

# David N Beratan

## List of Publications by Year in descending order

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259  
papers

18,597  
citations

14124

69  
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16186

128  
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271  
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271  
docs citations

271  
times ranked

15078  
citing authors

#	ARTICLE	IF	CITATIONS
1	Twisted molecular wires polarize spin currents at room temperature. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	8
2	Discovery of the Xenon-Protein Interactome Using Large-Scale Measurements of Protein Folding and Stability. <i>Journal of the American Chemical Society</i> , 2022, 144, 3925-3938.	6.6	7
3	Improving the efficiency of open-quantum-system simulations using matrix product states in the interaction picture. <i>Physical Review A</i> , 2022, 105, .	1.0	5
4	A Chirality-Based Quantum Leap. <i>ACS Nano</i> , 2022, 16, 4989-5035.	7.3	74
5	Synthetic Control of Exciton Dynamics in Bioinspired Cofacial Porphyrin Dimers. <i>Journal of the American Chemical Society</i> , 2022, 144, 6298-6310.	6.6	17
6	Cofactor Dynamics Couples the Protein Surface to the Heme in Cytochrome <i>c</i> , Facilitating Electron Transfer. <i>Journal of Physical Chemistry B</i> , 2022, 126, 3522-3529.	1.2	0
7	Delocalization-Assisted Transport through Nucleic Acids in Molecular Junctions. <i>Biochemistry</i> , 2021, 60, 1368-1378.	1.2	4
8	Temperature Dependence of Charge and Spin Transfer in Azurin. <i>Journal of Physical Chemistry C</i> , 2021, 125, 9875-9883.	1.5	26
9	Why Do Most Aromatics Fail to Support Hole Hopping in the Cytochrome <i>c</i> Peroxidase-Cytochrome <i>c</i> Complex?. <i>Journal of Physical Chemistry B</i> , 2021, 125, 7763-7773.	1.2	2
10	Oxalate decarboxylase uses electron hole hopping for catalysis. <i>Journal of Biological Chemistry</i> , 2021, 297, 100857.	1.6	5
11	Efficient and reversible electron bifurcation with either normal or inverted potentials at the bifurcating cofactor. <i>CheM</i> , 2021, 7, 1870-1886.	5.8	6
12	Electron ratcheting in self-assembled soft matter. <i>Journal of Chemical Physics</i> , 2021, 155, 055102.	1.2	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 Supramolecular Electro-Optic Properties. <i>Inorganic Chemistry</i> , 2021, 60, 15404-15412.	1.9	2
14	Energy transduction by reversible electron bifurcation. <i>Current Opinion in Electrochemistry</i> , 2021, 29, 100767.	2.5	1
15	Charge Transfer and Spin Dynamics in a Zinc Porphyrin Donor Covalently Linked to One or Two Naphthalenediimide Acceptors. <i>Journal of Physical Chemistry A</i> , 2021, 125, 825-834.	1.1	6
16	Multiple hops move electrons from bacteria to rocks. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, e2115620118.	3.3	1
17	Correlation between Charge Transport and Base Excision Repair in the MutY-DNA Glycosylase. <i>Journal of Physical Chemistry B</i> , 2021, 125, 17-23.	1.2	4
18	Mechanism of Side Chain-Controlled Proton Conductivity in Bioinspired Peptidic Nanostructures. <i>Journal of Physical Chemistry B</i> , 2021, 125, 12741-12752.	1.2	3

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19	Mutation effects on charge transport through the p58c iron-sulfur protein. <i>Chemical Science</i> , 2020, 11, 7076-7085.	3.7	5
20	Electrostatic Field-Induced Oscillator Strength Focusing in Molecules. <i>Journal of Physical Chemistry B</i> , 2020, 124, 6376-6388.	1.2	5
21	Predicting Dexter Energy Transfer Interactions from Molecular Orbital Overlaps. <i>Journal of Physical Chemistry C</i> , 2020, 124, 18956-18960.	1.5	15
22	A robust bioderived wavelength-specific photosensor based on BLUF proteins. <i>Sensors and Actuators B: Chemical</i> , 2020, 310, 127838.	4.0	4
23	Autobiography of David N. Beratan. <i>Journal of Physical Chemistry B</i> , 2020, 124, 3441-3446.	1.2	0
24	Conductance and Configuration of Molecular Gold-Water-Gold Junctions under Electric Fields. <i>Matter</i> , 2020, 3, 166-179.	5.0	21
25	Revisiting the Hole Size in Double Helical DNA with Localized Orbital Scaling Corrections. <i>Journal of Physical Chemistry B</i> , 2020, 124, 3428-3435.	1.2	5
26	Symmetry controlled photo-selection and charge separation in butadiyne-bridged donor-bridge-acceptor compounds. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9664-9676.	1.3	6
27	Mapping hole hopping escape routes in proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 15811-15816.	3.3	35
28	Photo-induced electron transfer: general discussion. <i>Faraday Discussions</i> , 2019, 216, 434-459.	1.6	0
29	Unsymmetrical Bis-Alkynyl Complexes Based on Co(III)(cyclam): Synthesis, Ultrafast Charge Separation, and Analysis. <i>Inorganic Chemistry</i> , 2019, 58, 15487-15497.	1.9	10
30	Electron bifurcation: progress and grand challenges. <i>Chemical Communications</i> , 2019, 55, 11823-11832.	2.2	25
31	A single AT-GC exchange can modulate charge transfer-induced p53-DNA dissociation. <i>Chemical Communications</i> , 2019, 55, 206-209.	2.2	11
32	Engineering opposite electronic polarization of singlet and triplet states increases the yield of high-energy photoproducts. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 14465-14470.	3.3	10
33	Quantum interferences among Dexter energy transfer pathways. <i>Faraday Discussions</i> , 2019, 216, 301-318.	1.6	16
34	Assessing Possible Mechanisms of Micrometer-Scale Electron Transfer in Heme-Free <i>Geobacter sulfurreducens</i> Pili. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5035-5047.	1.2	33
35	Voltage-induced long-range coherent electron transfer through organic molecules. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 5931-5936.	3.3	39
36	Why Are DNA and Protein Electron Transfer So Different?. <i>Annual Review of Physical Chemistry</i> , 2019, 70, 71-97.	4.8	70

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37	Orientational Dependence of Cofacial Porphyrin-Quinone Electronic Interactions within the Strong Coupling Regime. <i>Journal of Physical Chemistry B</i> , 2019, 123, 10456-10462.	1.2	8
38	Charge Transfer between [4Fe4S] Proteins and DNA Is Unidirectional: Implications for Biomolecular Signaling. <i>CheM</i> , 2019, 5, 122-137.	5.8	25
39	Charge splitters and charge transport junctions based on guanine quadruplexes. <i>Nature Nanotechnology</i> , 2018, 13, 316-321.	15.6	46
40	Improving Solar Cell Performance Using Quantum Dot Triad Charge-Separation Engines. <i>Journal of Physical Chemistry C</i> , 2018, 122, 5924-5934.	1.5	10
41	Determinants of Photolyase's DNA Repair Mechanism in Mesophiles and Extremophiles. <i>Journal of the American Chemical Society</i> , 2018, 140, 2853-2861.	6.6	19
42	On the nature of organic and inorganic centers that bifurcate electrons, coupling exergonic and endergonic oxidation-reduction reactions. <i>Chemical Communications</i> , 2018, 54, 4091-4099.	2.2	50
43	Directing Charge Transfer in Quantum Dot Assemblies. <i>Accounts of Chemical Research</i> , 2018, 51, 2565-2573.	7.6	24
44	Editorial overview: Biological pathways for electrons, protons and photo-excitations. <i>Current Opinion in Chemical Biology</i> , 2018, 47, A1-A3.	2.8	5
45	Electron transfer characteristics of 2-deoxy-2-fluoro-arabinonucleic acid, a nucleic acid with enhanced chemical stability. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 26063-26067.	1.3	8
46	Control of electron transfer in nitrogenase. <i>Current Opinion in Chemical Biology</i> , 2018, 47, 54-59.	2.8	43
47	How can infra-red excitation both accelerate and slow charge transfer in the same molecule?. <i>Chemical Science</i> , 2018, 9, 6395-6405.	3.7	15
48	A new era for electron bifurcation. <i>Current Opinion in Chemical Biology</i> , 2018, 47, 32-38.	2.8	54
49	A Nonequilibrium Molecular Dynamics Study of Infrared Perturbed Electron Transfer. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4818-4832.	2.3	1
50	Energy Transduction in Nitrogenase. <i>Accounts of Chemical Research</i> , 2018, 51, 2179-2186.	7.6	101
51	Effects of the Backbone and Chemical Linker on the Molecular Conductance of Nucleic Acid Duplexes. <i>Journal of the American Chemical Society</i> , 2017, 139, 6726-6735.	6.6	32
52	Controlling the excited-state dynamics of low band gap, near-infrared absorbers via proquinoidal unit electronic structural modulation. <i>Chemical Science</i> , 2017, 8, 5889-5901.	3.7	16
53	Chirality Control of Electron Transfer in Quantum Dot Assemblies. <i>Journal of the American Chemical Society</i> , 2017, 139, 9038-9043.	6.6	91
54	Charge and spin transport through nucleic acids. <i>Current Opinion in Electrochemistry</i> , 2017, 4, 175-181.	2.5	18

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55	De novo design of a hyperstable non-natural proteinâ€“ligand complex with sub-Å... accuracy. <i>Nature Chemistry</i> , 2017, 9, 1157-1164.	6.6	93
56	Electron Bifurcation: Thermodynamics and Kinetics of Two-Electron Brokering in Biological Redox Chemistry. <i>Accounts of Chemical Research</i> , 2017, 50, 2410-2417.	7.6	44
57	Controlling the Electron-Transfer Kinetics of Quantum-Dot Assemblies. <i>Journal of Physical Chemistry C</i> , 2017, 121, 14401-14412.	1.5	8
58	Dexter energy transfer pathways. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 8115-8120.	3.3	105
59	Large Hyperpolarizabilities at Telecommunication-Relevant Wavelengths in Donorâ€“Acceptorâ€“Donor Nonlinear Optical Chromophores. <i>ACS Central Science</i> , 2016, 2, 954-966.	5.3	48
60	Coarse-Grained Theory of Biological Charge Transfer with Spatially and Temporally Correlated Noise. <i>Journal of Physical Chemistry B</i> , 2016, 120, 3624-3633.	1.2	12
61	DNA charge transport: Moving beyond 1D. <i>Surface Science</i> , 2016, 652, 33-38.	0.8	16
62	Mean Firstâ€“Passage Times in Biology. <i>Israel Journal of Chemistry</i> , 2016, 56, 816-824.	1.0	54
63	Hot holes break the speed limit. <i>Nature Chemistry</i> , 2016, 8, 992-993.	6.6	9
64	Engineering nanometre-scale coherence in soft matter. <i>Nature Chemistry</i> , 2016, 8, 941-945.	6.6	51
65	Photoinduced Electron Transfer Elicits a Change in the Static Dielectric Constant of a <i>de Novo</i> Designed Protein. <i>Journal of the American Chemical Society</i> , 2016, 138, 2130-2133.	6.6	22
66	Where Is the Electronic Oscillator Strength? Mapping Oscillator Strength across Molecular Absorption Spectra. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1933-1943.	1.1	38
67	Diverse Optimal Molecular Libraries for Organic Light-Emitting Diodes. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1942-1952.	2.3	15
68	Conformationally Gated Charge Transfer in DNA Three-Way Junctions. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 2434-2438.	2.1	23
69	Open-Access, Interactive Explorations for Teaching and Learning Quantum Dynamics. <i>Journal of Chemical Education</i> , 2015, 92, 2161-2164.	1.1	3
70	Two-Electron Transfer Pathways. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7589-7597.	1.2	10
71	Electron transfer rate modulation in a compact Re( <i>donor</i> )â€“acceptor complex. <i>Dalton Transactions</i> , 2015, 44, 8609-8616.	1.6	25
72	Strategy To Discover Diverse Optimal Molecules in the Small Molecule Universe. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 529-537.	2.5	57

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73	Sensing of molecules using quantum dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E2419-28.	3.3	14
74	Charge Transport across DNA-Based Three-Way Junctions. Journal of the American Chemical Society, 2015, 137, 5113-5122.	6.6	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.	1.3	15
76	Defusing redox bombs?. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 10821-10822.	3.3	30
77	Charge Transfer in Dynamical Biosystems, or The Treachery of (Static) Images. Accounts of Chemical Research, 2015, 48, 474-481.	7.6	145
78	Breaking the simple proportionality between molecular conductances and charge transfer rates. Faraday Discussions, 2014, 174, 57-78.	1.6	44
79	Full-Electron Ligand-to-Ligand Charge Transfer in a Compact Re(I) Complex. Journal of Physical Chemistry A, 2014, 118, 10407-10415.	1.1	19
80	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. Journal of Physical Chemistry C, 2014, 118, 7094-7109.	1.5	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.	3.3	140
82	Biochemistry and Theory of Proton-Coupled Electron Transfer. Chemical Reviews, 2014, 114, 3381-3465.	23.0	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.	6.6	214
84	Ligand-Induced Changes in the Characteristic Size-Dependent Electronic Energies of CdSe Nanocrystals. Journal of Physical Chemistry C, 2013, 117, 22401-22411.	1.5	53
85	Distance-Independent Charge Recombination Kinetics in Cytochrome <i>c</i> –Cytochrome <i>c</i> /i> Peroxidase Complexes: Compensating Changes in the Electronic Coupling and Reorganization Energies. Journal of Physical Chemistry B, 2013, 117, 9129-9141.	1.2	23
86	Evaluating the Extent of Intramolecular Charge Transfer in the Excited States of Rhenium(I) Donor–Acceptor Complexes with Time-Resolved Vibrational Spectroscopy. Journal of Physical Chemistry B, 2013, 117, 15903-15916.	1.2	19
87	Enthalpic Signature of Methonium Desolvation Revealed in a Synthetic Host–Guest System Based on Cucurbit[7]uril. Journal of the American Chemical Society, 2013, 135, 6084-6091.	6.6	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.	7.3	65
90	Triplet Excitation Energy Dynamics in Metal–Organic Frameworks. Journal of Physical Chemistry C, 2013, 117, 22250-22259.	1.5	54

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91	Effect of Backbone Flexibility on Charge Transfer Rates in Peptide Nucleic Acid Duplexes. Journal of the American Chemical Society, 2012, 134, 9335-9342.	6.6	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.	0.9	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.	1.3	16
94	Design of Coupled Porphyrin Chromophores with Unusually Large Hyperpolarizabilities. Journal of Physical Chemistry C, 2012, 116, 9724-9733.	1.5	33
95	Redox redux. Physical Chemistry Chemical Physics, 2012, 14, 13728.	1.3	1
96	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). Journal of Physical Chemistry C, 2012, 116, 6817-6830.	1.5	31
97	Inverse design of molecules with optimal reactivity properties: acidity of 2-naphthol derivatives. Physical Chemistry Chemical Physics, 2012, 14, 16002.	1.3	24
98	Physical constraints on charge transport through bacterial nanowires. Faraday Discussions, 2012, 155, 43-61.	1.6	139
99	Exploring biological electron transfer pathway dynamics with the <i>Pathways</i> Plugin for VMD. Journal of Computational Chemistry, 2012, 33, 906-910.	1.5	74
100	Electronic Structure of Self-Assembled Peptide Nucleic Acid Thin Films. Journal of Physical Chemistry C, 2011, 115, 17123-17135.	1.5	17
101	Floquet Analysis for Vibronically Modulated Electron Tunneling. Journal of Physical Chemistry B, 2011, 115, 5510-5518.	1.2	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.	6.6	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.	1.1	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.	1.1	25
105	NCIPLOT: A Program for Plotting Noncovalent Interaction Regions. Journal of Chemical Theory and Computation, 2011, 7, 625-632.	2.3	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.	9.5	109
108	Synthesis and chemical diversity analysis of bicyclo[3.3.1]non-3-en-2-ones. Tetrahedron, 2010, 66, 5852-5862.	1.0	17

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109	A gradient-directed Monte Carlo approach for protein design. <i>Journal of Computational Chemistry</i> , 2010, 31, 2164-2168.	1.5	12
110	Analysis of the unusual wavelength dependence of the first hyperpolarizability of porphyrin derivatives. <i>Proceedings of SPIE</i> , 2010, , .	0.8	1
111	Chiral Control of Current Transfer in Molecules. <i>Topics in Current Chemistry</i> , 2010, 298, 259-278.	4.0	2
112	Optimizing Single-Molecule Conductivity of Conjugated Organic Oligomers with Carbodithioate Linkers. <i>Journal of the American Chemical Society</i> , 2010, 132, 7946-7956.	6.6	102
113	Fluctuations in Biological and Bioinspired Electron-Transfer Reactions. <i>Annual Review of Physical Chemistry</i> , 2010, 61, 461-485.	4.8	182
114	Predicting the Frequency Dispersion of Electronic Hyperpolarizabilities on the Basis of Absorption Data and Thomas-Kuhn Sum Rules. <i>Journal of Physical Chemistry C</i> , 2010, 114, 2349-2359.	1.5	56
115	Steady-State Theory of Current Transfer. <i>Journal of Physical Chemistry C</i> , 2010, 114, 8005-8013.	1.5	20
116	Is MD Geometry Sampling Sufficient for Nucleobase Electronic Structure Analysis of ET Reactions? Comparing Classical MD and QM/MM Methods. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20496-20502.	1.5	13
117	Coarse-grained modeling of allosteric regulation in protein receptors. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 14253-14258.	3.3	43
118	A gradient-directed Monte Carlo method for global optimization in a discrete space: Application to protein sequence design and folding. <i>Journal of Chemical Physics</i> , 2009, 131, 154117.	1.2	15
119	Emergent strategies for inverse molecular design. <i>Science in China Series B: Chemistry</i> , 2009, 52, 1769-1776.	0.8	9
120	Discrete Optimization of Electronic Hyperpolarizabilities in a Chemical Subspace. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 3321-3329.	2.3	21
121	Role of Nucleobase Energetics and Nucleobase Interactions in Single-Stranded Peptide Nucleic Acid Charge Transfer. <i>Journal of the American Chemical Society</i> , 2009, 131, 6498-6507.	6.6	55
122	Modulating Unimolecular Charge Transfer by Exciting Bridge Vibrations. <i>Journal of the American Chemical Society</i> , 2009, 131, 18060-18062.	6.6	97
123	Turning Charge Transfer On and Off in a Molecular Interferometer with Vibronic Pathways. <i>Nano Letters</i> , 2009, 9, 1818-1823.	4.5	54
124	Optical Signatures of Molecular Dissymmetry: Combining Theory with Experiments To Address Stereochemical Puzzles. <i>Accounts of Chemical Research</i> , 2009, 42, 809-819.	7.6	65
125	Steering Electrons on Moving Pathways. <i>Accounts of Chemical Research</i> , 2009, 42, 1669-1678.	7.6	168
126	Identification of 3-hydroxy-2-(3-hydroxyphenyl)-4H-1-benzopyran-4-ones as isoform-selective PKC- $\eta$ inhibitors and potential therapeutics for psychostimulant abuse. <i>Molecular BioSystems</i> , 2009, 5, 927.	2.9	11



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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.	1.0	13
129	Chiral Control of Electron Transmission through Molecules. Physical Review Letters, 2008, 101, 238103.	2.9	49
130	Characterizing Aqueous Solution Conformations of a Peptide Backbone Using Raman Optical Activity Computations. Biophysical Journal, 2008, 95, 5574-5586.	0.2	61
131	A Donor- $\pi$ -Nanotube Paradigm for Nonlinear Optical Materials. Nano Letters, 2008, 8, 2814-2818.	4.5	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.	1.5	45
133	Molecular Design of Porphyrin-Based Nonlinear Optical Materials. Journal of Physical Chemistry A, 2008, 112, 12203-12207.	1.1	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.	6.6	112
135	Hepatitis C Virus NS5B Polymerase: QM/MM Calculations Show the Important Role of the Internal Energy in Ligand Binding. Journal of Physical Chemistry B, 2008, 112, 3168-3176.	1.2	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.	6.6	50
137	Heme- $\pi$ -copper oxidases use tunneling pathways. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 403-404.	3.3	32
138	Exploring chemical space with discrete, gradient, and hybrid optimization methods. Journal of Chemical Physics, 2008, 129, 174105.	1.2	36
139	Inverse molecular design in a tight-binding framework. Journal of Chemical Physics, 2008, 129, 044106.	1.2	35
140	A gradient-directed Monte Carlo approach to molecular design. Journal of Chemical Physics, 2008, 129, 064102.	1.2	39
141	Persistence of Structure Over Fluctuations in Biological Electron-Transfer Reactions. Physical Review Letters, 2008, 101, 158102.	2.9	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.	3.3	70
143	A Molecular Double Slit Paradigm. AIP Conference Proceedings, 2007, , .	0.3	8
144	Flavin Charge Transfer Transitions Assist DNA Photolyase Electron Transfer. AIP Conference Proceedings, 2007, 963, 674-677.	0.3	4

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145	Coupling Coherence Distinguishes Structure Sensitivity in Protein Electron Transfer. <i>Science</i> , 2007, 315, 622-625.	6.0	179
146	Designing Molecules with Optimal Properties Using the Linear Combination of Atomic Potentials Approach in an AM1 Semiempirical Framework. <i>Journal of Physical Chemistry A</i> , 2007, 111, 176-181.	1.1	50
147	Theories of Structure-Function Relationships for Bridge-Mediated Electron Transfer Reactions. <i>Advances in Chemical Physics</i> , 2007, , 377-452.	0.3	54
148	BIOCHEMISTRY: Photosynthesis from the Protein's Perspective. <i>Science</i> , 2007, 316, 703-704.	6.0	14
149	Protein Phosphorylation and Intermolecular Electron Transfer: A Joint Experimental and Computational Study of a Hormone Biosynthesis Pathway. <i>Journal of the American Chemical Society</i> , 2007, 129, 4206-4216.	6.6	21
150	Contribution of a Solute's Chiral Solvent Imprint to Optical Rotation. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 6450-6452.	7.2	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. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 63-67.	1.3	134
153	Conformationally Averaged Score Functions for Electronic Propagation in Proteins. <i>Journal of Physical Chemistry B</i> , 2006, 110, 5747-5757.	1.2	13
154	Designing Molecules by Optimizing Potentials. <i>Journal of the American Chemical Society</i> , 2006, 128, 3228-3232.	6.6	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. <i>Molecular Endocrinology</i> , 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. <i>Photochemistry and Photobiology</i> , 2006, 82, 1365.	1.3	27
157	Electron transfer between cofactors in protein domains linked by a flexible tether. <i>Chemical Physics</i> , 2006, 326, 259-269.	0.9	16
158	Solvent Effect on Optical Rotation: A Case Study of Methyloxirane in Water. <i>ChemPhysChem</i> , 2006, 7, 2483-2486.	1.0	92
159	Guest editorial: Electron transfer. <i>Molecular Simulation</i> , 2006, 32, 675-676.	0.9	0
160	Designing Molecules by Optimizing Potentials. , 2006, , 1245-1246.		0
161	Charge transfer through chemisorbed organic molecules " Neutralization of ionization processes at local sites in the molecule. <i>Chemical Physics Letters</i> , 2005, 412, 171-175.	1.2	7
162	Towards Raman Optical Activity Calculations of Large Molecules. <i>ChemPhysChem</i> , 2005, 6, 595-597.	1.0	32

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