

# Alexei A Stuchebrukhov

## List of Publications by Year in descending order

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89  
papers

3,909  
citations

136950

32  
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123424

61  
g-index

89  
all docs

89  
docs citations

89  
times ranked

3181  
citing authors

#	ARTICLE	IF	CITATIONS
1	Respiratory complex I: Bottleneck at the entrance of quinone site requires conformational change for its opening. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2021, 1862, 148326.	1.0	12
2	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. <i>Photochemical and Photobiological Sciences</i> , 2021, , 1.	2.9	7
3	Kinetics of autoxidation of tartaric acid in presence of iron. <i>Journal of Chemical Physics</i> , 2020, 153, 064503.	3.0	9
4	Kinetic advantage of forming respiratory supercomplexes. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2020, 1861, 148193.	1.0	38
5	Kinetics and Efficiency of Energy-Transducing Enzymes. <i>Journal of Physical Chemistry B</i> , 2019, 123, 9456-9465.	2.6	5
6	Mutations in NDUFS1 Cause Metabolic Reprogramming and Disruption of the Electron Transfer. <i>Cells</i> , 2019, 8, 1149.	4.1	30
7	Concerted Two-Electron Reduction of Ubiquinone in Respiratory Complex I. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5265-5273.	2.6	9
8	Dynamic and Electronic Polarization Corrections to the Dielectric Constant of Water. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9243-9250.	2.5	12
9	Investigating the Many Roles of Internal Water in Cytochrome <i>c</i> Oxidase. <i>Journal of Physical Chemistry B</i> , 2018, 122, 7625-7635.	2.6	10
10	Redox-Driven Proton Pumps of the Respiratory Chain. <i>Biophysical Journal</i> , 2018, 115, 830-840.	0.5	14
11	Electron tunneling in proteins program. <i>Journal of Computational Chemistry</i> , 2016, 37, 1388-1395.	3.3	3
12	Monte Carlo Simulations of Glu-242 in Cytochrome <i>c</i> Oxidase. <i>Journal of Physical Chemistry B</i> , 2016, 120, 2095-2105.	2.6	10
13	Novel Inhibitors for a Novel Binding Site in Respiratory Complex III. <i>Journal of Physical Chemistry B</i> , 2016, 120, 2701-2708.	2.6	4
14	Internal switches modulating electron tunneling currents in respiratory complex III. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2016, 1857, 749-758.	1.0	2
15	Tunneling Time and the Breakdown of Born–Oppenheimer Approximation. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1408-1417.	2.6	5
16	Internal Switches Modulating Electron Flow in bc <sub>1</sub> Complex. <i>Biophysical Journal</i> , 2015, 108, 603a.	0.5	0
17	Transition Flux Formula for the Electronic Coupling Matrix Element. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7712-7721.	2.6	8
18	Docking and Migration of Carbon Monoxide in Nitrogenase: The Case for Gated Pockets from Infrared Spectroscopy and Molecular Dynamics. <i>Biochemistry</i> , 2015, 54, 3314-3319.	2.5	21

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19	Quantum Calculations of Electron Tunneling in Respiratory Complex III. <i>Journal of Physical Chemistry B</i> , 2015, 119, 14637-14651.	2.6	8
20	Polarizable molecular interactions in condensed phase and their equivalent nonpolarizable models. <i>Journal of Chemical Physics</i> , 2014, 141, 014103.	3.0	73
21	Mechanism of long-range proton translocation along biological membranes. <i>FEBS Letters</i> , 2013, 587, 345-349.	2.8	33
22	Polarizable Mean-Field Model of Water for Biological Simulations with AMBER and CHARMM Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3207-3216.	5.3	91
23	Proteins as strongly correlated protonic systems. <i>FEBS Letters</i> , 2012, 586, 519-525.	2.8	2
24	Coupled electron and proton transfer reactions during the O <sub>2</sub> →O <sub>2</sub> <sup>-</sup> transition in bovine cytochrome c oxidase. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2012, 1817, 506-517.	1.0	20
25	Accounting for electronic polarization in non-polarizable force fields. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 2613.	2.8	372
26	Quantum Electron Tunneling in Respiratory Complex I. <i>Journal of Physical Chemistry B</i> , 2011, 115, 5354-5364.	2.6	22
27	Redox-Coupled Protonation of Respiratory Complex I: The Hydrophilic Domain. <i>Biophysical Journal</i> , 2011, 101, 431-438.	0.5	5
28	First principles studies of electron tunneling in proteins. <i>Computational and Theoretical Chemistry</i> , 2011, 975, 61-68.	2.5	4
29	Histidine in continuum electrostatics protonation state calculations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 3410-3419.	2.6	9
30	Watching DNA repair in real time. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 19445-19446.	7.1	17
31	Theory of Coupled Electron and Proton Transfer Reactions. <i>Chemical Reviews</i> , 2010, 110, 6939-6960.	47.7	665
32	Electron tunneling in respiratory complex I. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 19157-19162.	7.1	112
33	Coupled Electron and Proton Transfer in Complex I and Complex IV of the Respiratory Chain: Insights from Computer Simulations. <i>Biophysical Journal</i> , 2010, 98, 733a.	0.5	0
34	Mechanisms of proton transfer in proteins: Localized charge transfer versus delocalized soliton transfer. <i>Physical Review E</i> , 2009, 79, 031927.	2.1	33
35	Molecular dynamics simulation of water in cytochrome c oxidase reveals two water exit pathways and the mechanism of transport. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2009, 1787, 1140-1150.	1.0	43
36	Theoretical and computational analysis of the membrane potential generated by cytochrome c oxidase upon single electron injection into the enzyme. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2008, 1777, 1129-1139.	1.0	55

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37	Theoretical Study of Excitation Energy Transfer in DNA Photolyase. <i>Journal of Physical Chemistry B</i> , 2008, 112, 8724-8729.	2.6	29
38	Toward Ab Initio Theory of Longdistance Electron Tunneling in Proteins: Tunneling Currents Approach. <i>Advances in Chemical Physics</i> , 2007, , 1-44.	0.3	26
39	Photoactivated excited states of DNA repair photolyase: Dynamical and semiempirical identification. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 3126-3131.	2.0	6
40	Two conformational states of Glu242 and pKas in bovine cytochrome c oxidase. <i>Photochemical and Photobiological Sciences</i> , 2006, 5, 611.	2.9	19
41	Combined DFT and electrostatics study of the proton pumping mechanism in cytochrome c oxidase. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2006, 1757, 1035-1046.	1.0	57
42	Improved Density Functional Theory/Electrostatic Calculation of the His291 Protonation State in Cytochrome c Oxidase: A Self-Consistent Charges for Solvation Energy Calculation. <i>Journal of Physical Chemistry B</i> , 2006, 110, 12162-12166.	2.6	24
43	Protein dynamics control of electron transfer in reaction centers from <i>Rps. viridis</i> . <i>Molecular Simulation</i> , 2006, 32, 735-750.	2.0	11
44	An accurate and efficient procedure of fitting electric field potential by point charges for QM/MM calculations. <i>Physica Status Solidi (B): Basic Research</i> , 2006, 243, 2030-2037.	1.5	0
45	Does internal water influence electron tunneling in proteins? Example of cytochromec oxidase. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 473-479.	2.0	7
46	Single-photon spectroscopy of singlet sulfur atoms and the autoionization lifetime measurements of the superexcited singlet states. <i>Journal of Chemical Physics</i> , 2005, 122, 144321.	3.0	4
47	Thermodynamic Properties of Internal Water Molecules in the Hydrophobic Cavity around the Catalytic Center of CytochromecOxidase. <i>Journal of Physical Chemistry B</i> , 2005, 109, 1015-1022.	2.6	47
48	Proton Exit Channels in Bovine CytochromecOxidase. <i>Journal of Physical Chemistry B</i> , 2005, 109, 1999-2006.	2.6	53
49	DFT/Electrostatic Calculations of pKaValues in CytochromecOxidase. <i>Journal of Physical Chemistry B</i> , 2005, 109, 3616-3626.	2.6	54
50	Ab Initio Calculations of Long-Distance Electron Tunneling in Proteins with the Method of Tunneling Currents. <i>ACS Symposium Series</i> , 2004, , 119-144.	0.5	0
51	On the electron tunneling in molecules: A generalized orthogonalization procedure for finding tunneling orbitals. <i>Journal of Chemical Physics</i> , 2004, 121, 8680-8686.	3.0	7
52	Electrostatic Study of the Proton Pumping Mechanism in Bovine Heart CytochromecOxidase. <i>Journal of the American Chemical Society</i> , 2004, 126, 1858-1871.	13.7	122
53	Measurement of the autoionization lifetime of the superexcited atomic sulfur $S(3s23p3(2D)4d)$ state using tunable vacuum ultraviolet (VUV) radiation. <i>Canadian Journal of Chemistry</i> , 2004, 82, 885-890.	1.1	5
54	Redox-Dependent pKaof CuBHistidine Ligand in CytochromecOxidase. <i>Journal of Physical Chemistry B</i> , 2004, 108, 18383-18389.	2.6	34

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55	Proton pumping mechanism and catalytic cycle of cytochrome c oxidase: Coulomb pump model with kinetic gating. <i>FEBS Letters</i> , 2004, 566, 126-130.	2.8	116
56	Long-distance electron tunneling in proteins. <i>Theoretical Chemistry Accounts</i> , 2003, 110, 291-306.	1.4	85
57	Electron Tunneling in Proteins:Â Implementation of ZINDO Model for Tunneling Currents Calculations. <i>Journal of Physical Chemistry B</i> , 2003, 107, 6621-6628.	2.6	14
58	Electron Tunneling in the His126Ru-Modified Azurin:Â Tunneling Jumps between Protein Strands via Hydrogen Bonds. <i>Journal of Physical Chemistry B</i> , 2003, 107, 9579-9584.	2.6	15
59	Computer simulation of water in cytochrome c oxidase. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2003, 1557, 99-107.	1.0	90
60	Tunneling currents in long-distance electron transfer reactions. V. Effective one electron approximation. <i>Journal of Chemical Physics</i> , 2003, 118, 7898-7906.	3.0	31
61	ELECTRON TRANSFER REACTIONS COUPLED TO PROTON TRANSLOCATION: CYTOCHROME OXIDASE, PROTON PUMPS, AND BIOLOGICAL ENERGY TRANSDUCTION. <i>Journal of Theoretical and Computational Chemistry</i> , 2003, 02, 91-118.	1.8	31
62	Proton transport via coupled surface and bulk diffusion. <i>Journal of Chemical Physics</i> , 2002, 116, 1692-1699.	3.0	30
63	Electron Transfer in Ferredoxin: Are Tunneling Pathways Evolutionarily Conserved?. <i>Molecular Biology and Evolution</i> , 2002, 19, 406-415.	8.9	34
64	Proton Transport via the Membrane Surface. <i>Biophysical Journal</i> , 2002, 82, 2833-2846.	0.5	62
65	DNA Repair Mechanism by Photolyase: Electron Transfer Path from the Photolyase Catalytic Cofactor FADH <sup>+</sup> to DNA Thymine Dimer. <i>Journal of Theoretical Biology</i> , 2001, 210, 237-248.	1.7	59
66	Ab initio calculations of long-distance electron tunneling in organometallic systems of biological origin. <i>International Journal of Quantum Chemistry</i> , 2000, 77, 16-26.	2.0	10
67	DFT calculation of electron tunneling currents: Real-space (grid) molecular orbitals vs. Gaussian-type molecular orbitals. <i>International Journal of Quantum Chemistry</i> , 2000, 80, 591-597.	2.0	12
68	Concerted electron and proton transfer: Transition from nonadiabatic to adiabatic proton tunneling. <i>Journal of Chemical Physics</i> , 2000, 113, 10438-10450.	3.0	103
69	Effect of quantum modes in biological electron transfer reactions: A useful approximation for the harmonic model with frequency change and Duchinsky rotation. <i>Journal of Chemical Physics</i> , 2000, 112, 9015-9024.	3.0	32
70	Theoretical Study of Electron Transfer between the Photolyase Catalytic Cofactor FADH <sup>+</sup> and DNA Thymine Dimer. <i>Journal of the American Chemical Society</i> , 2000, 122, 1057-1065.	13.7	142
71	Calculation of Quantum Parameters for Nonadiabatic Redox Reactions. Application to Photoreduction of Flavin in DNA Photolyase. <i>Journal of Physical Chemistry B</i> , 2000, 104, 6894-6902.	2.6	15
72	Ab Initio Study of Long-Distance Electron Tunneling in a Model Peptide System. <i>Journal of Physical Chemistry B</i> , 2000, 104, 8606-8613.	2.6	26

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73	Electron Transfer Tunneling Pathways in Bovine Heart Cytochrome c Oxidase. <i>Journal of the American Chemical Society</i> , 2000, 122, 6571-6582.	13.7	63
74	Vortex structure of the tunneling flow in long-range electron transfer reactions. <i>Journal of Chemical Physics</i> , 1999, 110, 8865-8868.	3.0	30
75	Tunneling currents in long-distance electron transfer reactions. IV. Many-electron formulation. Nonorthogonal atomic basis sets and Mulliken population analysis. <i>Journal of Chemical Physics</i> , 1998, 108, 8510-8520.	3.0	29
76	Electron Tunneling in Quasi-One-Dimensional Resonant Molecular Systems. Ab Initio Study. <i>Journal of Physical Chemistry A</i> , 1998, 102, 2847-2856.	2.5	14
77	New expression for the effective transfer matrix element in long-range electron transfer reactions. <i>Journal of Chemical Physics</i> , 1998, 109, 4960-4970.	3.0	35
78	Tunneling currents in long-distance electron transfer reactions. III. Many-electron formulation. <i>Journal of Chemical Physics</i> , 1998, 108, 8499-8509.	3.0	31
79	Inelastic tunneling in long-distance biological electron transfer reactions. <i>Journal of Chemical Physics</i> , 1997, 107, 3821-3831.	3.0	117
80	Calculation of electronic tunneling matrix element in proteins: Comparison of exact and approximate one-electron methods for Ru-modified azurin. <i>Journal of Chemical Physics</i> , 1997, 106, 5658-5666.	3.0	57
81	Tunneling currents in proteins: Nonorthogonal atomic basis sets and Mulliken population analysis. <i>Journal of Chemical Physics</i> , 1997, 107, 6495-6498.	3.0	42
82	On the non-orthogonal basis set calculations of the bridge-mediated electronic matrix elements. <i>Chemical Physics Letters</i> , 1997, 265, 643-648.	2.6	24
83	Tunneling currents in electron transfer reactions in proteins. <i>Journal of Chemical Physics</i> , 1996, 104, 8424-8432.	3.0	103
84	Tunneling currents in electron transfer reaction in proteins. II. Calculation of electronic superexchange matrix element and tunneling currents using nonorthogonal basis sets. <i>Journal of Chemical Physics</i> , 1996, 105, 10819-10829.	3.0	81
85	Quantum effects in electron transfer reactions with strong electronic coupling. <i>Journal of Chemical Physics</i> , 1994, 101, 9354-9365.	3.0	32
86	Dispersion relations for electron and hole transfer in donor-bridge-acceptor systems. <i>Chemical Physics Letters</i> , 1994, 225, 55-61.	2.6	38
87	Outer-sphere electron transfer in polar solvents: Quantum scaling of strongly interacting systems. <i>Journal of Chemical Physics</i> , 1993, 99, 969-978.	3.0	37
88	The Kinetics of Autoxidation in Wine. , 0, , .		1
89	Mechanical Allosteric Couplings of Redox-Induced Conformational Changes in Respiratory Complex I. <i>Journal of Physical Chemistry B</i> , 0, , .	2.6	0