Alexei A Stuchebrukhov

List of Publications by Year
in descending order

89 papers	3,909 citations	136950 32 h-index	123424 61 g-index
89 all docs	89 docs citations	89 times ranked	3181 citing authors

#	Article	IF	Citations
1	Theory of Coupled Electron and Proton Transfer Reactions. Chemical Reviews, 2010, 110, 6939-6960.	47.7	665
2	Accounting for electronic polarization in non-polarizable force fields. Physical Chemistry Chemical Physics, 2011, 13, 2613.	2.8	372
3	Theoretical Study of Electron Transfer between the Photolyase Catalytic Cofactor FADH-and DNA Thymine Dimer. Journal of the American Chemical Society, 2000, 122, 1057-1065.	13.7	142
4	Electrostatic Study of the Proton Pumping Mechanism in Bovine Heart CytochromecOxidase. Journal of the American Chemical Society, 2004, 126, 1858-1871.	13.7	122
5	Inelastic tunneling in long-distance biological electron transfer reactions. Journal of Chemical Physics, 1997, 107, 3821-3831.	3.0	117
6	Proton pumping mechanism and catalytic cycle of cytochrome c oxidase: Coulomb pump model with kinetic gating. FEBS Letters, 2004, 566, 126-130.	2.8	116
7	Electron tunneling in respiratory complex I. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 19157-19162.	7.1	112
8	Tunneling currents in electron transfer reactions in proteins. Journal of Chemical Physics, 1996, 104, 8424-8432.	3.0	103
9	Concerted electron and proton transfer: Transition from nonadiabatic to adiabatic proton tunneling. Journal of Chemical Physics, 2000, 113, 10438-10450.	3.0	103
10	Polarizable Mean-Field Model of Water for Biological Simulations with AMBER and CHARMM Force Fields. Journal of Chemical Theory and Computation, 2012, 8, 3207-3216.	5.3	91
11	Computer simulation of water in cytochrome c oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2003, 1557, 99-107.	1.0	90
12	Long-distance electron tunneling in proteins. Theoretical Chemistry Accounts, 2003, 110, 291-306.	1.4	85
13	Tunneling currents in electron transfer reaction in proteins. II. Calculation of electronic superexchange matrix element and tunneling currents using nonorthogonal basis sets. Journal of Chemical Physics, 1996, 105, 10819-10829.	3.0	81
14	Polarizable molecular interactions in condensed phase and their equivalent nonpolarizable models. Journal of Chemical Physics, 2014, 141, 014103.	3.0	73
15	Electron Transfer Tunneling Pathways in Bovine Heart CytochromecOxidase. Journal of the American Chemical Society, 2000, 122, 6571-6582.	13.7	63
16	Proton Transport via the Membrane Surface. Biophysical Journal, 2002, 82, 2833-2846.	0.5	62
17	DNA Repair Mechanism by Photolyase: Electron Transfer Path from the Photolyase Catalytic Cofactor FADHâ˚to DNA Thymine Dimer. Journal of Theoretical Biology, 2001, 210, 237-248.	1.7	59
18	Calculation of electronic tunneling matrix element in proteins: Comparison of exact and approximate one-electron methods for Ru-modified azurin. Journal of Chemical Physics, 1997, 106, 5658-5666.	3.0	57

#	Article	IF	Citations
19	Combined DFT and electrostatics study of the proton pumping mechanism in cytochrome c oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2006, 1757, 1035-1046.	1.0	57
20	Theoretical and computational analysis of the membrane potential generated by cytochrome c oxidase upon single electron injection into the enzyme. Biochimica Et Biophysica Acta - Bioenergetics, 2008, 1777, 1129-1139.	1.0	55
21	DFT/Electrostatic Calculations of pKaValues in CytochromecOxidase. Journal of Physical Chemistry B, 2005, 109, 3616-3626.	2.6	54
22	Proton Exit Channels in Bovine CytochromecOxidase. Journal of Physical Chemistry B, 2005, 109, 1999-2006.	2.6	53
23	Thermodynamic Properties of Internal Water Molecules in the Hydrophobic Cavity around the Catalytic Center of CytochromecOxidase. Journal of Physical Chemistry B, 2005, 109, 1015-1022.	2.6	47
24	Molecular dynamics simulation of water in cytochrome c oxidase reveals two water exit pathways and the mechanism of transport. Biochimica Et Biophysica Acta - Bioenergetics, 2009, 1787, 1140-1150.	1.0	43
25	Tunneling currents in proteins: Nonorthogonal atomic basis sets and Mulliken population analysis. Journal of Chemical Physics, 1997, 107, 6495-6498.	3.0	42
26	Dispersion relations for electron and hole transfer in donorâ€"bridgeâ€"acceptor systems. Chemical Physics Letters, 1994, 225, 55-61.	2.6	38
27	Kinetic advantage of forming respiratory supercomplexes. Biochimica Et Biophysica Acta - Bioenergetics, 2020, 1861, 148193.	1.0	38
28	Outerâ€sphere electron transfer in polar solvents: Quantum scaling of strongly interacting systems. Journal of Chemical Physics, 1993, 99, 969-978.	3.0	37
29	New expression for the effective transfer matrix element in long-range electron transfer reactions. Journal of Chemical Physics, 1998, 109, 4960-4970.	3.0	35
30	Electron Transfer in Ferredoxin: Are Tunneling Pathways Evolutionarily Conserved?. Molecular Biology and Evolution, 2002, 19, 406-415.	8.9	34
31	Redox-Dependent pKaof CuBHistidine Ligand in CytochromecOxidase. Journal of Physical Chemistry B, 2004, 108, 18383-18389.	2.6	34
32	Mechanisms of proton transfer in proteins: Localized charge transfer versus delocalized soliton transfer. Physical Review E, 2009, 79, 031927.	2.1	33
33	Mechanism of longâ€range proton translocation along biological membranes. FEBS Letters, 2013, 587, 345-349.	2.8	33
34	Quantum effects in electron transfer reactions with strong electronic coupling. Journal of Chemical Physics, 1994, 101, 9354-9365.	3.0	32
35	Effect of quantum modes in biological electron transfer reactions: A useful approximation for the harmonic model with frequency change and Duchinsky rotation. Journal of Chemical Physics, 2000, 112, 9015-9024.	3.0	32
36	Tunneling currents in long-distance electron transfer reactions. III. Many-electron formulation. Journal of Chemical Physics, 1998, 108, 8499-8509.	3.0	31

#	Article	IF	Citations
37	Tunneling currents in long-distance electron transfer reactions. V. Effective one electron approximation. Journal of Chemical Physics, 2003, 118, 7898-7906.	3.0	31
38	ELECTRON TRANSFER REACTIONS COUPLED TO PROTON TRANSLOCATION: CYTOCHROME OXIDASE, PROTON PUMPS, AND BIOLOGICAL ENERGY TRANSDUCTION. Journal of Theoretical and Computational Chemistry, 2003, 02, 91-118.	1.8	31
39	Vortex structure of the tunneling flow in long-range electron transfer reactions. Journal of Chemical Physics, 1999, 110, 8865-8868.	3.0	30
40	Proton transport via coupled surface and bulk diffusion. Journal of Chemical Physics, 2002, 116, 1692-1699.	3.0	30
41	Mutations in NDUFS1 Cause Metabolic Reprogramming and Disruption of the Electron Transfer. Cells, 2019, 8, 1149.	4.1	30
42	Tunneling currents in long-distance electron transfer reactions. IV. Many-electron formulation. Nonorthogonal atomic basis sets and Mulliken population analysis. Journal of Chemical Physics, 1998, 108, 8510-8520.	3.0	29
43	Theoretical Study of Excitation Energy Transfer in DNA Photolyase. Journal of Physical Chemistry B, 2008, 112, 8724-8729.	2.6	29
44	Ab Initio Study of Long-Distance Electron Tunneling in a Model Peptide System. Journal of Physical Chemistry B, 2000, 104, 8606-8613.	2.6	26
45	Toward Ab Initio Theory of Longdistance Electron Tunneling in Proteins: Tunneling Currents Approach. Advances in Chemical Physics, 2007, , 1-44.	0.3	26
46	On the non-orthogonal basis set calculations of the bridge-mediated electronic matrix elements. Chemical Physics Letters, 1997, 265, 643-648.	2.6	24
47	Improved Density Functional Theory/Electrostatic Calculation of the His291 Protonation State in Cytochrome c Oxidase:Â Self-Consistent Charges for Solvation Energy Calculation. Journal of Physical Chemistry B, 2006, 110, 12162-12166.	2.6	24
48	Quantum Electron Tunneling in Respiratory Complex I. Journal of Physical Chemistry B, 2011, 115, 5354-5364.	2.6	22
49	Docking and Migration of Carbon Monoxide in Nitrogenase: The Case for Gated Pockets from Infrared Spectroscopy and Molecular Dynamics. Biochemistry, 2015, 54, 3314-3319.	2.5	21
50	Coupled electron and proton transfer reactions during the Oâ†'E transition in bovine cytochrome c oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2012, 1817, 506-517.	1.0	20
51	Two conformational states of Glu242 and pKas in bovine cytochrome c oxidase. Photochemical and Photobiological Sciences, 2006, 5, 611.	2.9	19
52	Watching DNA repair in real time. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 19445-19446.	7.1	17
53	Calculation of Quantum Parameters for Nonadiabatic Redox Reactions. Application to Photoreduction of Flavin in DNA Photolyase. Journal of Physical Chemistry B, 2000, 104, 6894-6902.	2.6	15
54	Electron Tunneling in the His126Ru-Modified Azurin:Â Tunneling Jumps between Protein Strands via Hydrogen Bonds. Journal of Physical Chemistry B, 2003, 107, 9579-9584.	2.6	15

#	Article	IF	Citations
55	Electron Tunneling in Quasi-One-Dimensional Resonant Molecular Systems. Ab Initio Study. Journal of Physical Chemistry A, 1998, 102, 2847-2856.	2.5	14
56	Electron Tunneling in Proteins:Â Implementation of ZINDO Model for Tunneling Currents Calculations. Journal of Physical Chemistry B, 2003, 107, 6621-6628.	2.6	14
57	Redox-Driven Proton Pumps of the Respiratory Chain. Biophysical Journal, 2018, 115, 830-840.	0.5	14
58	DFT calculation of electron tunneling currents: Real-space (grid) molecular orbitals vs. Gaussian-type molecular orbitals. International Journal of Quantum Chemistry, 2000, 80, 591-597.	2.0	12
59	Dynamic and Electronic Polarization Corrections to the Dielectric Constant of Water. Journal of Physical Chemistry A, 2018, 122, 9243-9250.	2.5	12
60	Respiratory complex I: Bottleneck at the entrance of quinone site requires conformational change for its opening. Biochimica Et Biophysica Acta - Bioenergetics, 2021, 1862, 148326.	1.0	12
61	Protein dynamics control of electron transfer in reaction centers fromRps. viridis. Molecular Simulation, 2006, 32, 735-750.	2.0	11
62	Ab initio calculations of long-distance electron tunneling in organometallic systems of biological origin. International Journal of Quantum Chemistry, 2000, 77, 16-26.	2.0	10
63	Monte Carlo Simulations of Glu-242 in Cytochrome c Oxidase. Journal of Physical Chemistry B, 2016, 120, 2095-2105.	2.6	10
64	Investigating the Many Roles of Internal Water in Cytochrome c Oxidase. Journal of Physical Chemistry B, 2018, 122, 7625-7635.	2.6	10
65	Histidine in continuum electrostatics protonation state calculations. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3410-3419.	2.6	9
66	Concerted Two-Electron Reduction of Ubiquinone in Respiratory Complex I. Journal of Physical Chemistry B, 2019, 123, 5265-5273.	2.6	9
67	Kinetics of autoxidation of tartaric acid in presence of iron. Journal of Chemical Physics, 2020, 153, 064503.	3.0	9
68	Transition Flux Formula for the Electronic Coupling Matrix Element. Journal of Physical Chemistry B, 2015, 119, 7712-7721.	2.6	8
69	Quantum Calculations of Electron Tunneling in Respiratory Complex III. Journal of Physical Chemistry B, 2015, 119, 14637-14651.	2.6	8
70	On the electron tunneling in molecules: A generalized orthogonalization procedure for finding tunneling orbitals. Journal of Chemical Physics, 2004, 121, 8680-8686.	3.0	7
71	Does internal water influence electron tunneling in proteins? Example of cytochromec oxidase. International Journal of Quantum Chemistry, 2005, 102, 473-479.	2.0	7
72	Quinone binding in respiratory complex I: Going through the eye of a needle. The squeeze-in mechanism of passing the narrow entrance of the quinone site. Photochemical and Photobiological Sciences, 2021, , 1.	2.9	7

#	Article	IF	Citations
73	Photoactivated excited states of DNA repair photolyase: Dynamical and semiempircal identification. International Journal of Quantum Chemistry, 2007, 107, 3126-3131.	2.0	6
74	Measurement of the autoionization lifetime of the superexcited atomic sulfur S(3s23p3(2Do)4d) state using tunable vacuum ultraviolet (VUV) radiation. Canadian Journal of Chemistry, 2004, 82, 885-890.	1.1	5
75	Redox-Coupled Protonation of Respiratory Complex I: The Hydrophilic Domain. Biophysical Journal, 2011, 101, 431-438.	0.5	5
76	Tunneling Time and the Breakdown of Bornâ€“Oppenheimer Approximation. Journal of Physical Chemistry B, 2016, 120, 1408-1417.	2.6	5
77	Kinetics and Efficiency of Energy-Transducing Enzymes. Journal of Physical Chemistry B, 2019, 123, 9456-9465.	2.6	5
78	Single-photon spectroscopy of singlet sulfur atoms and the autoionization lifetime measurements of the superexcited singlet states. Journal of Chemical Physics, 2005, 122, 144321.	3.0	4
79	First principles studies of electron tunneling in proteins. Computational and Theoretical Chemistry, 2011, 975, 61-68.	2.5	4
80	Novel Inhibitors for a Novel Binding Site in Respiratory Complex III. Journal of Physical Chemistry B, 2016, 120, 2701-2708.	2.6	4
81	Electron tunneling in proteins program. Journal of Computational Chemistry, 2016, 37, 1388-1395.	3.3	3
82	Proteins as strongly correlated protonic systems. FEBS Letters, 2012, 586, 519-525.	2.8	2
83	Internal switches modulating electron tunneling currents in respiratory complex III. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 749-758.	1.0	2
84	The Kinetics of Autoxidation in Wine. , 0, , .		1
85	Ab Initio Calculations of Long-Distance Electron Tunneling in Proteins with the Method of Tunneling Currents. ACS Symposium Series, 2004, , 119-144.	0.5	0
86	An accurate and efficient procedure of fitting electric field potential by point charges for QM/MM calculations. Physica Status Solidi (B): Basic Research, 2006, 243, 2030-2037.	1.5	0
87	Coupled Electron and Proton Transfer in Complex I and Complex IV of the Respiratory Chain: Insights from Computer Simulations. Biophysical Journal, 2010, 98, 733a.	0.5	0
88	Internal Switches Modulating Electron Flow in bc1 Complex. Biophysical Journal, 2015, 108, 603a.	0.5	0
89	Mechanical Allosteric Couplings of Redox-Induced Conformational Changes in Respiratory Complex I. Journal of Physical Chemistry B, 0, , .	2.6	0