Lyudmila V Slipchenko

List of Publications by Year
in descending order

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99 papers	11,728 citations	74677 40 h-index	49007 88 g-index
102 all docs	102 docs citations	102 times ranked	12722 citing authors

#	Article	IF	Citations
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,647
2	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	2.9	2,632
3	Fragmentation Methods: A Route to Accurate Calculations on Large Systems. Chemical Reviews, 2012, 112, 632-672.	51.4	970
4	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	3.1	827
5	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.1	619
6	Singlet-triplet gaps in diradicals by the spin-flip approach: A benchmark study. Journal of Chemical Physics, 2002, 117, 4694-4708.	3.1	323
7	Accurate Methods for Large Molecular Systems. Journal of Physical Chemistry B, 2009, 113, 9646-9663.	2.7	189
8	Conformationally Locked Chromophores as Models of Excited-State Proton Transfer in Fluorescent Proteins. Journal of the American Chemical Society, 2012, 134, 6025-6032.	14.6	171
9	Accurate First Principles Model Potentials for Intermolecular Interactions. Annual Review of Physical Chemistry, 2013, 64, 553-578.	11.3	152
10	Solvation of the Excited States of Chromophores in Polarizable Environment: Orbital Relaxation versus Polarization^{â€}. Journal of Physical Chemistry A, 2010, 114, 8824-8830.	2.6	134
11	Ï€-Hydrogen Bonding in Liquid Water. Journal of Physical Chemistry Letters, 2011, 2, 2930-2933.	4.9	132
12	Assessing Cholesterol Storage in Live Cells and C. elegans by Stimulated Raman Scattering Imaging of Phenyl-Diyne Cholesterol. Scientific Reports, 2015, 5, 7930.	3.4	126
13	Solvent Effects on the Electronic Transitions ofp-Nitroaniline: A QM/EFP Study. Journal of Physical Chemistry A, 2011, 115, 392-401.	2.6	114
14	Spin-conserving and spin-flipping equation-of-motion coupled-cluster method with triple excitations. Journal of Chemical Physics, 2005, 123, 084107.	3.1	110
15	Modeling Solvent Effects on Electronic Excited States. Journal of Physical Chemistry Letters, 2011, 2, 2184-2192.	4.9	109
16	Electrostatic energy in the effective fragment potential method: Theory and application to benzene dimer. Journal of Computational Chemistry, 2007, 28, 276-291.	3.5	108
17	Atmospheric Significance of Water Clusters and Ozoneâ€“Water Complexes. Journal of Physical Chemistry A, 2013, 117, 10381-10396.	2.6	107
18	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, 12739-12754.	2.6	102

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19	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, 2835-2843.	5.6	101
20	Effect of Solvation on the Vertical Ionization Energy of Thymine: From Microhydration to Bulk. Journal of Physical Chemistry A, 2011, 115, 6028-6038.	2.6	100
21	Damping functions in the effective fragment potential method. Molecular Physics, 2009, 107, 999-1016.	1.7	99
22	Waterâˆ'Benzene Interactions: An Effective Fragment Potential and Correlated Quantum Chemistry Study. Journal of Physical Chemistry A, 2009, 113, 2092-2102.	2.6	97
23	Electronic structure of the trimethylenemethane diradical in its ground and electronically excited states:â€,Bonding, equilibrium geometries, and vibrational frequencies. Journal of Chemical Physics, 2003, 118, 6874-6883.	3.1	92
24	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.	3.1	88
25	Evolution of Amide Stacking in Larger Î³-Peptides: Triamide H-Bonded Cycles. Journal of Physical Chemistry A, 2011, 115, 13783-13798.	2.6	77
26	Extension of the Effective Fragment Potential Method to Macromolecules. Journal of Physical Chemistry B, 2016, 120, 6562-6574.	2.7	76
27	Solvent-Induced Frequency Shifts: Configuration Interaction Singles Combined with the Effective Fragment Potential Method. Journal of Physical Chemistry A, 2010, 114, 6742-6750.	2.6	74
28	Modeling Ï€â€“Ï€ Interactions with the Effective Fragment Potential Method: The Benzene Dimer and Substituents. Journal of Physical Chemistry A, 2008, 112, 5286-5294.	2.6	71
29	Systematic Study of the Embedding Potential Description in the Fragment Molecular Orbital Method^{â€}. Journal of Physical Chemistry A, 2010, 114, 8742-8753.	2.6	61
30	Electronic structure of the 1,3,5-tridehydrobenzene triradical in its ground and excited states. Journal of Chemical Physics, 2003, 118, 9614-9622.	3.1	60
31	Intramolecular Amide Stacking and Its Competition with Hydrogen Bonding in a Small Foldamer. Journal of the American Chemical Society, 2009, 131, 14243-14245.	14.6	60
32	5-Dehydro-1,3-quinodimethane: A Hydrocarbon with an Open-Shell Doublet Ground State. Angewandte Chemie - International Edition, 2004, 43, 742-745.	14.8	58
33	The acid-catalyzed hydrolysis of an <i>Î±</i>-pinene-derived organic nitrate: kinetics, products, reaction mechanisms, and atmospheric impact. Atmospheric Chemistry and Physics, 2016, 16, 15425-15432.	5.0	57
34	LIBEFP: A new parallel implementation of the effective fragment potential method as a portable software library. Journal of Computational Chemistry, 2013, 34, 2284-2292.	3.5	55
35	Benzeneâˆ'Pyridine Interactions Predicted by the Effective Fragment Potential Method. Journal of Physical Chemistry A, 2011, 115, 4598-4609.	2.6	50
36	Effective fragment potential method in <scp>Qâ€CHEM</scp>: A guide for users and developers. Journal of Computational Chemistry, 2013, 34, 1060-1070.	3.5	49

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37	Interactions between halide anions and a molecular hydrophobic interface. Faraday Discussions, 2013, 160, 255-270.	3.7	48
38	A Comparison of the Crystallization Inhibition Properties of Bile Salts. Crystal Growth and Design, 2016, 16, 7286-7300.	3.2	47
39	Mechanistic Design of Chemically Diverse Polymers with Applications in Oral Drug Delivery. Biomacromolecules, 2016, 17, 3659-3671.	5.6	45
40	Intermolecular Interactions in Complex Liquids: Effective Fragment Potential Investigation of Waterâ€“tert-Butanol Mixtures. Journal of Physical Chemistry B, 2012, 116, 2775-2786.	2.7	42
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.	3.1	39
42	Effective Fragment Potential Study of the Interaction of DNA Bases. Journal of Physical Chemistry A, 2011, 115, 11269-11276.	2.6	37
43	Photochemical degradation of isoprene-derived 4,1-nitrooxy enal. Atmospheric Chemistry and Physics, 2016, 16, 5595-5610.	5.0	32
44	The Binding of Ag⁺ and Au⁺ to Ethene. Journal of Physical Chemistry A, 2009, 113, 7474-7481.	2.6	29
45	The dispersion interaction between quantum mechanics and effective fragment potential molecules. Journal of Chemical Physics, 2012, 136, 244107.	3.1	29
46	Vibronic coupling in asymmetric bichromophores: Theory and application to diphenylmethane. Journal of Chemical Physics, 2012, 137, 084112.	3.1	24
47	Dispersion Interactions in QM/EFP. Journal of Physical Chemistry A, 2017, 121, 9495-9507.	2.6	23
48	Effective Fragment Potential Method: Past, Present, and Future. , 2017, , 183-208.		22
49	Exchange-repulsion energy in QM/EFP. Journal of Chemical Physics, 2018, 149, 094103.	3.1	22
50	Crystallization Inhibition Properties of Cellulose Esters and Ethers for a Group of Chemically Diverse Drugs: Experimental and Computational Insight. Biomacromolecules, 2018, 19, 4593-4606.	5.6	22
51	Polarizable embedding for simulating redox potentials of biomolecules. Physical Chemistry Chemical Physics, 2019, 21, 11642-11650.	2.9	22
52	Excited states of OH-(H2O)n clusters for n = 1â€“4: An ab initio study. Journal of Chemical Physics, 2014, 141, 104315.	3.1	18
53	Hybrid MPI/OpenMP parallelization of the effective fragment potential method in the libefp software library. Journal of Computational Chemistry, 2015, 36, 129-135.	3.5	18
54	Predictive First-Principles Modeling of a Photosynthetic Antenna Protein: The Fennaâ€“Matthewsâ€“Olson Complex. Journal of Physical Chemistry Letters, 2020, 11, 1636-1643.	4.9	18

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55	Jet-Cooled Spectroscopy of the Î±-Methylbenzyl Radical: Probing the State-Dependent Effects of Methyl Rocking Against a Radical Site. Journal of Physical Chemistry A, 2013, 117, 13465-13480.	2.6	17
56	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.	4.7	17
57	Reactivity and Structure of the 5-Dehydro-m-xylylene Anion. Journal of Organic Chemistry, 2004, 69, 5735-5741.	3.3	16
58	Efficient Strategies for Accurate Calculations of Electronic Excitation and Ionization Energies:â€‰ Theory and Application to the Dehydro-m-xylylene Anion. Journal of Physical Chemistry A, 2006, 110, 291-298.	2.6	15
59	Effective Fragment Potentials for Flexible Molecules: Transferability of Parameters and Amino Acid Database. Journal of Chemical Theory and Computation, 2020, 16, 7735-7747.	5.6	15
60	Exchange Repulsion in Quantum Mechanical/Effective Fragment Potential Excitation Energies: Beyond Polarizable Embedding. Journal of Chemical Theory and Computation, 2020, 16, 6408-6417.	5.6	14
61	Copper(I)â€“Pyrazolate Complexes as Solid-State Phosphors: Deep-Blue Emission through a Remote Steric Effect. Journal of the American Chemical Society, 2022, 144, 10186-10192.	14.6	14
62	Vibronic coupling in asymmetric bichromophores: Experimental investigation of diphenylmethane-d5. Journal of Chemical Physics, 2014, 141, 064316.	3.1	13
63	FMOxFMO: Elucidating Excitonic Interactions in the Fennaâ€“Matthewsâ€“Olson Complex with the Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2020, 16, 1175-1187.	5.6	12
64	Breaking the Curse of the Non-Dynamical Correlation Problem: The Spin-Flip Method. ACS Symposium Series, 2007, , 89-102.	0.0	11
65	Computational Investigation of Amineâ€“Oxygen Exciplex Formation. Journal of Physical Chemistry A, 2011, 115, 10159-10165.	2.6	11
66	Introduction: Calculations on Large Systems. Chemical Reviews, 2015, 115, 5605-5606.	51.4	11
67	Ground-State Charge Transfer: Lithiumâ€“Benzene and the Role of Hartreeâ€“Fock Exchange. Journal of Physical Chemistry A, 2016, 120, 8190-8198.	2.6	11
68	A new structural arrangement in proteins involving lysine NH3 + group and carbonyl. Scientific Reports, 2017, 7, 16402.	3.4	11
69	Interaction of Polymers with Enzalutamide Nanodropletsâ€”Impact on Droplet Properties and Induction Times. Molecular Pharmaceutics, 2021, 18, 836-849.	4.7	11
70	Vibronic coupling in asymmetric bichromophores: Theory and application to diphenylmethane-d5. Journal of Chemical Physics, 2014, 141, 134119.	3.1	9
71	Radical damage in lipids investigated with the fragment molecular orbital method. Chemical Physics Letters, 2016, 651, 56-61.	2.7	8
72	Tripletâ€“Triplet Coupling in Chromophore Dimers: Theory and Experiment. Journal of Physical Chemistry A, 2018, 122, 6713-6723.	2.6	8

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73	Hydration and Seamless Integration of Hydrogen Peroxide in Water. Journal of Physical Chemistry B, 2021, 125, 6986-6993.	2.7	8
74	Multipole Moments in the Effective Fragment Potential Method. Journal of Physical Chemistry A, 2017, 121, 2056-2067.	2.6	7
75	Ion-Size Dependent Adsorption Crossover on the Surface of a Water Droplet. Journal of Physical Chemistry B, 2023, 127, 4658-4665.	2.7	7
76	Effects of Ethynyl Substituents on the Electronic Structure of Cyclobutadiene. Journal of Physical Chemistry A, 2012, 116, 3194-3201.	2.6	6
77	Thermal Isomerizations of Diethynyl Cyclobutadienes and Implications for Fullerene Formation. Journal of Organic Chemistry, 2015, 80, 11863-11868.	3.3	5
78	Effective Fragment Potential Method for H-Bonding: How To Obtain Parameters for Nonrigid Fragments. Journal of Physical Chemistry A, 2017, 121, 5301-5312.	2.6	5
79	Molecular and Structural Characterization of Isomeric Compounds in Atmospheric Organic Aerosol Using Ion Mobility-Mass Spectrometry. Journal of Physical Chemistry A, 2023, 127, 1656-1674.	2.6	5
80	Predicting Mutation-Induced Changes in the Electronic Properties of Photosynthetic Proteins from First Principles: The Fennaâ€“Matthewsâ€“Olson Complex Example. Journal of Physical Chemistry Letters, 2023, 14, 7038-7044.	4.9	5
81	Thermodynamics and Kinetics for the Free Radical Oxygen Protein Oxidation Pathway in a Model for Î²-Structured Peptides. Journal of Physical Chemistry A, 2016, 120, 2493-2503.	2.6	4
82	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.	0.0	3
83	The effects of site asymmetry on near-degenerate state-to-state vibronic mixing in flexible bichromophores. Journal of Chemical Physics, 2019, 151, 084313.	3.1	3
84	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
85	Expulsion of Hydroxide Ions from Methyl Hydration Shells. Journal of Physical Chemistry B, 2022, 126, 869-877.	2.7	2
86	Quantifying the Nearly Random Microheterogeneity of Aqueous tert-Butyl Alcohol Solutions Using Vibrational Spectroscopy. Journal of Physical Chemistry Letters, 2023, 14, 11376-11383.	4.9	2
87	5-Dehydro-1,3-quinodimethane: A Hydrocarbon with an Open-Shell Doublet Ground State. Angewandte Chemie, 2004, 116, 760-763.	2.1	1
88	The unusual symmetry of hexafluoro-o-xyleneâ€”A microwave spectroscopy and computational study. Journal of Chemical Physics, 2020, 152, 064302.	3.1	1
89	Capturing CO₂ in Quadrupolar Binding Pockets: Broadband Microwave Spectroscopy of Pyrimidine-(CO₂)_n, n = 1,2. Journal of Physical Chemistry A, 2024, 128, 1124-1133.	2.6	1
90	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.	2.1	0

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91	Multiagent Consensus Equilibrium in Molecular Structure Determination. Journal of Physical Chemistry A, 2020, 124, 9105-9112.	2.6	0
92	Early-Career and Emerging Researchers in Physical Chemistry Volume 2. Journal of Physical Chemistry B, 2023, 127, 9211-9214.	2.7	0
93	Early-Career and Emerging Researchers in Physical Chemistry Volume 2. Journal of Physical Chemistry A, 2023, 127, 8967-8970.	2.6	0
94	Early-Career and Emerging Researchers in Physical Chemistry Volume 2. Journal of Physical Chemistry C, 2023, 127, 20975-20978.	3.3	0
95	Detangling Solvatochromic Effects by the Effective Fragment Potential Method. Journal of Physical Chemistry A, 2024, 128, 656-669.	2.6	0
96	Impact of Peripheral Hydrogen Bond on Electronic Properties of the Primary Acceptor Chlorophyll in the Reaction Center of Photosystem I. International Journal of Molecular Sciences, 2024, 25, 4815.	4.2	0
97	Controlling Vibronic Coupling in Chlorophyll Proteins: The Effects of Excitonic Delocalization and Vibrational Localization. Journal of Physical Chemistry Letters, 0, , 9456-9465.	4.9	0
98	Rigidochromism of Tetranuclear Cu(I)â€“Pyrazolate Macrocycles: Steric Crowding with Trifluoromethyl Groups. Chemical Communications, 0, , .	4.2	0
99	ANI/EFP: Modeling Long-Range Interactions in ANI Neural Network with Effective Fragment Potentials. Journal of Chemical Theory and Computation, 0, , .	5.6	0