

# Alexander A Voityuk

## List of Publications by Year in descending order

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182  
papers

5,419  
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87723

38  
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98622

67  
g-index

187  
all docs

187  
docs citations

187  
times ranked

3348  
citing authors

#	ARTICLE	IF	CITATIONS
1	Fragment charge difference method for estimating donor-acceptor electronic coupling: Application to DNA $\pi$ -stacks. <i>Journal of Chemical Physics</i> , 2002, 117, 5607-5616.	1.2	294
2	Extension of MNDO to d Orbitals: Parameters and Results for the Second-Row Elements and for the Zinc Group. <i>The Journal of Physical Chemistry</i> , 1996, 100, 616-626.	2.9	266
3	Electronic Coupling for Charge Transfer and Transport in DNA. <i>Journal of Physical Chemistry B</i> , 2000, 104, 9740-9745.	1.2	249
4	Electronic coupling between Watson-Crick pairs for hole transfer and transport in deoxyribonucleic acid. <i>Journal of Chemical Physics</i> , 2001, 114, 5614-5620.	1.2	228
5	Extension of the MNDO formalism to d orbitals: Integral approximations and preliminary numerical results. <i>Theoretica Chimica Acta</i> , 1992, 81, 391-404.	0.9	196
6	Energetics of hole transfer in DNA. <i>Chemical Physics Letters</i> , 2000, 324, 430-434.	1.2	185
7	Superexchange Mediated Charge Hopping in DNA. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7599-7606.	1.1	155
8	Charge transfer in DNA. Sensitivity of electronic couplings to conformational changes Dedicated to Professor F. Durr on the occasion of his 80th birthday.. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 5421-5425.	1.3	130
9	Environmental Fluctuations Facilitate Electron-Hole Transfer from Guanine to Adenine in DNA $\pi$ -Stacks. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 624-627.	7.2	120
10	Quantum chemical modeling of structure and absorption spectra of the chromophore in green fluorescent proteins. <i>Chemical Physics</i> , 1998, 231, 13-25.	0.9	110
11	Estimate of the Reorganization Energy for Charge Transfer in DNA. <i>Journal of Physical Chemistry B</i> , 2003, 107, 2595-2601.	1.2	104
12	Structure and rotation barriers for ground and excited states of the isolated chromophore of the green fluorescent protein. <i>Chemical Physics Letters</i> , 1998, 296, 269-276.	1.2	99
13	CASSCF/CAS-PT2 Study of Hole Transfer in Stacked DNA Nucleobases. <i>Journal of Physical Chemistry A</i> , 2006, 110, 6426-6432.	1.1	94
14	Electronic couplings and on-site energies for hole transfer in DNA: Systematic quantum mechanical/molecular dynamic study. <i>Journal of Chemical Physics</i> , 2008, 128, 115101.	1.2	87
15	Protonation effects on the chromophore of green fluorescent protein. Quantum chemical study of the absorption spectrum. <i>Chemical Physics Letters</i> , 1997, 272, 162-167.	1.2	86
16	AM1/d Parameters for Molybdenum. <i>Journal of Physical Chemistry A</i> , 2000, 104, 4089-4094.	1.1	82
17	Extension of MNDO to d orbitals: Parameters and results for the halogens. <i>International Journal of Quantum Chemistry</i> , 1992, 44, 807-829.	1.0	78
18	Cyclo[18]carbon: the smallest all-carbon electron acceptor. <i>Chemical Communications</i> , 2020, 56, 352-355.	2.2	78

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19	Absorption spectra of the GFP chromophore in solution: comparison of theoretical and experimental results. <i>Chemical Physics</i> , 2001, 269, 83-91.	0.9	77
20	Energetics of excess electron transfer in DNA. <i>Chemical Physics Letters</i> , 2001, 342, 231-238.	1.2	69
21	Charge transfer in DNA: Hole charge is confined to a single base pair due to solvation effects. <i>Journal of Chemical Physics</i> , 2005, 122, 204904.	1.2	68
22	Estimation of electronic coupling in $\pi$ -stacked donor-bridge-acceptor systems: Correction of the two-state model. <i>Journal of Chemical Physics</i> , 2006, 124, 064505.	1.2	66
23	Quantum Chemical Calculation of Donor-acceptor Coupling for Charge Transfer in DNA. <i>Topics in Current Chemistry</i> , 0, , 37-72.	4.0	62
24	A combined quantum chemical/molecular mechanical study of hydrogen-bonded systems. <i>International Journal of Quantum Chemistry</i> , 1992, 44, 897-930.	1.0	57
25	Extension of MNDO to d orbitals: parameters and results for silicon. <i>Computational and Theoretical Chemistry</i> , 1994, 313, 141-154.	1.5	54
26	A Quantum Chemical Study of Photoinduced DNA Repair: On the Splitting of Pyrimidine Model Dimers Initiated by Electron Transfer. <i>Journal of the American Chemical Society</i> , 1996, 118, 9750-9758.	6.6	54
27	Electronic Coupling Mediated by Stacked [Thymine-Hg-Thymine] Base Pairs. <i>Journal of Physical Chemistry B</i> , 2006, 110, 21010-21013.	1.2	54
28	Assessment of semiempirical methods for the computation of charge transfer in DNA $\pi$ -stacks. <i>Chemical Physics Letters</i> , 2006, 427, 177-180.	1.2	51
29	Substrate Oxidation in the Active Site of Xanthine Oxidase and Related Enzymes. A Model Density Functional Study. <i>Inorganic Chemistry</i> , 1998, 37, 176-180.	1.9	50
30	Quantum Chemical Modeling of Electron Hole Transfer through $\pi$ Stacks of Normal and Modified Pairs of Nucleobases. <i>Journal of Physical Chemistry B</i> , 2002, 106, 3013-3018.	1.2	49
31	Initiating Electron Transfer in Doubly Curved Nanographene Upon Supramolecular Complexation of $C_{60}$ . <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	48
32	MNDO calculations of systems containing hydrogen bonds. <i>Theoretica Chimica Acta</i> , 1987, 72, 223-228.	0.9	47
33	Exciton delocalization, charge transfer, and electronic coupling for singlet excitation energy transfer between stacked nucleobases in DNA: An MS-CASPT2 study. <i>Journal of Chemical Physics</i> , 2014, 140, 095102.	1.2	46
34	Are Radical Cation States Delocalized over GG and GGG Hole Traps in DNA?. <i>Journal of Physical Chemistry B</i> , 2005, 109, 10793-10796.	1.2	45
35	Electron-Hole Transfer in G-Quadruplexes with Different Tetrad Stacking Geometries: A Combined QM and MD Study. <i>Journal of Physical Chemistry B</i> , 2013, 117, 9851-9856.	1.2	45
36	Fragment transition density method to calculate electronic coupling for excitation energy transfer. <i>Journal of Chemical Physics</i> , 2014, 140, 244117.	1.2	44

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37	Prediction of Alternative Structures of the Molybdenum Site in the Xanthine Oxidase-Related Aldehyde Oxido Reductase. <i>Journal of the American Chemical Society</i> , 1997, 119, 3159-3160.	6.6	43
38	Ab Initio Study on the Structure and Splitting of the Uracil Dimer Anion Radical. <i>Journal of Physical Chemistry A</i> , 1997, 101, 8335-8338.	1.1	42
39	Electronic coupling for charge transfer in donor-bridge-acceptor systems. Performance of the two-state FCD model. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 13789.	1.3	42
40	Extension of the Neglect of Diatomic Differential Overlap Method to Spectroscopy. NDDO-G Parametrization and Results for Organic Molecules. <i>Journal of Physical Chemistry A</i> , 1999, 103, 4553-4559.	1.1	37
41	Femtosecond study of light-induced fluorescence increase of the dark chromoprotein asFP595. <i>Chemical Physics</i> , 2006, 323, 149-160.	0.9	36
42	Fast and accurate calculation of hydration energies of molecules and ions. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 14591-14598.	1.3	36
43	Effects of intra base-pairs flexibility on hole transfer coupling in DNA. <i>Chemical Physics Letters</i> , 2006, 429, 546-550.	1.2	35
44	Electron transfer in DNA. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2012, 2, 780-794.	6.2	35
45	All-Fullerene Electron Donor-Acceptor Conjugates. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 6932-6937.	7.2	35
46	Fluctuation of the electronic coupling in DNA: Multistate versus two-state model. <i>Chemical Physics Letters</i> , 2007, 439, 162-165.	1.2	33
47	On the mechanism of photoinduced dimer dissociation in the plant UVR8 photoreceptor. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 5219-5224.	3.3	32
48	Multiple Decay Mechanisms and 2D-UV Spectroscopic Fingerprints of Singlet Excited Solvated Adenine-Uracil Monophosphate. <i>Chemistry - A European Journal</i> , 2016, 22, 7497-7507.	1.7	31
49	Can Charge Transfer in DNA Significantly Be Modulated by Varying the $\pi$ Stack Conformation?. <i>Journal of Physical Chemistry B</i> , 2009, 113, 14365-14368.	1.2	30
50	Estimation of Electronic Coupling for Photoinduced Charge Separation and Charge Recombination Using the Fragment Charge Difference Method. <i>Journal of Physical Chemistry C</i> , 2013, 117, 2670-2675.	1.5	30
51	MS-CASPT2 Calculation of Excess Electron Transfer in Stacked DNA Nucleobases. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4714-4719.	1.1	28
52	Triplet-Triplet Energy Transfer in DNA: A Process that Occurs on the Nanosecond Timescale. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 1820-1822.	7.2	28
53	Influence of Base Stacking Geometry on the Nature of Excited States in G-Quadruplexes: A Time-Dependent DFT Study. <i>Journal of Physical Chemistry B</i> , 2015, 119, 3697-3705.	1.2	28
54	Estimates of electronic coupling for excess electron transfer in DNA. <i>Journal of Chemical Physics</i> , 2005, 123, 034903.	1.2	27

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55	Intermediate neglect of differential overlap for spectroscopy. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 515-527.	6.2	27
56	A simple model for calculating atomic charges in molecules. Physical Chemistry Chemical Physics, 2018, 20, 23328-23337.	1.3	27
57	A simple COSMO-based method for calculation of hydration energies of neutral molecules. Physical Chemistry Chemical Physics, 2019, 21, 18706-18713.	1.3	27
58	Effect of proton transfer on the electronic coupling in DNA. Chemical Physics, 2006, 325, 567-574.	0.9	26
59	INDO/X: A New Semiempirical Method for Excited States of Organic and Biological Molecules. Journal of Chemical Theory and Computation, 2014, 10, 4950-4958.	2.3	26
60	The Effect of Pyrimidine Bases on the Hole-Transfer Coupling in DNA. Journal of Physical Chemistry B, 2002, 106, 7919-7926.	1.2	24
61	Distance Dependence of Triplet Energy Transfer in Water and Organic Solvents: A QM/MD Study. Journal of Physical Chemistry C, 2012, 116, 22179-22185.	1.5	24
62	Effects of dynamic disorder on exciton delocalization and photoinduced charge separation in DNA. Photochemical and Photobiological Sciences, 2013, 12, 1303.	1.6	24
63	Electronic Couplings in DNA $\pi$ -Stacks: Multistate Effects. Journal of Physical Chemistry B, 2005, 109, 17917-17921.	1.2	23
64	Conformations of poly{G}-poly{C} $\pi$ stacks with high hole mobility. Journal of Chemical Physics, 2008, 128, 045104.	1.2	23
65	DFT performance for the hole transfer parameters in DNA $\pi$ stacks. International Journal of Quantum Chemistry, 2011, 111, 191-201.	1.0	23
66	In-silico Assessment of Protein-Protein Electron Transfer. A Case Study: Cytochrome c Peroxidase. PLoS Computational Biology, 2013, 9, e1002990.	1.5	23
67	Conformationally Gated Charge Transfer in DNA Three-Way Junctions. Journal of Physical Chemistry Letters, 2015, 6, 2434-2438.	2.1	23
68	Hypsochromic solvent shift of the charge separation band in ionic donor-acceptor Li <sup>+</sup> @C <sub>60</sub> -[10]CPP. Chemical Communications, 2019, 55, 11195-11198.	2.2	23
69	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.	1.5	22
70	Photoinduced electron transfer and unusual environmental effects in fullerene-Zn-porphyrin-BODIPY triads. Physical Chemistry Chemical Physics, 2019, 21, 25098-25107.	1.3	22
71	Splitting of Cyclobutane-Type Uracil Dimer Cation Radicals. Hartree-Fock, MP2, and Density Functional Studies. Journal of Physical Chemistry A, 1998, 102, 7168-7175.	1.1	21
72	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.	1.1	21

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73	π-Stack Structure and Hole Transfer Couplings in DNA Hairpins and DNA. A Combined QM/MD Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 8181-8187.	1.2	21
74	Fast non-iterative calculation of solvation energies for water and aqueous solvents. <i>Journal of Computational Chemistry</i> , 2021, 42, 1184-1194.	1.5	21
75	Excited-State Photophysics of an Acridine Derivative Selectively Intercalated in Duplex DNA. <i>ChemPhysChem</i> , 2002, 3, 452.	1.0	20
76	Parameters For Excess Electron Transfer in DNA. Estimation Using Unoccupied Kohn-Sham Orbitals and TD DFT. <i>Journal of Physical Chemistry A</i> , 2008, 112, 9043-9049.	1.1	20
77	DNA Base Pair Stacks with High Electric Conductance: A Systematic Structural Search. <i>ACS Nano</i> , 2012, 6, 8216-8225.	7.3	20
78	Long-Range Electron Transfer in Biomolecules. Tunneling or Hopping?. <i>Journal of Physical Chemistry B</i> , 2011, 115, 12202-12207.	1.2	19
79	Conformational dependence of the electronic coupling for singlet excitation energy transfer in DNA. An INDO/S study. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 7403.	1.3	18
80	Iterative Atomic Charge Partitioning of Valence Electron Density. <i>Journal of Computational Chemistry</i> , 2019, 40, 875-884.	1.5	18
81	Evaluation of charge-transfer rates in fullerene-based donor-acceptor dyads with different density functional approximations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 5376-5384.	1.3	18
82	Stereocontrolled Photoinduced Electron Transfer in Metal-Fullerene Hybrids. <i>Chemistry - A European Journal</i> , 2018, 24, 13020-13025.	1.7	17
83	Buckycatcher. A New Opportunity for Charge-Transfer Mediation?. <i>Journal of Physical Chemistry C</i> , 2008, 112, 1672-1678.	1.5	16
84	Photoinduced electron transfer in nanotube-C <sub>70</sub> inclusion complexes: phenine vs. nanographene nanotubes. <i>Chemical Communications</i> , 2020, 56, 12624-12627.	2.2	16
85	Electron Transfer in a Li-Doped Zn-Porphyrin [10]CPP Fullerene Junction and Charge-Separated Bands with Opposite Response to Polar Environments. <i>Journal of Physical Chemistry B</i> , 2020, 124, 9095-9102.	1.2	16
86	Donor-acceptor electronic couplings in π-stacks: How many states must be accounted for?. <i>Chemical Physics Letters</i> , 2006, 422, 15-19.	1.2	15
87	Electron transfer between [4Fe-4S] clusters. <i>Chemical Physics Letters</i> , 2010, 495, 131-134.	1.2	15
88	Electronic Couplings for Photoinduced Electron Transfer and Excitation Energy Transfer Computed Using Excited States of Noninteracting Molecules. <i>Journal of Physical Chemistry A</i> , 2017, 121, 5414-5419.	1.1	15
89	Application of the MNDO method to investigation of properties and reactivity of molecules. <i>Journal of Structural Chemistry</i> , 1988, 29, 120-146.	0.3	14
90	Solvent Effects on Donor-Acceptor Couplings in Peptides. A Combined QM and MD Study. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 3312-3320.	2.3	14

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91	Estimation of Electronic Coupling for Singlet Excitation Energy Transfer. <i>Journal of Physical Chemistry C</i> , 2014, 118, 1478-1483.	1.5	14
92	Hole Transfer Energetics in Structurally Distorted DNA: The Nucleosome Core Particle. <i>Journal of Physical Chemistry B</i> , 2007, 111, 2976-2985.	1.2	13
93	Chromophore/DNA Interactions: Femto- to Nanosecond Spectroscopy, NMR Structure, and Electron Transfer Theory. <i>Journal of Physical Chemistry B</i> , 2008, 112, 973-989.	1.2	13
94	Triplet Excitation Energy Transfer through Fluorene $\pi$ Stack. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20236-20239.	1.5	13
95	An <i>in Silico</i> Design for a DNA Nanomechanical Switch. <i>ACS Nano</i> , 2010, 4, 5737-5742.	7.3	13
96	Extent of charge separation and exciton delocalization for electronically excited states in a triphenylamine-C <sub>60</sub> donor-acceptor conjugate: a combined molecular dynamics and TD-DFT study. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	13
97	Photoinduced Charge Shift in Li <sup>+</sup> -Doped Giant Nested Fullerenes. <i>Journal of Physical Chemistry C</i> , 2019, 123, 16525-16532.	1.5	13
98	All-Fluorene Electron Donor-Acceptor Conjugates. <i>Angewandte Chemie</i> , 2019, 131, 7006-7011.	1.6	13
99	Accurate Treatment of Energetics and Geometry of Carbon and Hydrocarbon Compounds within Tight-Binding Model. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1038-1044.	2.3	12
100	Stabilization of radical anion states of nucleobases in DNA. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 10608.	1.3	10
101	Theoretical estimation of the rate of photoinduced charge transfer reactions in triphenylamine C <sub>60</sub> donor-acceptor conjugate. <i>Journal of Computational Chemistry</i> , 2016, 37, 1396-1405.	1.5	10
102	Photoinduced Charge Separation in the Carbon Nano-Onion C <sub>60</sub> @C <sub>240</sub> . <i>Journal of Physical Chemistry A</i> , 2016, 120, 5798-5804.	1.1	10
103	Thermally induced hopping model for long-range triplet excitation energy transfer in DNA. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4997-5000.	1.3	10
104	Triquinoline-versus Fullerene-Based Cycloparaphenylene Ionic Complexes: Comparison of Photoinduced Charge-Shift Reactions. <i>Chemistry - A European Journal</i> , 2020, 26, 10896-10902.	1.7	10
105	[10]CPP-Based Inclusion Complexes of Charged Fulleropyrrolidines. Effect of the Charge Location on the Photoinduced Electron Transfer. <i>Chemistry - A European Journal</i> , 2021, 27, 8737-8744.	1.7	10
106	Thermochemistry of Hydrocarbons. Back to Extended H <sub>2</sub> ckel Theory. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1877-1885.	2.3	9
107	Excess charge delocalization in organic and biological molecules: some theoretical notions. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 29-40.	0.5	9
108	Peculiar Photoinduced Electron Transfer in Porphyrin-Fluorene Akamptisomers. <i>Chemistry - A European Journal</i> , 2019, 25, 2577-2585.	1.7	9

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109	Photoinduced electron transfer in mechanically interlocked suit[3]ane systems. <i>Journal of Materials Chemistry C</i> , 2021, 9, 9436-9445.	2.7	9
110	Unexpected Disparity in Photoinduced Reactions of C <sub>60</sub> and C <sub>70</sub> in Water with the Generation of O <sub>2</sub> <sup>•-</sup> or <sup>1</sup> O <sub>2</sub> . <i>Jacs Au</i> , 2021, 1, 1601-1611.	3.6	9
111	Initiating Electron Transfer in Doubly Curved Nanographene Upon Supramolecular Complexation of C <sub>60</sub> . <i>Angewandte Chemie</i> , 2022, 134, .	1.6	9
112	The Hunter Falls Prey: Photoinduced Oxidation of C <sub>60</sub> in Inclusion Complex with Perfluorocycloparaphenylene. <i>ChemPhysChem</i> , 2022, 23, .	1.0	9
113	Charge-on-site scheme to estimate the electronic coupling in electron transfer systems. <i>Chemical Physics Letters</i> , 2008, 451, 153-157.	1.2	8
114	Photoinduced electron transfer in nano-Saturn complexes of fullerene. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2126-2133.	1.3	8
115	Solvation Free Energies for Aqueous and Nonaqueous Solutions Computed Using PM7 Atomic Charges. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4544-4553.	2.5	8
116	Temperature Effects on Donor-Acceptor Couplings in Peptides. A Combined Quantum Mechanics and Molecular Dynamics Study. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3241-3248.	2.3	7
117	Environment effects on triplet-triplet energy transfer in DNA. <i>Chemical Physics Letters</i> , 2011, 512, 118-122.	1.2	7
118	Interaction of Dark Excited States. Comparison of Computational Approaches. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7417-7421.	1.2	7
119	How Do Defects in Carbon Nanostructures Regulate the Photoinduced Electron Transfer Processes? The Case of Phenine Nanotubes. <i>ChemPhysChem</i> , 2021, 22, 1178-1186.	1.0	7
120	Change in the electronic structure of the thiocyanate ion on coordination. <i>Journal of Structural Chemistry</i> , 1982, 23, 364-368.	0.3	6
121	Superexchange Pathways in Charge Transfer through a DNA $\pi$ -Stack. <i>Israel Journal of Chemistry</i> , 2004, 44, 109-117.	1.0	6
122	Modified tight-binding model for fast and accurate estimation of thermochemistry and molecular structure. Parameters and results for hydrocarbons. <i>Chemical Physics Letters</i> , 2006, 433, 216-220.	1.2	6
123	How to Switch the Direction of Photoinduced Charge Injection into DNA?. <i>Journal of Physical Chemistry C</i> , 2007, 111, 7207-7210.	1.5	6
124	Conformational dependence of the electronic coupling for hole transfer between adenine and tryptophan. <i>Computational and Theoretical Chemistry</i> , 2011, 975, 38-41.	1.1	6
125	How abasic sites impact hole transfer dynamics in GC-rich DNA sequences. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 23123-23131.	1.3	6
126	Covalent Functionalization of Single-Walled Carbon Nanotubes by the Bingel Reaction for Building Charge-Transfer Complexes. <i>Journal of Organic Chemistry</i> , 2020, 85, 11721-11731.	1.7	6



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127	Nitrogen-doped molecular bowls as electron donors in photoinduced electron transfer reactions. <i>Nanoscale Advances</i> , 2022, 4, 2180-2188.	2.2	6
128	Single Amino Acid Mutation Controls Hole Transfer Dynamics in DNA-Methyltransferase <i>HhaI</i> Complexes. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 3749-3753.	2.1	5
129	The Driving Force of Photoinduced Charge Separation in Metal-Cluster-Encapsulated Triphenylamine- $C_{80}$ fullerenes. <i>Chemistry - A European Journal</i> , 2016, 22, 17305-17310.	1.7	5
130	Reliable charge assessment on encapsulated fragment for endohedral systems. <i>Scientific Reports</i> , 2018, 8, 2882.	1.6	5
131	Computational modeling of Charge Transfer in DNA. , 2006, , 485-511.		5
132	A cyclic intermediate of the splitting reaction of cyclobutane-type pyrimidine dimer cation radicals. A computational finding as challenge for experimental techniques. <i>Computational and Theoretical Chemistry</i> , 1999, 488, 163-168.	1.5	4
133	Energetics of the splitting of pyrimidine photodimers induced by electron transfer to rhodium(III) complexes. A quantum chemical study. <i>International Journal of Quantum Chemistry</i> , 2000, 77, 128-138.	1.0	4
134	Thermochemistry of Pt <sup>II</sup> -Fullerene Complexes: Semiempirical Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11801-11808.	1.1	4
135	MS-CASPT2 Study of Hole Transfer in Guanine-Indole Complexes Using the Generalized Mulliken-Hush Method: Effective Two-State Treatment. <i>Journal of Physical Chemistry B</i> , 2012, 116, 7815-7820.	1.2	4
136	On the performance of the Kohn-Sham orbital approach in the calculation of electron transfer parameters. The three state model. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 17154-17162.	1.3	4
137	Relaxation of the molecular orbitals in palladium complexes. <i>Journal of Structural Chemistry</i> , 1982, 23, 50-55.	0.3	3
138	MNDO calculations of systems with hydrogen bonds S-H. <i>Theoretica Chimica Acta</i> , 1987, 71, 327-331.	0.9	3
139	Revised semiempirical parameters for Br, I, Sn, Hg, and Pb in the MNDO method. <i>Journal of Structural Chemistry</i> , 1987, 28, 9-12.	0.3	3
140	Molecular mechanics calculations of systems with strong hydrogen bonds. <i>Journal of Molecular Structure</i> , 1992, 265, 179-187.	1.8	3
141	Direct estimation of the transfer integral for photoinduced electron transfer from TD DFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 31007-31010.	1.3	3
142	Photoinduced electron transfer in non-covalent complexes of C60 and phosphangulene oxide derivatives. <i>Dalton Transactions</i> , 2021, 50, 16214-16222.	1.6	3
143	Mutual influence of the ligands in the complexes [Pd(NH3)2X2]. <i>Journal of Structural Chemistry</i> , 1980, 21, 276-280.	0.3	2
144	X-ray spectra and model quantum-chemical calculation of SO2 in clathrates based on hydroquinone. <i>Journal of Structural Chemistry</i> , 1984, 25, 371-376.	0.3	2

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145	MNDO calculations of Mg compounds. <i>Journal of Structural Chemistry</i> , 1988, 28, 926-929.	0.3	2
146	Quantum-chemical study of the mechanism of the hydrolysis of amides in the gas phase and in aqueous solution. <i>Bulletin of the Academy of Sciences of the USSR Division of Chemical Science</i> , 1989, 38, 1635-1641.	0.0	2
147	Can Charge Recombination in DNA Hairpins Be Controlled by Counterions?. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20503-20509.	1.5	2
148	Effects of various halogen anions and cations of alkali metals on energetics of excess charge recombination in stilbene donor-acceptor capped DNA hairpins. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 16028.	1.3	2
149	Conformational dependence of the electronic coupling in guanine-tryptophan complexes: A DFT study. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 1838-1843.	1.0	2
150	Interligand interaction in planar complexes of palladium (II) and platinum (II). <i>Journal of Structural Chemistry</i> , 1981, 22, 282-285.	0.3	1
151	Study of rotational isomerism in thiophenol, thioanisole, and their polyfluorinated derivatives. <i>Journal of Structural Chemistry</i> , 1982, 23, 194-197.	0.3	1
152	MNDO calculations on systems containing S-H hydrogen bonds. <i>Journal of Structural Chemistry</i> , 1987, 28, 5-8.	0.3	1
153	The MNDO-85 system of programs for calculating the electronic structure, physicochemical properties, and reactivity of molecular systems by the MDNO, MNDOC, and AM1 semiempirical methods. <i>Journal of Structural Chemistry</i> , 1987, 27, 674-676.	0.3	1
154	Complexes with hydrogen bonds by the MNDO/M method. <i>Journal of Structural Chemistry</i> , 1988, 29, 192-197.	0.3	1
155	Structural features of labile N-phosphorylammonium zwitterions and cations according to data from MNDO calculations and <sup>15</sup> N NMR spectroscopy. <i>Bulletin of the Academy of Sciences of the USSR Division of Chemical Science</i> , 1989, 38, 1177-1182.	0.0	1
156	Diazabicycloalkanes with nitrogen atoms in bridgehead positions.. <i>Chemistry of Heterocyclic Compounds</i> , 1989, 25, 305-310.	0.6	1
157	Structure and energy characteristic of [Mg(H <sub>3</sub> O) <sub>n</sub> ] <sup>2+</sup> and [Mg(H <sub>2</sub> O) <sub>n-1</sub> OH] <sup>+</sup> complexes according to data from MNDO calculations. <i>Journal of Structural Chemistry</i> , 1992, 32, 590-593.	0.3	1
158	Quantum chemical study of molecular ion complexes with hydrogen bonds (Review). <i>Journal of Structural Chemistry</i> , 1993, 33, 899-924.	0.3	1
159	Innen-Äußertitelbild: All-Fullerene Electron Donor-Acceptor Conjugates ( <i>Angew. Chem.</i> 21/2019). <i>Angewandte Chemie</i> , 2019, 131, 7217-7217.	1.6	1
160	An indo study of the electronic structure of the planar complexes [Pd(NH <sub>3</sub> ) <sub>n</sub> Cl <sub>4-n</sub> ] <sup>2-</sup> . <i>Journal of Structural Chemistry</i> , 1980, 21, 281-286.	0.3	0
161	Use of the eigenvalues of the matrix of the resonance interaction of the orbitals for an analysis of the M-lig bonds in the complexes cis- and trans-[Pd(NH <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub> ]. <i>Journal of Structural Chemistry</i> , 1981, 22, 504-507.	0.3	0
162	One-center parameters dependent on the valence state of the atom. <i>Journal of Structural Chemistry</i> , 1981, 22, 614-616.	0.3	0

#	ARTICLE	IF	CITATIONS
163	Electronic structure of anions of organic dithioacids and their oxidation-reduction and electron-donor properties. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1981, 30, 765-769.	0.0	0
164	One-center parameters dependent on the valence state of the atom. III. Transition elements of periods IV and V. Journal of Structural Chemistry, 1982, 22, 783-786.	0.3	0
165	Use of X-ray spectra to determine the semiempirical parameters of 4d transition metals. Journal of Structural Chemistry, 1982, 23, 355-359.	0.3	0
166	Program for calculating the electronic structure of molecules, complexes, and clusters in the INDO approximation. Journal of Structural Chemistry, 1983, 23, 821-822.	0.3	0
167	A generalization of the half-electron method for calculations for complex compounds. Journal of Structural Chemistry, 1983, 24, 344-348.	0.3	0
168	The transition state in the half-electron method. Journal of Structural Chemistry, 1984, 24, 593-596.	0.3	0
169	Investigation of electronic structure of chloro complexes of Rhodium(III). Journal of Structural Chemistry, 1984, 25, 351-355.	0.3	0
170	X-ray spectra and electronic structure of the $PCl_3$ molecule. Journal of Structural Chemistry, 1984, 24, 676-682.	0.3	0
171	An x-ray spectral and quantum-chemical study of the electronic structure of ruthenium complexes. Journal of Structural Chemistry, 1984, 24, 837-842.	0.3	0
172	Quantum-chemical study of the influence of the electronegativity of substituents on the reactivity of $\alpha$ -chloroethylamine derivatives. Journal of Structural Chemistry, 1986, 27, 367-371.	0.3	0
173	A program for searching for semiempirical parameters by the MNDO method. Journal of Structural Chemistry, 1987, 28, 312-314.	0.3	0
174	Parameters of MNDO method for Zn atom. Journal of Structural Chemistry, 1988, 28, 649-652.	0.3	0
175	Quantum-chemical study of the effect of solvation on the strength of the phosphamide bond in N-phosphorylammonium cations and zwitterions. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1989, 38, 267-270.	0.0	0
176	Quantum-chemical investigation of the mechanism of nucleophilic addition in the HCNO molecule. Theoretical and Experimental Chemistry, 1989, 25, 662-665.	0.2	0
177	MNDO parameters for the Ca atom. Journal of Structural Chemistry, 1989, 29, 793-795.	0.3	0
178	Stereoelectronic effect in reactions of phosphoester bond rupture. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1990, 39, 2286-2289.	0.0	0
179	Use of AM1 and PM3 methods for the investigation of energies and structures of compounds $O=PXYZ$ , $S=PXYZ$ . Journal of Structural Chemistry, 1991, 31, 684-685.	0.3	0
180	Quantum chemical modeling of charge transfer in DNA. , 2006, , 99-119.		0

#	ARTICLE	IF	CITATIONS
181	(Invited) Photoinduced Charge Separation in Several Dyads Involving Fullerenes. ECS Meeting Abstracts, 2019, , .	0.0	0
182	(Invited) Reactivity of Li+@C60@C240 and Photoinduced Charge Shift in Li+ Doped Giant Nested Fullerenes. ECS Meeting Abstracts, 2020, MA2020-01, 809-809.	0.0	0