David N Beratan

List of Publications by Year
in descending order

259 papers	18,597 citations	12330 69 h-index	14208 128 g-index
271 all docs	271 docs citations	271 times ranked	13376 citing authors

#	Article	IF	Citations
1	Twisted molecular wires polarize spin currents at room temperature. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	8
2	Discovery of the Xenonâ€“Protein Interactome Using Large-Scale Measurements of Protein Folding and Stability. Journal of the American Chemical Society, 2022, 144, 3925-3938.	13.7	7
3	Improving the efficiency of open-quantum-system simulations using matrix product states in the interaction picture. Physical Review A, 2022, 105, .	2.5	5
4	A Chirality-Based Quantum Leap. ACS Nano, 2022, 16, 4989-5035.	14.6	74
5	Synthetic Control of Exciton Dynamics in Bioinspired Cofacial Porphyrin Dimers. Journal of the American Chemical Society, 2022, 144, 6298-6310.	13.7	17
6	Cofactor Dynamics Couples the Protein Surface to the Heme in Cytochrome c, Facilitating Electron Transfer. Journal of Physical Chemistry B, 2022, 126, 3522-3529.	2.6	0
7	Delocalization-Assisted Transport through Nucleic Acids in Molecular Junctions. Biochemistry, 2021, 60, 1368-1378.	2.5	4
8	Temperature Dependence of Charge and Spin Transfer in Azurin. Journal of Physical Chemistry C, 2021, 125, 9875-9883.	3.1	26
9	Why Do Most Aromatics Fail to Support Hole Hopping in the Cytochrome c Peroxidaseâ€“Cytochrome c Complex?. Journal of Physical Chemistry B, 2021, 125, 7763-7773.	2.6	2
10	Oxalate decarboxylase uses electron hole hopping for catalysis. Journal of Biological Chemistry, 2021, 297, 100857.	3.4	5
11	Efficient and reversible electron bifurcation with either normal or inverted potentials at the bifurcating cofactor. CheM, 2021, 7, 1870-1886.	11.7	6
12	Electron ratcheting in self-assembled soft matter. Journal of Chemical Physics, 2021, 155, 055102.	3.0	2
13	Excited-State Dynamics and Nonlinear Optical Properties of Hyperpolarizable Chromophores Based on Conjugated Bis(terpyridyl)Ru(II) and Palladium and Platinum Porphyrinic Components: Impact of Heavy Metals upon Supermolecular Electro-Optic Properties. Inorganic Chemistry, 2021, 60, 15404-15412.	4.0	2
14	Energy transduction by reversible electron bifurcation. Current Opinion in Electrochemistry, 2021, 29, 100767.	4.8	1
15	Charge Transfer and Spin Dynamics in a Zinc Porphyrin Donor Covalently Linked to One or Two Naphthalenediimide Acceptors. Journal of Physical Chemistry A, 2021, 125, 825-834.	2.5	6
16	Multiple hops move electrons from bacteria to rocks. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, e2115620118.	7.1	1
17	Correlation between Charge Transport and Base Excision Repair in the MutYâ€“DNA Glycosylase. Journal of Physical Chemistry B, 2021, 125, 17-23.	2.6	4
18	Mechanism of Side Chain-Controlled Proton Conductivity in Bioinspired Peptidic Nanostructures. Journal of Physical Chemistry B, 2021, 125, 12741-12752.	2.6	3

#	Article	IF	Citations
19	Mutation effects on charge transport through the p58c ironâ€“sulfur protein. Chemical Science, 2020, 11, 7076-7085.	7.4	5
20	Electrostatic Field-Induced Oscillator Strength Focusing in Molecules. Journal of Physical Chemistry B, 2020, 124, 6376-6388.	2.6	5
21	Predicting Dexter Energy Transfer Interactions from Molecular Orbital Overlaps. Journal of Physical Chemistry C, 2020, 124, 18956-18960.	3.1	15
22	A robust bioderived wavelength-specific photosensor based on BLUF proteins. Sensors and Actuators B: Chemical, 2020, 310, 127838.	7.8	4
23	Autobiography of David N. Beratan. Journal of Physical Chemistry B, 2020, 124, 3441-3446.	2.6	0
24	Conductance and Configuration of Molecular Gold-Water-Gold Junctions under Electric Fields. Matter, 2020, 3, 166-179.	10.0	21
25	Revisiting the Hole Size in Double Helical DNA with Localized Orbital Scaling Corrections. Journal of Physical Chemistry B, 2020, 124, 3428-3435.	2.6	5
26	Symmetry controlled photo-selection and charge separation in butadiyne-bridged donorâ€“bridgeâ€“acceptor compounds. Physical Chemistry Chemical Physics, 2020, 22, 9664-9676.	2.8	6
27	Mapping hole hopping escape routes in proteins. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 15811-15816.	7.1	35
28	Photo-induced electron transfer: general discussion. Faraday Discussions, 2019, 216, 434-459.	3.2	0
29	Unsymmetrical Bis-Alkynyl Complexes Based on Co(III)(cyclam): Synthesis, Ultrafast Charge Separation, and Analysis. Inorganic Chemistry, 2019, 58, 15487-15497.	4.0	10
30	Electron bifurcation: progress and grand challenges. Chemical Communications, 2019, 55, 11823-11832.	4.1	25
31	A single ATâ€“GC exchange can modulate charge transfer-induced p53â€“DNA dissociation. Chemical Communications, 2019, 55, 206-209.	4.1	11
32	Engineering opposite electronic polarization of singlet and triplet states increases the yield of high-energy photoproducts. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 14465-14470.	7.1	10
33	Quantum interferences among Dexter energy transfer pathways. Faraday Discussions, 2019, 216, 301-318.	3.2	16
34	Assessing Possible Mechanisms of Micrometer-Scale Electron Transfer in Heme-Free Geobacter sulfurreducens Pili. Journal of Physical Chemistry B, 2019, 123, 5035-5047.	2.6	33
35	Voltage-induced long-range coherent electron transfer through organic molecules. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 5931-5936.	7.1	39
36	Why Are DNA and Protein Electron Transfer So Different?. Annual Review of Physical Chemistry, 2019, 70, 71-97.	10.8	70

#	Article	IF	Citations
37	Orientational Dependence of Cofacial Porphyrinâ€“Quinone Electronic Interactions within the Strong Coupling Regime. Journal of Physical Chemistry B, 2019, 123, 10456-10462.	2.6	8
38	Charge Transfer between [4Fe4S] Proteins and DNA Is Unidirectional: Implications for Biomolecular Signaling. CheM, 2019, 5, 122-137.	11.7	25
39	Charge splitters and charge transport junctions based on guanine quadruplexes. Nature Nanotechnology, 2018, 13, 316-321.	31.5	46
40	Improving Solar Cell Performance Using Quantum Dot Triad Charge-Separation Engines. Journal of Physical Chemistry C, 2018, 122, 5924-5934.	3.1	10
41	Determinants of Photolyaseâ€™s DNA Repair Mechanism in Mesophiles and Extremophiles. Journal of the American Chemical Society, 2018, 140, 2853-2861.	13.7	19
42	On the nature of organic and inorganic centers that bifurcate electrons, coupling exergonic and endergonic oxidationâ€“reduction reactions. Chemical Communications, 2018, 54, 4091-4099.	4.1	50
43	Directing Charge Transfer in Quantum Dot Assemblies. Accounts of Chemical Research, 2018, 51, 2565-2573.	15.6	24
44	Editorial overview: Biological pathways for electrons, protons and photo-excitations. Current Opinion in Chemical Biology, 2018, 47, A1-A3.	6.1	5
45	Electron transfer characteristics of 2â€²-deoxy-2â€²-fluoro-arabinonucleic acid, a nucleic acid with enhanced chemical stability. Physical Chemistry Chemical Physics, 2018, 20, 26063-26067.	2.8	8
46	Control of electron transfer in nitrogenase. Current Opinion in Chemical Biology, 2018, 47, 54-59.	6.1	43
47	How can infra-red excitation both accelerate and slow charge transfer in the same molecule?. Chemical Science, 2018, 9, 6395-6405.	7.4	15
48	A new era for electron bifurcation. Current Opinion in Chemical Biology, 2018, 47, 32-38.	6.1	54
49	A Nonequilibrium Molecular Dynamics Study of Infrared Perturbed Electron Transfer. Journal of Chemical Theory and Computation, 2018, 14, 4818-4832.	5.3	1
50	Energy Transduction in Nitrogenase. Accounts of Chemical Research, 2018, 51, 2179-2186.	15.6	101
51	Effects of the Backbone and Chemical Linker on the Molecular Conductance of Nucleic Acid Duplexes. Journal of the American Chemical Society, 2017, 139, 6726-6735.	13.7	32
52	Controlling the excited-state dynamics of low band gap, near-infrared absorbers via proquinoidal unit electronic structural modulation. Chemical Science, 2017, 8, 5889-5901.	7.4	16
53	Chirality Control of Electron Transfer in Quantum Dot Assemblies. Journal of the American Chemical Society, 2017, 139, 9038-9043.	13.7	91
54	Charge and spin transport through nucleic acids. Current Opinion in Electrochemistry, 2017, 4, 175-181.	4.8	18

#	Article	IF	Citations
55	De novo design of a hyperstable non-natural proteinâ€“ligand complex with sub-Ã... accuracy. Nature Chemistry, 2017, 9, 1157-1164.	13.6	93
56	Electron Bifurcation: Thermodynamics and Kinetics of Two-Electron Brokering in Biological Redox Chemistry. Accounts of Chemical Research, 2017, 50, 2410-2417.	15.6	44
57	Controlling the Electron-Transfer Kinetics of Quantum-Dot Assemblies. Journal of Physical Chemistry C, 2017, 121, 14401-14412.	3.1	8
58	Dexter energy transfer pathways. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 8115-8120.	7.1	105
59	Large Hyperpolarizabilities at Telecommunication-Relevant Wavelengths in Donorâ€“Acceptorâ€“Donor Nonlinear Optical Chromophores. ACS Central Science, 2016, 2, 954-966.	11.3	48
60	Coarse-Grained Theory of Biological Charge Transfer with Spatially and Temporally Correlated Noise. Journal of Physical Chemistry B, 2016, 120, 3624-3633.	2.6	12
61	DNA charge transport: Moving beyond 1D. Surface Science, 2016, 652, 33-38.	1.9	16
62	Mean Firstâ€Passage Times in Biology. Israel Journal of Chemistry, 2016, 56, 816-824.	2.3	54
63	Hot holes break the speed limit. Nature Chemistry, 2016, 8, 992-993.	13.6	9
64	Engineering nanometre-scale coherence in soft matter. Nature Chemistry, 2016, 8, 941-945.	13.6	51
65	Photoinduced Electron Transfer Elicits a Change in the Static Dielectric Constant of a de Novo Designed Protein. Journal of the American Chemical Society, 2016, 138, 2130-2133.	13.7	22
66	Where Is the Electronic Oscillator Strength? Mapping Oscillator Strength across Molecular Absorption Spectra. Journal of Physical Chemistry A, 2016, 120, 1933-1943.	2.5	38
67	Diverse Optimal Molecular Libraries for Organic Light-Emitting Diodes. Journal of Chemical Theory and Computation, 2016, 12, 1942-1952.	5.3	15
68	Conformationally Gated Charge Transfer in DNA Three-Way Junctions. Journal of Physical Chemistry Letters, 2015, 6, 2434-2438.	4.6	23
69	Open-Access, Interactive Explorations for Teaching and Learning Quantum Dynamics. Journal of Chemical Education, 2015, 92, 2161-2164.	2.3	3
70	Two-Electron Transfer Pathways. Journal of Physical Chemistry B, 2015, 119, 7589-7597.	2.6	10
71	Electron transfer rate modulation in a compact Re(<scp>i</scp>) donorâ€“acceptor complex. Dalton Transactions, 2015, 44, 8609-8616.	3.3	25
72	Strategy To Discover Diverse Optimal Molecules in the Small Molecule Universe. Journal of Chemical Information and Modeling, 2015, 55, 529-537.	5.4	57

#	Article	IF	Citations
73	Sensing of molecules using quantum dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E2419-28.	7.1	14
74	Charge Transport across DNA-Based Three-Way Junctions. Journal of the American Chemical Society, 2015, 137, 5113-5122.	13.7	39
75	Vibrational control of electron-transfer reactions: a feasibility study for the fast coherent transfer regime. Physical Chemistry Chemical Physics, 2015, 17, 30854-30866.	2.8	15
76	Defusing redox bombs?. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 10821-10822.	7.1	30
77	Charge Transfer in Dynamical Biosystems, or The Treachery of (Static) Images. Accounts of Chemical Research, 2015, 48, 474-481.	15.6	145
78	Breaking the simple proportionality between molecular conductances and charge transfer rates. Faraday Discussions, 2014, 174, 57-78.	3.2	44
79	Full-Electron Ligand-to-Ligand Charge Transfer in a Compact Re(I) Complex. Journal of Physical Chemistry A, 2014, 118, 10407-10415.	2.5	19
80	Structural and Electronic Properties of Bare and Capped Cd₃₃Se₃₃ and Cd₃₃Te₃₃ Quantum Dots. Journal of Physical Chemistry C, 2014, 118, 7094-7109.	3.1	32
81	Biological charge transfer via flickering resonance. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 10049-10054.	7.1	140
82	Biochemistry and Theory of Proton-Coupled Electron Transfer. Chemical Reviews, 2014, 114, 3381-3465.	47.7	399
83	Stochastic Voyages into Uncharted Chemical Space Produce a Representative Library of All Possible Drug-Like Compounds. Journal of the American Chemical Society, 2013, 135, 7296-7303.	13.7	214
84	Ligand-Induced Changes in the Characteristic Size-Dependent Electronic Energies of CdSe Nanocrystals. Journal of Physical Chemistry C, 2013, 117, 22401-22411.	3.1	53
85	Distance-Independent Charge Recombination Kinetics in Cytochrome câ€“Cytochrome c Peroxidase Complexes: Compensating Changes in the Electronic Coupling and Reorganization Energies. Journal of Physical Chemistry B, 2013, 117, 9129-9141.	2.6	23
86	Evaluating the Extent of Intramolecular Charge Transfer in the Excited States of Rhenium(I) Donorâ€“Acceptor Complexes with Time-Resolved Vibrational Spectroscopy. Journal of Physical Chemistry B, 2013, 117, 15903-15916.	2.6	19
87	Enthalpic Signature of Methonium Desolvation Revealed in a Synthetic Hostâ€“Guest System Based on Cucurbit[7]uril. Journal of the American Chemical Society, 2013, 135, 6084-6091.	13.7	9
88	Electron Transfer Through Proteins. , 2013, , 625-630.		3
89	The Single-Molecule Conductance and Electrochemical Electron-Transfer Rate Are Related by a Power Law. ACS Nano, 2013, 7, 5391-5401.	14.6	65
90	Triplet Excitation Energy Dynamics in Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2013, 117, 22250-22259.	3.1	54

#	Article	IF	Citations
91	Effect of Backbone Flexibility on Charge Transfer Rates in Peptide Nucleic Acid Duplexes. Journal of the American Chemical Society, 2012, 134, 9335-9342.	13.7	38
92	Effects of S-containing ligands on the structure and electronic properties of CdnSen/CdnTen nanoparticles (n=3, 4, 6, and 9). Chemical Physics, 2012, 407, 97-109.	1.9	12
93	Interfacial hydration, dynamics and electron transfer: multi-scale ET modeling of the transient [myoglobin, cytochrome b5] complex. Physical Chemistry Chemical Physics, 2012, 14, 13881.	2.8	16
94	Design of Coupled Porphyrin Chromophores with Unusually Large Hyperpolarizabilities. Journal of Physical Chemistry C, 2012, 116, 9724-9733.	3.1	33
95	Redox redux. Physical Chemistry Chemical Physics, 2012, 14, 13728.	2.8	1
96	Structural and Electronic Properties of Bare and Capped Cd_nSe_n/Cd_nTe_n Nanoparticles (n = 6, 9). Journal of Physical Chemistry C, 2012, 116, 6817-6830.	3.1	31
97	Inverse design of molecules with optimal reactivity properties: acidity of 2-naphthol derivatives. Physical Chemistry Chemical Physics, 2012, 14, 16002.	2.8	24
98	Physical constraints on charge transport through bacterial nanowires. Faraday Discussions, 2012, 155, 43-61.	3.2	139
99	Exploring biological electron transfer pathway dynamics with the Pathways Plugin for VMD. Journal of Computational Chemistry, 2012, 33, 906-910.	3.3	74
100	Electronic Structure of Self-Assembled Peptide Nucleic Acid Thin Films. Journal of Physical Chemistry C, 2011, 115, 17123-17135.	3.1	17
101	Floquet Analysis for Vibronically Modulated Electron Tunneling. Journal of Physical Chemistry B, 2011, 115, 5510-5518.	2.6	17
102	Evidence for a Near-Resonant Charge Transfer Mechanism for Double-Stranded Peptide Nucleic Acid. Journal of the American Chemical Society, 2011, 133, 62-72.	13.7	45
103	Two-Photon Absorption Properties of Proquinoidal D-A-D and A-D-A Quadrupolar Chromophores. Journal of Physical Chemistry A, 2011, 115, 5525-5539.	2.5	69
104	B-DNA to Zip-DNA: Simulating a DNA Transition to a Novel Structure with Enhanced Charge-Transport Characteristics. Journal of Physical Chemistry A, 2011, 115, 9377-9391.	2.5	25
105	NCIPLOT: A Program for Plotting Noncovalent Interaction Regions. Journal of Chemical Theory and Computation, 2011, 7, 625-632.	5.3	2,897
106	Coherence in electron transfer pathways. Procedia Chemistry, 2011, 3, 99-104.	0.7	10
107	Nucleic acid charge transfer: Black, white and gray. Coordination Chemistry Reviews, 2011, 255, 635-648.	18.8	109
108	Synthesis and chemical diversity analysis of bicyclo[3.3.1]non-3-en-2-ones. Tetrahedron, 2010, 66, 5852-5862.	1.9	17

#	Article	IF	Citations
109	A gradientâ€directed Monte Carlo approach for protein design. Journal of Computational Chemistry, 2010, 31, 2164-2168.	3.3	12
110	Analysis of the unusual wavelength dependence of the first hyperpolarizability of porphyrin derivatives. Proceedings of SPIE, 2010, , .	0.8	1
111	Chiral Control of Current Transfer in Molecules. Topics in Current Chemistry, 2010, 298, 259-278.	4.0	2
112	Optimizing Single-Molecule Conductivity of Conjugated Organic Oligomers with Carbodithioate Linkers. Journal of the American Chemical Society, 2010, 132, 7946-7956.	13.7	102
113	Fluctuations in Biological and Bioinspired Electron-Transfer Reactions. Annual Review of Physical Chemistry, 2010, 61, 461-485.	10.8	182
114	Predicting the Frequency Dispersion of Electronic Hyperpolarizabilities on the Basis of Absorption Data and Thomasâ^'Kuhn Sum Rules. Journal of Physical Chemistry C, 2010, 114, 2349-2359.	3.1	56
115	Steady-State Theory of Current Transfer. Journal of Physical Chemistry C, 2010, 114, 8005-8013.	3.1	20
116	Is MD Geometry Sampling Sufficient for Nucleobase Electronic Structure Analysis of ET Reactions? Comparing Classical MD and QM/MM Methods. Journal of Physical Chemistry C, 2010, 114, 20496-20502.	3.1	13
117	Coarse-grained modeling of allosteric regulation in protein receptors. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 14253-14258.	7.1	43
118	A gradient-directed Monte Carlo method for global optimization in a discrete space: Application to protein sequence design and folding. Journal of Chemical Physics, 2009, 131, 154117.	3.0	15
119	Emergent strategies for inverse molecular design. Science in China Series B: Chemistry, 2009, 52, 1769-1776.	0.8	9
120	Discrete Optimization of Electronic Hyperpolarizabilities in a Chemical Subspace. Journal of Chemical Theory and Computation, 2009, 5, 3321-3329.	5.3	21
121	Role of Nucleobase Energetics and Nucleobase Interactions in Single-Stranded Peptide Nucleic Acid Charge Transfer. Journal of the American Chemical Society, 2009, 131, 6498-6507.	13.7	55
122	Modulating Unimolecular Charge Transfer by Exciting Bridge Vibrations. Journal of the American Chemical Society, 2009, 131, 18060-18062.	13.7	97
123	Turning Charge Transfer On and Off in a Molecular Interferometer with Vibronic Pathways. Nano Letters, 2009, 9, 1818-1823.	9.1	54
124	Optical Signatures of Molecular Dissymmetry: Combining Theory with Experiments To Address Stereochemical Puzzles. Accounts of Chemical Research, 2009, 42, 809-819.	15.6	65
125	Steering Electrons on Moving Pathways. Accounts of Chemical Research, 2009, 42, 1669-1678.	15.6	168
126	Identification of 3-hydroxy-2-(3-hydroxyphenyl)-4H-1-benzopyran-4-ones as isoform-selective PKC-Î¶ inhibitors and potential therapeutics for psychostimulant abuse. Molecular BioSystems, 2009, 5, 927.	2.9	11

#	Article	IF	Citations
127	Photoconductivity and current-voltage characteristics of thin DNA films: experiments and modeling. , 2009, , .		1
128	Exploring the Optical Activity Tensor by Anisotropic Rayleigh Optical Activity Scattering. ChemPhysChem, 2008, 9, 265-271.	2.1	13
129	Chiral Control of Electron Transmission through Molecules. Physical Review Letters, 2008, 101, 238103.	7.8	49
130	Characterizing Aqueous Solution Conformations of a Peptide Backbone Using Raman Optical Activity Computations. Biophysical Journal, 2008, 95, 5574-5586.	0.5	61
131	A Donorâ"Nanotube Paradigm for Nonlinear Optical Materials. Nano Letters, 2008, 8, 2814-2818.	9.1	106
132	Computational design, synthesis and biological evaluation of para-quinone-based inhibitors for redox regulation of the dual-specificity phosphatase Cdc25B. Organic and Biomolecular Chemistry, 2008, 6, 3256.	2.8	45
133	Molecular Design of Porphyrin-Based Nonlinear Optical Materials. Journal of Physical Chemistry A, 2008, 112, 12203-12207.	2.5	100
134	PNA versus DNA: Effects of Structural Fluctuations on Electronic Structure and Hole-Transport Mechanisms. Journal of the American Chemical Society, 2008, 130, 11752-11761.	13.7	112
135	Hepatitis C Virus NS5B Polymerase:â€‰ QM/MM Calculations Show the Important Role of the Internal Energy in Ligand Binding. Journal of Physical Chemistry B, 2008, 112, 3168-3176.	2.6	14
136	Solution Structure of a Peptide Nucleic Acid Duplex from NMR Data: Features and Limitations. Journal of the American Chemical Society, 2008, 130, 13264-13273.	13.7	50
137	Hemeâ€"copper oxidases use tunneling pathways. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 403-404.	7.1	32
138	Exploring chemical space with discrete, gradient, and hybrid optimization methods. Journal of Chemical Physics, 2008, 129, 174105.	3.0	36
139	Inverse molecular design in a tight-binding framework. Journal of Chemical Physics, 2008, 129, 044106.	3.0	35
140	A gradient-directed Monte Carlo approach to molecular design. Journal of Chemical Physics, 2008, 129, 064102.	3.0	39
141	Persistence of Structure Over Fluctuations in Biological Electron-Transfer Reactions. Physical Review Letters, 2008, 101, 158102.	7.8	80
142	Photoselected electron transfer pathways in DNA photolyase. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 802-807.	7.1	70
143	A Molecular Double Slit Paradigm. AIP Conference Proceedings, 2007, , .	0.4	8
144	Flavin Charge Transfer Transitions Assist DNA Photolyase Electron Transfer. AIP Conference Proceedings, 2007, 963, 674-677.	0.4	4

#	Article	IF	Citations
145	Coupling Coherence Distinguishes Structure Sensitivity in Protein Electron Transfer. Science, 2007, 315, 622-625.	12.6	179
146	Designing Molecules with Optimal Properties Using the Linear Combination of Atomic Potentials Approach in an AM1 Semiempirical Framework. Journal of Physical Chemistry A, 2007, 111, 176-181.	2.5	50
147	Theories of Structure-Function Relationships for Bridge-Mediated Electron Transfer Reactions. Advances in Chemical Physics, 2007, , 377-452.	0.3	54
148	BIOCHEMISTRY: Photosynthesis from the Protein's Perspective. Science, 2007, 316, 703-704.	12.6	14
149	Protein Phosphorylation and Intermolecular Electron Transfer:Â A Joint Experimental and Computational Study of a Hormone Biosynthesis Pathway. Journal of the American Chemical Society, 2007, 129, 4206-4216.	13.7	21
150	Contribution of a Solute's Chiral Solvent Imprint to Optical Rotation. Angewandte Chemie - International Edition, 2007, 46, 6450-6452.	13.8	102
151	The effects of bridge motion on electron transfer reactions mediated by tunneling. , 2006, , 357-382.		7
152	The chiroptical signature of achiral metal clusters induced by dissymmetric adsorbates. Physical Chemistry Chemical Physics, 2006, 8, 63-67.	2.8	134
153	Conformationally Averaged Score Functions for Electronic Propagation in Proteins. Journal of Physical Chemistry B, 2006, 110, 5747-5757.	2.6	13
154	Designing Molecules by Optimizing Potentials. Journal of the American Chemical Society, 2006, 128, 3228-3232.	13.7	138
155	Linking Ligand-Induced Alterations in Androgen Receptor Structure to Differential Gene Expression: A First Step in the Rational Design of Selective Androgen Receptor Modulators. Molecular Endocrinology, 2006, 20, 1201-1217.	3.7	66
156	Binding of Warfarin Influences the Acid-Base Equilibrium of H242 in Sudlow Site I of Human Serum Albumin. Photochemistry and Photobiology, 2006, 82, 1365.	2.5	27
157	Electron transfer between cofactors in protein domains linked by a flexible tether. Chemical Physics, 2006, 326, 259-269.	1.9	16
158	Solvent Effect on Optical Rotation: A Case Study of Methyloxirane in Water. ChemPhysChem, 2006, 7, 2483-2486.	2.1	92
159	Guest editorial: Electron transfer. Molecular Simulation, 2006, 32, 675-676.	2.0	0
160	Designing Molecules by Optimizing Potentials. , 2006, , 1245-1246.		0
161	Charge transfer through chemisorbed organic molecules â€“ Neutralization of ionization processes at local sites in the molecule. Chemical Physics Letters, 2005, 412, 171-175.	2.6	7
162	Towards Raman Optical Activity Calculations of Large Molecules. ChemPhysChem, 2005, 6, 595-597.	2.1	32

#	Article	IF	Citations
163	Assignment of the absolute configuration of [n]-ladderanes by TD-DFT optical rotation calculations. Chirality, 2005, 17, 507-510.	2.6	24
164	Protein dynamics and electron transfer: Electronic decoherence and non-Condon effects. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 3552-3557.	7.1	170
165	The Nature of Aqueous Tunneling Pathways Between Electron-Transfer Proteins. Science, 2005, 310, 1311-1313.	12.6	237
166	Simulation of Scanning Tunneling Microscope Images of 1,3-Cyclohexadiene Bound to a Silicon Surface. Journal of Physical Chemistry B, 2005, 109, 1473-1480.	2.6	8
167	Ab Initio Based Calculations of Electron-Transfer Rates in Metalloproteins. Journal of Physical Chemistry B, 2005, 109, 1618-1625.	2.6	75
168	Simulation of Electron Transfer between Cytochrome c2and the Bacterial Photosynthetic Reaction Center:Â Brownian Dynamics Analysis of the Native Proteins and Double Mutants. Journal of Physical Chemistry B, 2005, 109, 7529-7534.	2.6	30
169	Systematic Assignment of the Configuration of Flexible Natural Products by Spectroscopic and Computational Methods:â€‰ The Bistramide C Analysis. Organic Letters, 2005, 7, 5269-5272.	4.6	28
170	Electron Transfer through Proteins. , 2005, , 15-33.		20
171	Generalized Mullikenâ^'Hush Analysis of Electronic Coupling Interactions in Compressed Ï€-Stacked Porphyrinâ^'Bridgeâ^'Quinone Systems. Journal of the American Chemical Society, 2005, 127, 11303-11310.	13.7	57
172	Dynamic Docking and Electron-Transfer between Cytochromeb5and a Suite of Myoglobin Surface-Charge Mutants. Introduction of a Functional-Docking Algorithm for Proteinâ^'Protein Complexes. Journal of the American Chemical Society, 2004, 126, 2785-2798.	13.7	88
173	Inelastic Electron Tunneling Erases Coupling-Pathway Interferences. Journal of Physical Chemistry B, 2004, 108, 15511-15518.	2.6	63
174	The Degree of Charge Transfer in Ground and Charge-Separated States Revealed by Ultrafast Visible Pump/Mid-IR Probe Spectroscopy. Journal of the American Chemical Society, 2004, 126, 5022-5023.	13.7	36
175	Tunneling while Pulling:â€‰ The Dependence of Tunneling Current on End-to-End Distance in a Flexible Molecule. Journal of Physical Chemistry A, 2004, 108, 5655-5661.	2.5	25
176	Structure of the Ochratoxin A Binding Site within Human Serum Albumin. Journal of Physical Chemistry B, 2004, 108, 16960-16964.	2.6	20
177	How Does Protein Architecture Facilitate the Transduction of ATP Chemical-Bond Energy into Mechanical Work? The Cases of Nitrogenase and ATP Binding-Cassette Proteins. Biophysical Journal, 2004, 87, 1369-1377.	0.5	23
178	DNA Electron Transfer Processes: Some Theoretical Notions. Topics in Current Chemistry, 2004, , 1-36.	4.0	93
179	Binding of Ochratoxin A to Human Serum Albumin Stabilized by a Proteinâ^'Ligand Ion Pair. Journal of Physical Chemistry B, 2003, 107, 7884-7888.	2.6	31
180	Optical Rotation of Noncovalent Aggregates. Journal of the American Chemical Society, 2003, 125, 15696-15697.	13.7	63

#	Article	IF	Citations
181	Molecular Control of Electron Transfer Events Within and Between Biomolecules. , 2003, , 227-236.		1
182	Donor-bridge-acceptor energetics determine the distance dependence of electron tunneling in DNA. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 12536-12541.	7.1	155
183	The Nature of Tunneling Pathway and Average Packing Density Models for Protein-Mediated Electron Transferâ€. Journal of Physical Chemistry A, 2002, 106, 2002-2006.	2.5	100
184	Hole Size and Energetics in Double Helical DNA:â€‰ Competition between Quantum Delocalization and Solvation Localization. Journal of Physical Chemistry B, 2002, 106, 7-10.	2.6	106
185	Dynamic Docking and Electron Transfer between Zn-myoglobin and Cytochromeb5. Journal of the American Chemical Society, 2002, 124, 6849-6859.	13.7	98
186	Tunneling Energy Effects on GC Oxidation in DNA. Journal of Physical Chemistry B, 2002, 106, 2381-2392.	2.6	117
187	Optical Activity: From Structure-Function to Structure Prediction. ACS Symposium Series, 2002, , 104-118.	0.5	3
188	Determining Absolute Configuration in Flexible Molecules: A Case Study. Journal of the American Chemical Society, 2001, 123, 8961-8966.	13.7	67
189	From ATP to Electron Transfer:Â Electrostatics and Free-Energy Transduction in Nitrogenase. Journal of Physical Chemistry B, 2001, 105, 5359-5367.	2.6	39
190	New peroxylactones from the Jamaican sponge Plakinastrella onkodes, with inhibitory activity against the AIDS opportunistic parasitic infection Toxoplasma gondii. Tetrahedron, 2001, 57, 1483-1487.	1.9	61
191	Bond-Mediated Electron Tunneling in Ruthenium-Modified High-Potential Ironâ^'Sulfur Protein. Journal of the American Chemical Society, 2000, 122, 4532-4533.	13.7	70
192	Optical Rotation Computation, Total Synthesis, and Stereochemistry Assignment of the Marine Natural Product Pitiamide A. Journal of the American Chemical Society, 2000, 122, 4608-4617.	13.7	104
193	The Nature of Tunnel Splitting Mediated by Stacked Aromatics. Journal of Physical Chemistry A, 2000, 104, 7593-7599.	2.5	15
194	Chiral Action at a Distance:â€‰ Remote Substituent Effects on the Optical Activity of Calyculins A and B. Organic Letters, 2000, 2, 1509-1512.	4.6	16
195	Electrostatic Control of Electron Transfer between Myoglobin and Cytochrome b5:â€‰ Effect of Methylating the Heme Propionates of Zn-Myoglobin. Journal of the American Chemical Society, 2000, 122, 3552-3553.	13.7	40
196	Electron transfer in three-center chemical systems. Journal of Chemical Physics, 1999, 110, 10468-10481.	3.0	30
197	Determination of the absolute configuration of 1,3,5,7-tetramethyl-1,3-dihydroindol-2-one by optical rotation computation. Tetrahedron: Asymmetry, 1999, 10, 4143-4150.	1.8	29
198	Structural and Conformational Dependence of Optical Rotation Angles. Journal of Physical Chemistry A, 1999, 103, 6603-6611.	2.5	70

#	Article	IF	Citations
199	DNA-mediated electron transfer. Journal of Biological Inorganic Chemistry, 1998, 3, 196-200.	2.6	40
200	Electron transfer in the photosynthetic reaction center: mechanistic implications of mutagenesis studies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1998, 54, 1211-1218.	3.9	8
201	Electron transfer mechanisms. Current Opinion in Chemical Biology, 1998, 2, 235-243.	6.1	83
202	Use of Modern Electron Transfer Theories To Determine Electronic Coupling Matrix Elements in Intramolecular Systems. Journal of Physical Chemistry A, 1998, 102, 5529-5541.	2.5	106
203	Binding and Electron Transfer between Putidaredoxin and Cytochrome P450cam. Theory and Experiments. Journal of the American Chemical Society, 1998, 120, 8927-8932.	13.7	83
204	Theory-Assisted Determination of Absolute Stereochemistry for Complex Natural Products via Computation of Molar Rotation Angles. Journal of the American Chemical Society, 1998, 120, 2204-2205.	13.7	127
205	Atomic Contributions to the Optical Rotation Angle as a Quantitative Probe of Molecular Chirality. Science, 1998, 282, 2247-2250.	12.6	138
206	Structure of the Electrical Double Layer in High-Temperature Superconductors. Origin of the Dip in the Double-Layer Capacitance near the Superconducting Transition. Journal of Physical Chemistry B, 1997, 101, 7095-7099.	2.6	3
207	Structural Fluctuations, Spin, Reorganization Energy, and Tunneling Energy Control of Intramolecular Electron Transfer:Â The Surprising Case of Electron Transfer in a d8â^'d8Bimetallic System. Journal of the American Chemical Society, 1997, 119, 5690-5700.	13.7	44
208	Electron Transfer Contact Maps. Journal of Physical Chemistry B, 1997, 101, 1215-1234.	2.6	50
209	Secondary Structure Conformations and Long Range Electronic Interactions in Oligopeptides. Journal of Physical Chemistry B, 1997, 101, 2986-2991.	2.6	76
210	Three-State Model for Two-Electron Transfer Reactions. Journal of Physical Chemistry A, 1997, 101, 4136-4141.	2.5	32
211	High and low resolution theories of protein electron transfer. Journal of Biological Inorganic Chemistry, 1997, 2, 378-386.	2.6	46
212	DNA: insulator or wire?. Chemistry and Biology, 1997, 4, 3-8.	6.0	161
213	Synthetic and model computational studies of molar rotation additivity for interacting chiral centers: A reinvestigation of van't Hoff's principle. , 1997, 9, 469-477.		34
214	Theory and Practice of Electron Transfer within Proteinâ^'Protein Complexes:Â Application to the Multidomain Binding of Cytochromecby CytochromecPeroxidase. Chemical Reviews, 1996, 96, 2459-2490.	47.7	202
215	Acetylenyl-Linked, Porphyrin-Bridged, Donorâ^'Acceptor Molecules:â€‰ A Theoretical Analysis of the Molecular First Hyperpolarizability in Highly Conjugated Pushâ^'Pull Chromophore Structures. Journal of the American Chemical Society, 1996, 118, 1504-1510.	13.7	238
216	Bridgeâ€mediated electronic interactions: Differences between Hamiltonian and Green function partitioning in a nonâ€orthogonal basis. Journal of Chemical Physics, 1996, 104, 9473-9481.	3.0	112

#	Article	IF	Citations
217	Twoâ€electron transfer reactions in polar solvents. Journal of Chemical Physics, 1996, 105, 165-176.	3.0	47
218	Ab initio based effective Hamiltonians for longâ€range electron transfer: Hartreeâ€“Fock analysis. Journal of Chemical Physics, 1996, 105, 9561-9573.	3.0	98
219	Donorâ€”Acceptor Electronic Coupling in Ruthenium-Modified Heme Proteins. Advances in Chemistry Series, 1996, , 471-485.	0.6	5
220	DNA double-helix-mediated long-range electron transfer. International Journal of Quantum Chemistry, 1996, 60, 1789-1795.	2.0	14
221	A method to analyze multi-pathway effects on protein mediated donor-acceptor coupling interactions. Inorganica Chimica Acta, 1996, 243, 167-175.	2.4	27
222	Inverse Strategies for Molecular Design. The Journal of Physical Chemistry, 1996, 100, 10595-10599.	2.9	61
223	Pathways, pathway tubes, pathway docking, and propagators in electron transfer proteins. Journal of Bioenergetics and Biomembranes, 1995, 27, 285-293.	2.3	71
224	Docking and electron transfer between cytochrome c2 and the photosynthetic reaction center. Chemical Physics, 1995, 197, 277-288.	1.9	33
225	What is the Anharmonicity of a Molecule's Electronic Wave Function?. The Journal of Physical Chemistry, 1995, 99, 1935-1942.	2.9	3
226	The two-state reduction for electron and hole transfer in bridge-mediated electron-transfer reactions. Chemical Physics, 1993, 176, 501-520.	1.9	64
227	Molecular Electronics: Observation of Molecular Rectification. Science, 1993, 261, 576-577.	12.6	56
228	Electron transfer in DNA: predictions of exponential growth and decay of coupling with donor-acceptor distance. Journal of the American Chemical Society, 1993, 115, 2508-2510.	13.7	71
229	Structure-function relationships for .beta., the first molecular hyperpolarizability. Journal of the American Chemical Society, 1993, 115, 7719-7728.	13.7	85
230	Electronic coupling in starburst dendrimers: connectivity, disorder, and finite size effects in macromolecular Bethe lattices. The Journal of Physical Chemistry, 1993, 97, 4523-4527.	2.9	30
231	Electron-tunneling pathways in proteins. Science, 1992, 258, 1740-1741.	12.6	517
232	Tunneling pathway and redox-state-dependent electronic couplings at nearly fixed distance in electron transfer proteins. The Journal of Physical Chemistry, 1992, 96, 2852-2855.	2.9	131
233	Mapping electron tunneling pathways: an algorithm that finds the "minimum length"/maximum coupling pathway between electron donors and acceptors in proteins. Journal of the American Chemical Society, 1992, 114, 4043-4046.	13.7	129
234	Pathway Analysis of Protein Electron-Transfer Reactions. Annual Review of Biophysics and Biomolecular Structure, 1992, 21, 349-377.	18.3	378

#	Article	IF	Citations
235	Electron Transfer. Advances in Chemistry Series, 1991, , 71-90.	0.6	17
236	Electronic Hyperpolarizability and Chemical Structure. ACS Symposium Series, 1991, , 89-102.	0.5	12
237	Approaches for Optimizing the First Electronic Hyperpolarizability of Conjugated Organic Molecules. Science, 1991, 252, 103-106.	12.6	721
238	Protein electron transfer rates set by the bridging secondary and tertiary structure. Science, 1991, 252, 1285-1288.	12.6	721
239	Electron tunneling pathways in proteins: A method to compute tunneling matrix elements in very large systems. Journal of Chemical Physics, 1991, 95, 1131-1138.	3.0	79
240	Structure/property relationships for molecular second-order nonlinear optics. , 1991, 1560, 86.		2
241	Electron tunneling pathways in ruthenated proteins. Journal of the American Chemical Society, 1990, 112, 7915-7921.	13.7	220
242	A predictive theoretical model for electron tunneling pathways in proteins. Journal of Chemical Physics, 1990, 92, 722-733.	3.0	220
243	Influence of gap states on the nonresonant second hyperpolarizabilities of conjugated organic polymers. The Journal of Physical Chemistry, 1989, 93, 3915-3920.	2.9	4
244	Electronic shift register memory based on molecular electron-transfer reactions. The Journal of Physical Chemistry, 1989, 93, 6350-6357.	2.9	109
245	Electron tunneling pathways in proteins: influences on the transfer rate. Photosynthesis Research, 1989, 22, 173-186.	2.9	84
246	Design of a True Molecular Electronic Device: The Electron Transfer Shift Register Memory. , 1989, , 353-360.		1
247	Long-Range Electron Transfer in Myoblobin. Annals of the New York Academy of Sciences, 1988, 550, 68-84.	3.8	61
248	Adiabaticity and nonadiabaticity in bimolecular outerâ€sphere charge transfer reactions. Journal of Chemical Physics, 1988, 89, 6195-6203.	3.0	47
249	Adiabaticity criteria for outer-sphere bimolecular electron-transfer reactions. The Journal of Physical Chemistry, 1988, 92, 4817-4820.	2.9	25
250	A Molecular Shift Register Based on Electron Transfer. Science, 1988, 241, 817-820.	12.6	187
251	Electron tunneling through covalent and noncovalent pathways in proteins. Journal of Chemical Physics, 1987, 86, 4488-4498.	3.0	306
252	Molecular bridge effects on distant charge tunneling. Journal of the American Chemical Society, 1987, 109, 6771-6778.	13.7	91

#	Article	IF	Citations
253	Nonlinear susceptibilities of finite conjugated organic polymers. The Journal of Physical Chemistry, 1987, 91, 2696-2698.	2.9	96
254	Some aspects of electron-transfer reaction dynamics.. The Journal of Physical Chemistry, 1986, 90, 3707-3721.	2.9	169
255	Electron tunneling through rigid molecular bridges: bicyclo[2.2.2]octane. Journal of the American Chemical Society, 1986, 108, 4321-4326.	13.7	77
256	Limiting forms of the tunneling matrix element in the long distance bridge mediated electron transfer problem. Journal of Chemical Physics, 1985, 83, 5325-5329.	3.0	60
257	Failure of the Bornâ€“Oppenheimer and Franckâ€“Condon approximations for long distance electron transfer rate calculations. Journal of Chemical Physics, 1984, 81, 5753-5759.	3.0	60
258	Calculation of tunneling matrix elements in rigid systems: mixed-valence dithiaspirocyclobutane molecules. Journal of the American Chemical Society, 1984, 106, 1584-1594.	13.7	192
259	Localized orbitals and the Fermi hole. Theoretica Chimica Acta, 1982, 61, 265-281.	0.8	111