Alexander A Voityuk

List of Publications by Citations

178 papers	4,648 citations	36 h-index	63 g-index
187 ext. papers	4,991 ext. citations	3.7 avg, IF	6.04 L-index

#	Paper	IF	Citations
178	Fragment charge difference method for estimating donor–acceptor electronic coupling: Application to DNA π-stacks. *Journal of Chemical Physics*, **2002**, 117, 5607-5616	3.9	251
177	Extension of MNDO to d Orbitals: Parameters and Results for the Second-Row Elements and for the Zinc Group. *The Journal of Physical Chemistry*, **1996**, 100, 616-626		231
176	Electronic Coupling for Charge Transfer and Transport in DNA. *Journal of Physical Chemistry B*, **2000**, 104, 9740-9745	3.4	219
175	Electronic coupling between Watson–Crick pairs for hole transfer and transport in desoxyribonucleic acid. *Journal of Chemical Physics*, **2001**, 114, 5614-5620	3.9	213
174	Energetics of hole transfer in DNA. *Chemical Physics Letters*, **2000**, 324, 430-434	2.5	175
173	Extension of the MNDO formalism tod orbitals: Integral approximations and preliminary numerical results. *Theoretica Chimica Acta*, **1992**, 81, 391-404		168
172	Superexchange Mediated Charge Hopping in DNA. *Journal of Physical Chemistry A*, **2002**, 106, 7599-7606	2.8	139
171	Charge transfer in DNA. Sensitivity of electronic couplings to conformational changes. *Physical Chemistry Chemical Physics*, **2001**, 3, 5421-5425	3.6	119
170	Environmental fluctuations facilitate electron-hole transfer from guanine to adenine in DNA pi stacks. *Angewandte Chemie - International Edition*, **2004**, 43, 624-7	16.4	114
169	Quantum chemical modeling of structure and absorption spectra of the chromophore in green fluorescent proteins. *Chemical Physics*, **1998**, 231, 13-25	2.3	102
168	Structure and rotation barriers for ground and excited states of the isolated chromophore of the green fluorescent protein. *Chemical Physics Letters*, **1998**, 296, 269-276	2.5	96
167	Estimate of the Reorganization Energy for Charge Transfer in DNA. *Journal of Physical Chemistry B*, **2003**, 107, 2595-2601	3.4	96
166	CASSCF/CAS-PT2 study of hole transfer in stacked DNA nucleobases. *Journal of Physical Chemistry A*, **2006**, 110, 6426-32	2.8	90
165	Electronic couplings and on-site energies for hole transfer in DNA: systematic quantum mechanical/molecular dynamic study. *Journal of Chemical Physics*, **2008**, 128, 115101	3.9	84
164	Protonation effects on the chromophore of green fluorescent protein. Quantum chemical study of the absorption spectrum. *Chemical Physics Letters*, **1997**, 272, 162-167	2.5	82
163	Absorption spectra of the GFP chromophore in solution: comparison of theoretical and experimental results. *Chemical Physics*, **2001**, 269, 83-91	2.3	73
162	AM1/d Parameters for Molybdenum. *Journal of Physical Chemistry A*, **2000**, 104, 4089-4094	2.8	72

161	Extension of MNDO to d orbitals: Parameters and results for the halogens. *International Journal of Quantum Chemistry*, **1992**, 44, 807-829	2.1	68
160	Energetics of excess electron transfer in DNA. *Chemical Physics Letters*, **2001**, 342, 231-238	2.5	62
159	Charge transfer in DNA: hole charge is confined to a single base pair due to solvation effects. *Journal of Chemical Physics*, **2005**, 122, 204904	3.9	61
158	Quantum Chemical Calculation of Donor□Acceptor Coupling for Charge Transfer in DNA. *Topics in Current Chemistry*,37-72		58
157	Estimation of electronic coupling in pi-stacked donor-bridge-acceptor systems: correction of the two-state model. *Journal of Chemical Physics*, **2006**, 124, 64505	3.9	57
156	Electronic coupling mediated by stacked [Thymine-Hg-Thymine] base pairs. *Journal of Physical Chemistry B*, **2006**, 110, 21010-3	3.4	54
155	A Quantum Chemical Study of Photoinduced DNA Repair: On the Splitting of Pyrimidine Model Dimers Initiated by Electron Transfer. *Journal of the American Chemical Society*, **1996**, 118, 9750-9758	16.4	52
154	A combined quantum chemical/molecular mechanical study of hydrogen-bonded systems. *International Journal of Quantum Chemistry*, **1992**, 44, 897-930	2.1	52
153	Assessment of semiempirical methods for the computation of charge transfer in DNA □stacks. *Chemical Physics Letters*, **2006**, 427, 177-180	2.5	49
152	Extension of MNDO to d orbitals: parameters and results for silicon. *Computational and Theoretical Chemistry*, **1994**, 313, 141-154		49
151	Quantum Chemical Modeling of Electron Hole Transfer through □Stacks of Normal and Modified Pairs of Nucleobases. *Journal of Physical Chemistry B*, **2002**, 106, 3013-3018	3.4	46
150	MNDO calculations of systems containing hydrogen bonds. *Theoretica Chimica Acta*, **1987**, 72, 223-228		46
149	Substrate Oxidation in the Active Site of Xanthine Oxidase and Related Enzymes. A Model Density Functional Study. *Inorganic Chemistry*, **1998**, 37, 176-180	5.1	43
148	Cyclo[18]carbon: the smallest all-carbon electron acceptor. *Chemical Communications*, **2020**, 56, 352-355	5.8	43
147	Are radical cation states delocalized over GG and GGG hole traps in DNA?. *Journal of Physical Chemistry B*, **2005**, 109, 10793-6	3.4	41
146	Electron-hole transfer in G-quadruplexes with different tetrad stacking geometries: a combined QM and MD study. *Journal of Physical Chemistry B*, **2013**, 117, 9851-6	3.4	40
145	Prediction of Alternative Structures of the Molybdenum Site in the Xanthine Oxidase-Related Aldehyde Oxido Reductase. *Journal of the American Chemical Society*, **1997**, 119, 3159-3160	16.4	40
144	Ab Initio Study on the Structure and Splitting of the Uracil Dimer Anion Radical. *Journal of Physical Chemistry A*, **1997**, 101, 8335-8338	2.8	38

143	Exciton delocalization, charge transfer, and electronic coupling for singlet excitation energy transfer between stacked nucleobases in DNA: an MS-CASPT2 study. *Journal of Chemical Physics*, **2014**, 140, 095102	3.9	37
142	Electronic coupling for charge transfer in donor-bridge-acceptor systems. Performance of the two-state FCD model. *Physical Chemistry Chemical Physics*, **2012**, 14, 13789-93	3.6	34
141	Femtosecond study of light-induced fluorescence increase of the dark chromoprotein asFP595. *Chemical Physics*, **2006**, 323, 149-160	2.3	34
140	Effects of intra base-pairs flexibility on hole transfer coupling in DNA. *Chemical Physics Letters*, **2006**, 429, 546-550	2.5	34
139	Fragment transition density method to calculate electronic coupling for excitation energy transfer. *Journal of Chemical Physics*, **2014**, 140, 244117	3.9	32
138	Electron transfer in DNA. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 780-794	7.9	31
137	Fluctuation of the electronic coupling in DNA: Multistate versus two-state model. *Chemical Physics Letters*, **2007**, 439, 162-165	2.5	31
136	Extension of the Neglect of Diatomic Differential Overlap Method to Spectroscopy. NDDO-G Parametrization and Results for Organic Molecules. *Journal of Physical Chemistry A*, **1999**, 103, 4553-4559	2.8	30
135	On the mechanism of photoinduced dimer dissociation in the plant UVR8 photoreceptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 5219-24	11.5	29
134	Can charge transfer in DNA significantly be modulated by varying the pi stack conformation?. *Journal of Physical Chemistry B*, **2009**, 113, 14365-8	3.4	29
133	MS-CASPT2 calculation of excess electron transfer in stacked DNA nucleobases. *Journal of Physical Chemistry A*, **2007**, 111, 4714-9	2.8	27
132	Multiple Decay Mechanisms and 2D-UV Spectroscopic Fingerprints of Singlet Excited Solvated Adenine-Uracil Monophosphate. *Chemistry - A European Journal*, **2016**, 22, 7497-507	4.8	26
131	Estimation of Electronic Coupling for Photoinduced Charge Separation and Charge Recombination Using the Fragment Charge Difference Method. *Journal of Physical Chemistry C*, **2013**, 117, 2670-2675	3.8	26
130	Estimates of electronic coupling for excess electron transfer in DNA. *Journal of Chemical Physics*, **2005**, 123, 34903	3.9	26
129	Effects of dynamic disorder on exciton delocalization and photoinduced charge separation in DNA. *Photochemical and Photobiological Sciences*, **2013**, 12, 1303-9	4.2	24
128	Triplet-triplet energy transfer in DNA: a process that occurs on the nanosecond timescale. *Angewandte Chemie - International Edition*, **2011**, 50, 1820-2	16.4	24
127	Effect of proton transfer on the electronic coupling in DNA. *Chemical Physics*, **2006**, 325, 567-574	2.3	24
126	Intermediate neglect of differential overlap for spectroscopy. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 515-527	7.9	23

125	INDO/X: A New Semiempirical Method for Excited States of Organic and Biological Molecules. *Journal of Chemical Theory and Computation*, **2014**, 10, 4950-8	6.4	22
124	Influence of base stacking geometry on the nature of excited states in G-quadruplexes: a time-dependent DFT study. *Journal of Physical Chemistry B*, **2015**, 119, 3697-705	3.4	22
123	In-silico assessment of protein-protein electron transfer. a case study: cytochrome c peroxidase--cytochrome c. *PLoS Computational Biology*, **2013**, 9, e1002990	5	22
122	DFT performance for the hole transfer parameters in DNA stacks. *International Journal of Quantum Chemistry*, **2011**, 111, 191-201	2.1	22
121	Electronic couplings in DNA pi-stacks: multistate effects. *Journal of Physical Chemistry B*, **2005**, 109, 17911-21	3.4	22
120	The Effect of Pyrimidine Bases on the Hole-Transfer Coupling in DNA. *Journal of Physical Chemistry B*, **2002**, 106, 7919-7926	3.4	22
119	Splitting of Cyclobutane-Type Uracil Dimer Cation Radicals. Hartree-Fock, MP2, and Density Functional Studies. *Journal of Physical Chemistry A*, **1998**, 102, 7168-7175	2.8	21
118	Pi stack structure and hole transfer couplings in DNA hairpins and DNA. A combined QM/MD study. *Journal of Physical Chemistry B*, **2008**, 112, 8181-7	3.4	21
117	Conformations of poly{G}-poly{C} pi stacks with high hole mobility. *Journal of Chemical Physics*, **2008**, 128, 045104	3.9	21
116	Conformationally Gated Charge Transfer in DNA Three-Way Junctions. *Journal of Physical Chemistry Letters*, **2015**, 6, 2434-8	6.4	20
115	Parameters for excess electron transfer in DNA. Estimation using unoccupied Kohn-Sham orbitals and TD DFT. *Journal of Physical Chemistry A*, **2008**, 112, 9043-9	2.8	20
114	Excited-state photophysics of an acridine derivative selectively intercalated in duplex DNA. *ChemPhysChem*, **2002**, 3, 452-5	3.2	20
113	Effect of Proton Transfer on the Anionic and Cationic Pathways of Pyrimidine Photodimer Cleavage. A Computational Study. *Journal of Physical Chemistry A*, **1999**, 103, 3569-3574	2.8	20
112	All-Fullerene Electron Donor-Acceptor Conjugates. *Angewandte Chemie - International Edition*, **2019**, 58, 6932-6937	16.4	19
111	Distance Dependence of Triplet Energy Transfer in Water and Organic Solvents: A QM/MD Study. *Journal of Physical Chemistry C*, **2012**, 116, 22179-22185	3.8	19
110	DNA base pair stacks with high electric conductance: a systematic structural search. *ACS Nano*, **2012**, 6, 8216-25	16.7	19
109	Electron transfer from aromatic amino acids to guanine and adenine radical cations in pi stacked and T-shaped complexes. *Organic and Biomolecular Chemistry*, **2010**, 8, 1870-5	3.9	19
108	A simple model for calculating atomic charges in molecules. *Physical Chemistry Chemical Physics*, **2018**, 20, 23328-23337	3.6	18

107	Conformational dependence of the electronic coupling for singlet excitation energy transfer in DNA. An INDO/S study. *Physical Chemistry Chemical Physics*, **2010**, 12, 7403-8	3.6	18
106	Long-range electron transfer in biomolecules. Tunneling or hopping?. *Journal of Physical Chemistry B*, **2011**, 115, 12202-7	3.4	18
105	Photoinduced electron transfer and unusual environmental effects in fullerene-Zn-porphyrin-BODIPY triads. *Physical Chemistry Chemical Physics*, **2019**, 21, 25098-25107	3.6	17
104	Buckycatcher. A New Opportunity for Charge-Transfer Mediation?. *Journal of Physical Chemistry C*, **2008**, 112, 1672-1678	3.8	16
103	Fast and accurate calculation of hydration energies of molecules and ions. *Physical Chemistry Chemical Physics*, **2020**, 22, 14591-14598	3.6	15
102	Donor–acceptor electronic couplings in π-stacks: How many states must be accounted for?. *Chemical Physics Letters*, **2006**, 422, 15-19	2.5	15
101	Solvent Effects on Donor-Acceptor Couplings in Peptides. A Combined QM and MD Study. *Journal of Chemical Theory and Computation*, **2009**, 5, 3312-20	6.4	14
100	Stereocontrolled Photoinduced Electron Transfer in Metal-Fullerene Hybrids. *Chemistry - A European Journal*, **2018**, 24, 13020-13025	4.8	14
99	Estimation of Electronic Coupling for Singlet Excitation Energy Transfer. *Journal of Physical Chemistry C*, **2014**, 118, 1478-1483	3.8	13
98	An in silico design for a DNA nanomechanical switch. *ACS Nano*, **2010**, 4, 5737-42	16.7	13
97	Chromophore/DNA interactions: femto- to nanosecond spectroscopy, NMR structure, and electron transfer theory. *Journal of Physical Chemistry B*, **2008**, 112, 973-89	3.4	13
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95	Extent of charge separation and exciton delocalization for electronically excited states in a triphenylamine-C60 donor–acceptor conjugate: a combined molecular dynamics and TD-DFT study. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	12
94	Triplet Excitation Energy Transfer through Fluorene π-Stack. *Journal of Physical Chemistry C*, **2010**, 114, 20236-20239	3.8	12
93	Electron transfer between [4Fe4S] clusters. *Chemical Physics Letters*, **2010**, 495, 131-134	2.5	12
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91	Application of the MNDO method to investigation of properties and reactivity of molecules. *Journal of Structural Chemistry*, **1988**, 29, 120-146	0.9	12
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88	Hole transfer energetics in structurally distorted DNA: the nucleosome core particle. *Journal of Physical Chemistry B*, **2007**, 111, 2976-85	3.4	11
87	Environmental Fluctuations Facilitate Electron-Hole Transfer from Guanine to Adenine in DNA Stacks. *Angewandte Chemie*, **2004**, 116, 634-637	3.6	11
86	A simple COSMO-based method for calculation of hydration energies of neutral molecules. *Physical Chemistry Chemical Physics*, **2019**, 21, 18706-18713	3.6	10
85	Stabilization of radical anion states of nucleobases in DNA. *Physical Chemistry Chemical Physics*, **2009**, 11, 10608-13	3.6	10
84	Photoinduced Charge Separation in the Carbon Nano-Onion C60@C240. *Journal of Physical Chemistry A*, **2016**, 120, 5798-804	2.8	10
83	Thermochemistry of Hydrocarbons. Back to Extended H kel Theory. *Journal of Chemical Theory and Computation*, **2008**, 4, 1877-85	6.4	9
82	All-Fullerene Electron Donor Acceptor Conjugates. *Angewandte Chemie*, **2019**, 131, 7006-7011	3.6	8
81	Excess charge delocalization in organic and biological molecules: some theoretical notions. *Theoretical Chemistry Accounts*, **2009**, 123, 29-40	1.9	8
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79	Theoretical estimation of the rate of photoinduced charge transfer reactions in triphenylamine C60 donor-acceptor conjugate. *Journal of Computational Chemistry*, **2016**, 37, 1396-405	3.5	8
78	Environment effects on triplet riplet energy transfer in DNA. *Chemical Physics Letters*, **2011**, 512, 118-122	2.5	7
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76	Peculiar Photoinduced Electron Transfer in Porphyrin-Fullerene Akamptisomers. *Chemistry - A European Journal*, **2019**, 25, 2577-2585	4.8	7
75	Photoinduced Charge Shift in Li+-Doped Giant Nested Fullerenes. *Journal of Physical Chemistry C*, **2019**, 123, 16525-16532	3.8	6
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70	Thermally induced hopping model for long-range triplet excitation energy transfer in DNA. *Physical Chemistry Chemical Physics*, **2018**, 20, 4997-5000	3.6	5
69	The Driving Force of Photoinduced Charge Separation in Metal-Cluster-Encapsulated Triphenylamine-[80]fullerenes. *Chemistry - A European Journal*, **2016**, 22, 17305-17310	4.8	5
68	Conformational dependence of the electronic coupling for hole transfer between adenine and tryptophan. *Computational and Theoretical Chemistry*, **2011**, 975, 38-41	2	5
67	Triplet□riplet Energy Transfer in DNA: A Process that Occurs on the Nanosecond Timescale. *Angewandte Chemie*, **2011**, 123, 1860-1862	3.6	5
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65	Covalent Functionalization of Single-Walled Carbon Nanotubes by the Bingel Reaction for Building Charge-Transfer Complexes. *Journal of Organic Chemistry*, **2020**, 85, 11721-11731	4.2	5
64	Computational modeling of Charge Transfer in DNA **2006**, 485-511		5
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61	Single Amino Acid Mutation Controls Hole Transfer Dynamics in DNA-Methyltransferase HhaI Complexes. *Journal of Physical Chemistry Letters*, **2015**, 6, 3749-53	6.4	4
60	MS-CASPT2 study of hole transfer in guanine-indole complexes using the generalized Mulliken-Hush method: effective two-state treatment. *Journal of Physical Chemistry B*, **2012**, 116, 7815-20	3.4	4
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57	Electron Transfer in a Li-Doped Zn-Porphyrin-[10]CPP?Fullerene Junction and Charge-Separated Bands with Opposite Response to Polar Environments. *Journal of Physical Chemistry B*, **2020**, 124, 9095-9102	3.4	4
56	Reliable charge assessment on encapsulated fragment for endohedral systems. *Scientific Reports*, **2018**, 8, 2882	4.9	3
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48	Relaxation of the molecular orbitals in palladium complexes. *Journal of Structural Chemistry*, **1982**, 23, 50-55	0.9	3
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45	Photoinduced electron transfer in mechanically interlocked suit[3]ane systems. *Journal of Materials Chemistry C*, **2021**, 9, 9436-9445	7.1	3
44	Evaluation of charge-transfer rates in fullerene-based donor-acceptor dyads with different density functional approximations. *Physical Chemistry Chemical Physics*, **2021**, 23, 5376-5384	3.6	3
43	Conformational dependence of the electronic coupling in guanine□ryptophan complexes: A DFT study. *International Journal of Quantum Chemistry*, **2012**, 112, 1838-1843	2.1	2
42	Can Charge Recombination in DNA Hairpins Be Controlled by Counterions?□*Journal of Physical Chemistry C*, **2010**, 114, 20503-20509	3.8	2
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35	Innenrücktitelbild: All-Fullerene Electron Donor–Acceptor Conjugates (Angew. Chem. 21/2019). *Angewandte Chemie*, **2019**, 131, 7217-7217	3.6	1
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