, D.S. Bendall, editor, BIOS Scientific Publishers, Oxford, pp 23-42, 1996.

J.N. Onuchic and D.N. Beratan, "Appendix A: Electron transfer rate calculations," in *Protein Electron Transfer*, D.S. Bendall, editor, Bios Scientific Publishers, Oxford, pp 273-283, 1996.

S.S. Skourtis, J.N. Onuchic, and D.N. Beratan, "A method to analyze multi-pathway effects on protein mediated donor-acceptor coupling interactions," *Inorg. Chim. Acta*, 243, 167-175 (1996).

L.D. Zusman and D.N. Beratan, "Two-electron transfer reactions in polar solvents," *J. Chem. Phys.*, 105, 165-176 (1996).

### **1995**

D.R. Casimiro, D.N. Beratan, J.N. Onuchic, J.R. Winkler, and H.B. Gray, "Donor-acceptor electronic coupling in ruthenium-modified heme proteins" in *Mechanistic Bioinorganic Chemistry*, H. Thorp and V. Pecoraro, eds., ACS Symp. Series, pp. 471-485, Washington, DC, 1995.

A.J.A. Aquino, P. Beroza, D.N. Beratan, and J.N. Onuchic, "Docking and electron transfer between cytochrome  $c_2$  and the photosynthetic reaction center," *Chem. Phys.*, 197, 277-288 (1995).

W.B. Curry, M.D. Grabe, I.V. Kurnikov, S.S. Skourtis, D.N. Beratan, J.J. Regan, A.J.A. Aquino, P. Beroza, and J.N. Onuchic, "Pathways, pathway tubes, pathway docking and propagators in electron transfer proteins," *J. Bioenerg. Biomemb.*, 27, 285-293 (1995).

S.M. Risser and D.N. Beratan, "What is the anharmonicity of a molecule's electronic wave function?" *J. Phys. Chem.*, 99, 1935-1942 (1995).

### **1993**

S.M. Risser, D.N. Beratan, and T.J. Meade, "Electron transfer in DNA: predictions of both exponential growth and decay of coupling with distance," *J. Am. Chem. Soc.*, 115, 2508-2510 (1993).

S.M. Risser, D.N. Beratan, and S.R. Marder, "Structure function relationships for  $\beta$ , the first molecular hyperpolarizability," *J. Am. Chem. Soc.*, 115, 7719-7728 (1993).

S.M. Risser, D.N. Beratan, and J.N. Onuchic, "Electronic coupling in starburst dendrimers: connectivity, disorder, and finite size effects in macromolecular Bethe lattices," *J. Phys. Chem.*, 97, 4523-4527 (1993).

D.H. Waldeck and D.N. Beratan, "Molecular electronics: observation of molecular Rectification," *Science*, 261, 576-578 (1993).

S.S. Skourtis, D.N. Beratan, and J.N. Onuchic, "The two-state reduction for electron and hole transfer in bridge mediated electron-transfer reactions," *Chem. Phys.*, 176, 501-520 (1993).

J.J. Regan, S.M. Risser, D.N. Beratan, and J.N. Onuchic, "Protein electron transport: single versus multiple pathways," *J. Phys. Chem.*, 97, 13083-13088 (1993).

### **1992**

D.N. Beratan, J.N. Onuchic, J.R. Winkler, and H.B. Gray, "Electron tunneling pathways in proteins," *Science*, 258, 1740-1741 (1992).

D.N. Beratan, J.N. Betts and J.N. Onuchic, "Tunneling pathway and redox state dependent electronic couplings at nearly fixed distance in electron transfer proteins," *J. Phys. Chem.*, 96, 2852-2855 (1992).

J.N. Betts, D.N. Beratan, and J.N. Onuchic, "Mapping electron tunneling pathways: an algorithm that finds the 'minimum length'/ maximum coupling pathway between electron donors and acceptors in proteins," *J. Am. Chem. Soc.*, 114, 4043-4046 (1992).

J.N. Onuchic, D.N. Beratan, J.R. Winkler, H.B. Gray, "Pathway analysis of protein electron-transfer reactions," *Ann. Rev. Biophys. Biomol. Struct.*, 21, 349-377 (1992).

J.J. Regan, D.N. Beratan, and J.N. Onuchic, "Finding electron transfer pathways," in *Princeton Lectures on Biophysics*, W. Bialek, ed., World Scientific Publishing Co., 1992, pp. 175-195.

D.N. Beratan, and J.N. Onuchic "Structural control of electron transfer in proteins," in *The molecular basis of oxidative damage by leukocytes*, A.J. Jesaitis and E.A. Dratz, eds., CRC Press, Boca Raton, pp. 57-67, 1992.

S.R. Marder, D.N. Beratan, and L-T. Cheng, "Structure/property relationships for molecular second-order nonlinear optics," *Molecular Electronics - Science and Technology*, AIP Conf. Proc. 262, 252-264 (1992).

D.N. Beratan, "Molecular electronic device concepts," in *1992 Encyclopedia of Physical Science and Technology*, Academic Press, Vol 10, pp. 411-417

### **1991**

D.N. Beratan, J.N. Betts, and J.N. Onuchic, "Protein electron transfer rates set by the bridging secondary and tertiary structure," *Science*, 252, 1285-1288 (1991).

S.R. Marder, D.N. Beratan, and L-T. Cheng, "Approaches for optimizing the first electronic hyperpolarizability of conjugated organic molecules," *Science*, 252, 103-106 (1991).

J.N. Onuchic and P.C.P. de Andrade, and D.N. Beratan, "Electron tunneling pathways in proteins: a method to compute tunneling matrix elements in very large systems," *J. Chem. Phys.*, 95, 1131-1138 (1991).

D.N. Beratan, J.N. Onuchic and J.J. Hopfield, "Design of a molecular memory device: the electron transfer shift register memory," in *Towards the Biochip*, C. Nicolini, editor, World Publishing Company, New Jersey, 1990, pp. 107-118.

S.R. Marder, B.G. Tiemann, D.N. Beratan, L-T. Cheng, and W. Tam, "Structure property relationships for organic and organometallic materials with second-order nonlinearities," in *Organic Materials for Nonlinear Optics*, II, R.A. Hann and D. Bloor, editors, Royal Society of Chemistry, Cambridge, pp. 165-175, 1991.

D.N. Beratan, "Electronic hyperpolarizability and chemical structure: a tutorial," in *ACS Symposium Series vol. 455, New Materials for Nonlinear Optics*, S.R. Marder, J.E. Sohn, and G.D. Stucky, editors, pp. 89-102, 1991.

D.N. Beratan, J.N. Onuchic, and H.B. Gray, "Electron tunneling pathways in proteins," in *Metal Ions in Biological Systems*, vol. 27, H. Sigel and A. Sigel, eds., Marcel Dekker Press, New York, 1991, pp. 97-127, 1991.

D.N. Beratan and J.N. Onuchic, "Electron tunneling pathways: from model compounds to proteins," in *ACS Advance in Chemistry Series vol. 228, Electron transfer in inorganic, organic, and biological systems*, J.R. Bolton, N. Mataga, G. McLendon, eds., pp. 71-90, 1991.

D.N. Beratan, "Molecular electronic device concepts," in *1991 Encyclopedia of Physical Science and Technology Yearbook*, Academic Press, pp. 359-364.

S.R. Marder, L-T. Cheng, and B.G. Tiemann, and D.N. Beratan, "Structure/property relationships for molecular second-order nonlinear optics," Proceedings of SPIE-The Society of Photo-Optical Instrumentation Engineers, 1560, 86-97 (1991).

### **1990**

J.N. Onuchic and D.N. Beratan, "A predictive theoretical model for electron tunneling pathways in proteins," J. Chem. Phys., 92, 722-733 (1990).

D.N. Beratan, J.N. Onuchic, J.N. Betts, B. Bowler, and H.B. Gray, "Electron mediation pathways in ruthenated proteins," J. Am. Chem. Soc., 112, 7915-7921 (1990).

D.N. Beratan, "Controlled electron transfer for molecular electronics," Mol. Cryst. Liq. Cryst., 190, 85-94 (1990).

### **1989**

D.N. Beratan and J.N. Onuchic, "Electron tunneling pathways in proteins: influences on the transfer rate," Photosynthesis Res., 22, 173-186 (1989).

D.N. Beratan, J.N. Onuchic, and J.J. Hopfield, "Information storage at the molecular level: the design of a molecular shift register memory," J. British Interplan. Soc., 42, 468-473 (1989).

D.N. Beratan, "Influence of gap states on the nonresonant second hyperpolarizabilities of conjugated organic polymers," J. Phys. Chem., 93, 3915-3920 (1989).

J.J. Hopfield and J.N. Onuchic, and D.N. Beratan, "Electronic shift register memory based on molecular electron transfer reactions," J. Phys. Chem., 93, 6350-6357 (1989).

D.N. Beratan, J.N. Onuchic and J.J. Hopfield, "Design of a true molecular electronic device: the electron transfer shift register memory," in *Molecular Electronics - Biosensors and Biocomputers*, F.T. Hong, editor, Plenum Press 1989, pp. 353-360. 20

D.N. Beratan, J.N. Onuchic and J.J. Hopfield, "Design of a molecular memory device based on electron transfer reactions," in *Molecular Electronics: Science and Technology*, Engineering Foundation, New York, 1989, pp. 331-337.

D.N. Beratan, M.A. Lee, D.W. Allender, and S. Risser, "Structural dependence of the pi-electron contributions to the optical second hyperpolarizability of linear conjugated organic molecules," Proceedings of SPIE-The Society of Photo-Optical Instrumentation Engineers, 1080, 101-107 (1989).

### **1988**

J.A. Cowan, R.K. Upmacis, D.N. Beratan, J.N. Onuchic, and H.B. Gray, "Long-range electron transfer in myoglobin," Ann. NY Acad. Sci., 550, 68-84 (1988).

J.J. Hopfield, J.N. Onuchic, D.N. Beratan, "A molecular shift register based on electron transfer," *Science*, 241, 817-820 (1988).

D.N. Beratan and J.N. Onuchic, "Adiabaticity and nonadiabaticity in bimolecular outer-sphere charge transfer reactions," *J. Chem. Phys.*, 89, 6195-6203 (1988).

J.N. Onuchic and D.N. Beratan, "Adiabaticity criteria for outer-sphere bimolecular electron transfer reactions," *J. Phys. Chem.*, 92, 4817-4820 (1988).

J.W. Perry, A.E. Stiegman, S.R. Marder, D.R. Coulter, D.N. Beratan, D.E. Brinza, F.L. Klavetter, R.H. Grubbs, "Second and third order nonlinear optical properties of conjugated molecules and polymers," *Proceedings of SPIE-The Society of Photo-Optical Instrumentation Engineers*, 971, 17-24 (1988).

### **1987**

D.N. Beratan, J.N. Onuchic and J.J. Hopfield, "Through bond and through space limits of the long distance electron transfer problem," in *Protein Structure, Molecular and Electronic Reactivity*, by R. Austin, *et al.*, eds. 1987, p. 488.

J.N. Onuchic and D.N. Beratan, "Molecular bridge effects on distant charge tunneling," *J. Am. Chem. Soc.*, 109, 6771-6778 (1987).

D.N. Beratan, J.N. Onuchic, and J.W. Perry, "Non-linear susceptibilities of finite organic polymers," *J. Phys. Chem.*, 91, 2696-2698 (1987).

D.N. Beratan, J.N. Onuchic and J.J. Hopfield, "Electron tunneling through covalent and non-covalent pathways in proteins," *J. Chem. Phys.*, 86, 4488-4498 (1987).

### **1986**

J.N. Onuchic, D.N. Beratan, and J.J. Hopfield, "Some aspects of electron transfer reaction dynamics," *J. Phys. Chem.*, 90, 3707-3721 (1986).

D.N. Beratan, "Electron tunneling through rigid molecular bridges: bicyclo[2.2.2]octane," *J. Am. Chem. Soc.*, 108, 4321-4326 (1986).

D.N. Beratan, "The theory of long distance electron transfer reactions," Ph.D. Thesis, California Institute of Technology (1986).

### **1985**

D.N. Beratan, J.N. Onuchic and J.J. Hopfield, "Limiting forms of the tunneling matrix element in the long distance bridge mediated electron transfer problem," *J. Chem. Phys.*, 83, 5325-5329 (1985).

### **1984**

D.N. Beratan and J.J. Hopfield, "Failure of the Born-Oppenheimer and Franck-Condon approximations for long distance electron transfer rate calculations," *J. Chem. Phys.* 81, 5753-5759 (1984).

D.N. Beratan and J.J. Hopfield, "Calculation of electron tunneling matrix elements in rigid systems: The mixed valence dithiaspirocyclobutane molecules," *J. Am. Chem. Soc.*, 106, 1584-1894 (1984).

### **1982**

W.L. Luken and D.N. Beratan, "Localized orbitals and the Fermi hole," *Theor. Chim. Acta*, 61, 265-281 (1982).

### **1980**

D.N. Beratan and W.L. Luken, "Electron Correlation and the Chemical Bond," Freewater Film Productions, Durham, NC, 1980.

<https://www.youtube.com/watch?v=4EORz9EM45w>

### **Patents, New Technology Disclosures, and Software**

- Electron bifurcation devices, New technology disclosure, 12/19
- ACSESS and PB-ACSESS: Software to construct diversity oriented molecular libraries.
- "Methods and systems for selecting molecular structures," provisional patent application submitted 2/16/07.
- *Pathways*, a program to identify electron-tunneling pathways in proteins, on file with COSMIC, the NASA software center, *NASA Tech Briefs*, 1994. This software is available as a plugin to the NAMD software package.
- Molecular Implementation of a Molecular Shift Register based on Electron Transfer, *NASA Tech Briefs* 14, 55 (1990). US Patent No. 5,016,063 issued May 14, 1991.
- A New Design Strategy for Molecules with Enhanced Hyperpolarizabilities Based on "Defect"-like States in Conjugated Polymers. US Patent No. 5,011,907 issued April 30, 1991.
- All Optical Photochromic Spatial Light Modulators based on Photoinduced Electron Transfer in Rigid Matrices, *NASA Tech Briefs* 13, 44 (1989). US Patent No. 5,062,693 issued Nov. 5, 1991.

### **Teaching Initiatives at Duke University**

- Developed and taught a function-oriented undergraduate course on Biophysical Chemistry in a "flipped" (active-learning) mode.
- Developed multi-university, web-based early graduate special topics courses.
- Developed electronic notebooks to teach graduate quantum dynamics using *Mathematica* (see: *J. Chem. Ed.* 92, 2161-2164).
- Developed a senior undergraduate Inorganic Chemistry course with emphasis on materials and bioinorganic chemistry.

- Developed freshman seminar course on Science Ethics as part of the “Faces of Science” focus cluster of four courses (with Chemistry, Philosophy, & History).
- Revised the freshman Introduction to Research in Chemistry course, providing an independent opportunity for freshman, coupled to substantive readings and guest lectures about the conduct of modern science.
- Developed an inquiry based first semester Physical Chemistry course, employing electronic and computational elements.
- Developed an Introduction to Molecular Modeling graduate course.

### **Special Teaching Initiatives at University of Pittsburgh**

- Developed *Mathematica* classroom demonstrations and homework assignments for Physical Chemistry using early LCD devices and laptops in the early 1990s.
- Built Joint Chemistry-Physics teaching classroom in 1995, aimed at active learning strategies for Physical Chemistry.
- Contributed to a (funded) Hewlett Foundation Proposal to develop an integrated introductory science course for non-science majors (1997).

### **Professional Associations**

ACS (Fellow), APS (Fellow), AAAS (Fellow), RSC (Fellow), Phi Lambda Upsilon, Sigma Xi inductee (1980)

### **Teaching at Duke University**

- Biophysical Chemistry
- Introduction to Modeling Complex Molecular Materials: From Energy Science to Bioscience
- Quantum Dynamics
- Modeling Charge Transfer and Transport
- Inorganic Chemistry
- Ethical Issues in Science (freshman seminar)
- Introduction to Molecular Modeling
- Statistical Mechanics
- Introduction to Research in Chemistry
- Physical Chemistry

### **Teaching at University of Pittsburgh (1992-2001)**

- Atoms, Molecules and Materials
- Quantum Mechanics
- Statistical Mechanics
- Advanced Quantum Mechanics
- Theory of Materials
- Special topics in Electron Transfer Chemistry
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