Lyudmila V Slipchenko

List of Publications by Year in Descending Order

84 papers	9,000 citations	37 h-index	88 g-index
88 ext. papers	10,114 ext. citations	6 avg, IF	5.78 L-index

#	Paper	IF	Citations
84	Hydration and Seamless Integration of Hydrogen Peroxide in Water. *Journal of Physical Chemistry B*, **2021**,	3.4	2
83	Interaction of Polymers with Enzalutamide Nanodroplets-Impact on Droplet Properties and Induction Times. *Molecular Pharmaceutics*, **2021**, 18, 836-849	5.6	4
82	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
81	The unusual symmetry of hexafluoro-o-xylene-A microwave spectroscopy and computational study. *Journal of Chemical Physics*, **2020**, 152, 064302	3.9	1
80	Predictive First-Principles Modeling of a Photosynthetic Antenna Protein: The Fenna-Matthews-Olson Complex. *Journal of Physical Chemistry Letters*, **2020**, 11, 1636-1643	6.4	10
79	Multiagent Consensus Equilibrium in Molecular Structure Determination. *Journal of Physical Chemistry A*, **2020**, 124, 9105-9112	2.8	
78	FMOxFMO: Elucidating Excitonic Interactions in the Fenna-Matthews-Olson Complex with the Fragment Molecular Orbital Method. *Journal of Chemical Theory and Computation*, **2020**, 16, 1175-1187	6.4	6
77	Effective Fragment Potentials for Flexible Molecules: Transferability of Parameters and Amino Acid Database. *Journal of Chemical Theory and Computation*, **2020**, 16, 7735-7747	6.4	3
76	Exchange Repulsion in Quantum Mechanical/Effective Fragment Potential Excitation Energies: Beyond Polarizable Embedding. *Journal of Chemical Theory and Computation*, **2020**, 16, 6408-6417	6.4	5
75	Recent developments in the general atomic and molecular electronic structure system. *Journal of Chemical Physics*, **2020**, 152, 154102	3.9	274
74	Polarizable embedding for simulating redox potentials of biomolecules. *Physical Chemistry Chemical Physics*, **2019**, 21, 11642-11650	3.6	12
73	The effects of site asymmetry on near-degenerate state-to-state vibronic mixing in flexible bichromophores. *Journal of Chemical Physics*, **2019**, 151, 084313	3.9	1
72	Triplet-Triplet Coupling in Chromophore Dimers: Theory and Experiment. *Journal of Physical Chemistry A*, **2018**, 122, 6713-6723	2.8	5
71	Phase Behavior of Drug-Hydroxypropyl Methylcellulose Amorphous Solid Dispersions Produced from Various Solvent Systems: Mechanistic Understanding of the Role of Polymer using Experimental and Theoretical Methods. *Molecular Pharmaceutics*, **2018**, 15, 3236-3251	5.6	13
70	Exchange-repulsion energy in QM/EFP. *Journal of Chemical Physics*, **2018**, 149, 094103	3.9	13
69	Crystallization Inhibition Properties of Cellulose Esters and Ethers for a Group of Chemically Diverse Drugs: Experimental and Computational Insight. *Biomacromolecules*, **2018**, 19, 4593-4606	6.9	14
68	Multipole Moments in the Effective Fragment Potential Method. *Journal of Physical Chemistry A*, **2017**, 121, 2056-2067	2.8	6

67	Effective Fragment Potential Method for H-Bonding: How To Obtain Parameters for Nonrigid Fragments. *Journal of Physical Chemistry A*, **2017**, 121, 5301-5312	2.8	4
66	To Be or Not To Be Symmetric: That Is the Question for Potentially Active Vibronic Modes. *Journal of Chemical Education*, **2017**, 94, 1232-1237	2.4	2
65	Dispersion Interactions in QM/EFP. *Journal of Physical Chemistry A*, **2017**, 121, 9495-9507	2.8	15
64	Effective Fragment Potential Method: Past, Present, and Future **2017**, 183-208		13
63	A new structural arrangement in proteins involving lysine NH group and carbonyl. *Scientific Reports*, **2017**, 7, 16402	4.9	6
62	A Comparison of the Crystallization Inhibition Properties of Bile Salts. *Crystal Growth and Design*, **2016**, 16, 7286-7300	3.5	37
61	The acid-catalyzed hydrolysis of an <i></i>-pinene-derived organic nitrate: kinetics, products, reaction mechanisms, and atmospheric impact. *Atmospheric Chemistry and Physics*, **2016**, 16, 15425-15432	6.8	39
60	Photochemical degradation of isoprene-derived 4,1-nitrooxy enal. *Atmospheric Chemistry and Physics*, **2016**, 16, 5595-5610	6.8	21
59	Extension of the Effective Fragment Potential Method to Macromolecules. *Journal of Physical Chemistry B*, **2016**, 120, 6562-74	3.4	65
58	Radical damage in lipids investigated with the fragment molecular orbital method. *Chemical Physics Letters*, **2016**, 651, 56-61	2.5	7
57	Thermodynamics and Kinetics for the Free Radical Oxygen Protein Oxidation Pathway in a Model for Structured Peptides. *Journal of Physical Chemistry A*, **2016**, 120, 2493-503	2.8	3
56	Mechanistic Design of Chemically Diverse Polymers with Applications in Oral Drug Delivery. *Biomacromolecules*, **2016**, 17, 3659-3671	6.9	36
55	Ground-State Charge Transfer: Lithium-Benzene and the Role of Hartree-Fock Exchange. *Journal of Physical Chemistry A*, **2016**, 120, 8190-8198	2.8	10
54	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
53	Thermal Isomerizations of Diethynyl Cyclobutadienes and Implications for Fullerene Formation. *Journal of Organic Chemistry*, **2015**, 80, 11863-8	4.2	3
52	Hybrid MPI/OpenMP parallelization of the effective fragment potential method in the libefp software library. *Journal of Computational Chemistry*, **2015**, 36, 129-35	3.5	14
51	Assessing cholesterol storage in live cells and C. elegans by stimulated Raman scattering imaging of phenyl-Diyne cholesterol. *Scientific Reports*, **2015**, 5, 7930	4.9	90
50	Vibronic coupling in asymmetric bichromophores: experimental investigation of diphenylmethane-d *Journal of Chemical Physics*, **2014**, 141, 064316	3.9	12

49	Excited states of OH-(H□)n clusters for n = 1-4: an ab initio study. *Journal of Chemical Physics*, **2014**, 141, 104315	3.9	18
48	Vibronic coupling in asymmetric bichromophores: theory and application to diphenylmethane-d(5). *Journal of Chemical Physics*, **2014**, 141, 134119	3.9	8
47	Atmospheric significance of water clusters and ozone-water complexes. *Journal of Physical Chemistry A*, **2013**, 117, 10381-96	2.8	78
46	LIBEFP: A new parallel implementation of the effective fragment potential method as a portable software library. *Journal of Computational Chemistry*, **2013**, 34, 2284-92	3.5	44
45	Effective fragment potential method in Q-CHEM: a guide for users and developers. *Journal of Computational Chemistry*, **2013**, 34, 1060-70	3.5	44
44	Accurate first principles model potentials for intermolecular interactions. *Annual Review of Physical Chemistry*, **2013**, 64, 553-78	15.7	126
43	Interactions between halide anions and a molecular hydrophobic interface. *Faraday Discussions*, **2013**, 160, 255-70; discussion 311-27	3.6	42
42	Jet-cooled spectroscopy of the □methylbenzyl radical: probing the state-dependent effects of methyl rocking against a radical site. *Journal of Physical Chemistry A*, **2013**, 117, 13465-80	2.8	16
41	Open-shell pair interaction energy decomposition analysis (PIEDA): formulation and application to the hydrogen abstraction in tripeptides. *Journal of Chemical Physics*, **2013**, 138, 074111	3.9	36
40	Fragmentation methods: a route to accurate calculations on large systems. *Chemical Reviews*, **2012**, 112, 632-72	68.1	799
39	Accurate Prediction of Noncovalent Interaction Energies with the Effective Fragment Potential Method: Comparison of Energy Components to Symmetry-Adapted Perturbation Theory for the S22 Test Set. *Journal of Chemical Theory and Computation*, **2012**, 8, 2835-43	6.4	80
38	Effects of ethynyl substituents on the electronic structure of cyclobutadiene. *Journal of Physical Chemistry A*, **2012**, 116, 3194-201	2.8	6
37	Conformationally locked chromophores as models of excited-state proton transfer in fluorescent proteins. *Journal of the American Chemical Society*, **2012**, 134, 6025-32	16.4	136
36	Intermolecular interactions in complex liquids: effective fragment potential investigation of water-tert-butanol mixtures. *Journal of Physical Chemistry B*, **2012**, 116, 2775-86	3.4	37
35	The dispersion interaction between quantum mechanics and effective fragment potential molecules. *Journal of Chemical Physics*, **2012**, 136, 244107	3.9	22
34	Vibronic coupling in asymmetric bichromophores: theory and application to diphenylmethane. *Journal of Chemical Physics*, **2012**, 137, 084112	3.9	22
33	Effect of solvation on the vertical ionization energy of thymine: from microhydration to bulk. *Journal of Physical Chemistry A*, **2011**, 115, 6028-38	2.8	84
32	Evolution of amide stacking in larger □peptides: triamide H-bonded cycles. *Journal of Physical Chemistry A*, **2011**, 115, 13783-98	2.8	73

31	Modeling Solvent Effects on Electronic Excited States. *Journal of Physical Chemistry Letters*, **2011**, 2, 2184-2192	6.4	90
30	Computational investigation of amine-oxygen exciplex formation. *Journal of Physical Chemistry A*, **2011**, 115, 10159-65	2.8	9
29	Effective fragment potential study of the interaction of DNA bases. *Journal of Physical Chemistry A*, **2011**, 115, 11269-76	2.8	32
28	Hydrogen Bonding in Liquid Water. *Journal of Physical Chemistry Letters*, **2011**, 2, 2930-2933	6.4	113
27	Benzene-pyridine interactions predicted by the effective fragment potential method. *Journal of Physical Chemistry A*, **2011**, 115, 4598-609	2.8	44
26	Solvent effects on the electronic transitions of p-nitroaniline: a QM/EFP study. *Journal of Physical Chemistry A*, **2011**, 115, 392-401	2.8	100
25	Systematic study of the embedding potential description in the fragment molecular orbital method. *Journal of Physical Chemistry A*, **2010**, 114, 8742-53	2.8	49
24	Solvation of the excited states of chromophores in polarizable environment: orbital relaxation versus polarization. *Journal of Physical Chemistry A*, **2010**, 114, 8824-30	2.8	120
23	Noncovalent interactions in extended systems described by the effective fragment potential method: theory and application to nucleobase oligomers. *Journal of Physical Chemistry A*, **2010**, 114, 12739-54	2.8	91
22	Solvent-induced frequency shifts: configuration interaction singles combined with the effective fragment potential method. *Journal of Physical Chemistry A*, **2010**, 114, 6742-50	2.8	72
21	Damping functions in the effective fragment potential method. *Molecular Physics*, **2009**, 107, 999-1016	1.7	81
20	Double spin-flip approach within equation-of-motion coupled cluster and configuration interaction formalisms: Theory, implementation, and examples. *Journal of Chemical Physics*, **2009**, 130, 044103	3.9	82
19	Accurate methods for large molecular systems. *Journal of Physical Chemistry B*, **2009**, 113, 9646-63	3.4	170
18	Water-benzene interactions: an effective fragment potential and correlated quantum chemistry study. *Journal of Physical Chemistry A*, **2009**, 113, 2092-102	2.8	88
17	Intramolecular amide stacking and its competition with hydrogen bonding in a small foldamer. *Journal of the American Chemical Society*, **2009**, 131, 14243-5	16.4	54
16	The binding of Ag+ and Au+ to ethene. *Journal of Physical Chemistry A*, **2009**, 113, 7474-81	2.8	28
15	Coarse-Grained Intermolecular Potentials Derived From The Effective Fragment Potential: Application To Water, Benzene, And Carbon Tetrachloride. *Challenges and Advances in Computational Chemistry and Physics*, **2009**, 197-218	0.7	3
14	Modeling pi-pi interactions with the effective fragment potential method: the benzene dimer and substituents. *Journal of Physical Chemistry A*, **2008**, 112, 5286-94	2.8	60

13	Electrostatic energy in the effective fragment potential method: theory and application to benzene dimer. *Journal of Computational Chemistry*, **2007**, 28, 276-91	3.5	103
12	Breaking the Curse of the Non-Dynamical Correlation Problem: The Spin-Flip Method. *ACS Symposium Series*, **2007**, 89-102	0.4	10
11	Efficient strategies for accurate calculations of electronic excitation and ionization energies: theory and application to the dehydro-m-xylylene anion. *Journal of Physical Chemistry A*, **2006**, 110, 291-8	2.8	14
10	Advances in methods and algorithms in a modern quantum chemistry program package. *Physical Chemistry Chemical Physics*, **2006**, 8, 3172-91	3.6	2371
9	Spin-conserving and spin-flipping equation-of-motion coupled-cluster method with triple excitations. *Journal of Chemical Physics*, **2005**, 123, 084107	3.9	102
8	5-Dehydro-1,3-quinodimethane: a hydrocarbon with an open-shell doublet ground state. *Angewandte Chemie - International Edition*, **2004**, 43, 742-5	16.4	54
7	Cover Picture: 5-Dehydro-1,3-quinodimethane: A Hydrocarbon with an Open-Shell Doublet Ground State (Angew. Chem. Int. Ed. 6/2004). *Angewandte Chemie - International Edition*, **2004**, 43, 647-647	16.4	
6	5-Dehydro-1,3-quinodimethane: A Hydrocarbon with an Open-Shell Doublet Ground State. *Angewandte Chemie*, **2004**, 116, 760-763	3.6	1
5	Titelbild: 5-Dehydro-1,3-quinodimethane: A Hydrocarbon with an Open-Shell Doublet Ground State (Angew. Chem. 6/2004). *Angewandte Chemie*, **2004**, 116, 663-663	3.6	
4	Reactivity and structure of the 5-dehydro-m-xylylene anion. *Journal of Organic Chemistry*, **2004**, 69, 5735-41	4.1	16
3	Electronic structure of the trimethylenemethane diradical in its ground and electronically excited states: Bonding, equilibrium geometries, and vibrational frequencies. *Journal of Chemical Physics*, **2003**, 118, 6874-6883	3.9	83
2	Electronic structure of the 1,3,5-tridehydrobenzene triradical in its ground and excited states. *Journal of Chemical Physics*, **2003**, 118, 9614-9622	3.9	53
1	Singlet-triplet gaps in diradicals by the spin-flip approach: A benchmark study. *Journal of Chemical Physics*, **2002**, 117, 4694-4708	3.9	294