# Lyudmila V Slipchenko

List of Publications by Year
in descending order

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

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Detangling Solvatochromic Effects by the Effective Fragment Potential Method. Journal of Physical Chemistry A, 2024, 128, 656-669. | 2.6 | 0 |
| 2 | Capturing CO<sub>2</sub> in Quadrupolar Binding Pockets: Broadband Microwave Spectroscopy of Pyrimidine-(CO<sub>2</sub>)<sub>n</sub>, n = 1,2. Journal of Physical Chemistry A, 2024, 128, 1124-1133. | 2.6 | 1 |
| 3 | 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 |
| 4 | 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 |
| 5 | Ion-Size Dependent Adsorption Crossover on the Surface of a Water Droplet. Journal of Physical Chemistry B, 2023, 127, 4658-4665. | 2.7 | 7 |
| 6 | 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 |
| 7 | Early-Career and Emerging Researchers in Physical Chemistry Volume 2. Journal of Physical Chemistry B, 2023, 127, 9211-9214. | 2.7 | 0 |
| 8 | Early-Career and Emerging Researchers in Physical Chemistry Volume 2. Journal of Physical Chemistry A, 2023, 127, 8967-8970. | 2.6 | 0 |
| 9 | Early-Career and Emerging Researchers in Physical Chemistry Volume 2. Journal of Physical Chemistry C, 2023, 127, 20975-20978. | 3.3 | 0 |
| 10 | 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 |
| 11 | Expulsion of Hydroxide Ions from Methyl Hydration Shells. Journal of Physical Chemistry B, 2022, 126, 869-877. | 2.7 | 2 |
| 12 | 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 |
| 13 | Interaction of Polymers with Enzalutamide Nanodropletsâ€”Impact on Droplet Properties and Induction Times. Molecular Pharmaceutics, 2021, 18, 836-849. | 4.7 | 11 |
| 14 | Hydration and Seamless Integration of Hydrogen Peroxide in Water. Journal of Physical Chemistry B, 2021, 125, 6986-6993. | 2.7 | 8 |
| 15 | 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 |
| 16 | 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 |
| 17 | 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 |
| 18 | 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 |

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|---|---|---|---|
| 19 | The unusual symmetry of hexafluoro-o-xyleneâ€"A microwave spectroscopy and computational study. Journal of Chemical Physics, 2020, 152, 064302. | 3.1 | 1 |
| 20 | 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 |
| 21 | Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102. | 3.1 | 827 |
| 22 | Multiagent Consensus Equilibrium in Molecular Structure Determination. Journal of Physical Chemistry A, 2020, 124, 9105-9112. | 2.6 | 0 |
| 23 | 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 |
| 24 | Polarizable embedding for simulating redox potentials of biomolecules. Physical Chemistry Chemical Physics, 2019, 21, 11642-11650. | 2.9 | 22 |
| 25 | Exchange-repulsion energy in QM/EFP. Journal of Chemical Physics, 2018, 149, 094103. | 3.1 | 22 |
| 26 | 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 |
| 27 | Tripletâ€"Triplet Coupling in Chromophore Dimers: Theory and Experiment. Journal of Physical Chemistry A, 2018, 122, 6713-6723. | 2.6 | 8 |
| 28 | 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 |
| 29 | Multipole Moments in the Effective Fragment Potential Method. Journal of Physical Chemistry A, 2017, 121, 2056-2067. | 2.6 | 7 |
| 30 | 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 |
| 31 | 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 |
| 32 | Dispersion Interactions in QM/EFP. Journal of Physical Chemistry A, 2017, 121, 9495-9507. | 2.6 | 23 |
| 33 | Effective Fragment Potential Method: Past, Present, and Future. , 2017, , 183-208. | | 22 |
| 34 | A new structural arrangement in proteins involving lysine NH3 + group and carbonyl. Scientific Reports, 2017, 7, 16402. | 3.4 | 11 |
| 35 | 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 |
| 36 | Mechanistic Design of Chemically Diverse Polymers with Applications in Oral Drug Delivery. Biomacromolecules, 2016, 17, 3659-3671. | 5.6 | 45 |

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| 37 | 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 |
| 38 | A Comparison of the Crystallization Inhibition Properties of Bile Salts. Crystal Growth and Design, 2016, 16, 7286-7300. | 3.2 | 47 |
| 39 | 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 |
| 40 | Photochemical degradation of isoprene-derived 4,1-nitrooxy enal. Atmospheric Chemistry and Physics, 2016, 16, 5595-5610. | 5.0 | 32 |
| 41 | Extension of the Effective Fragment Potential Method to Macromolecules. Journal of Physical Chemistry B, 2016, 120, 6562-6574. | 2.7 | 76 |
| 42 | Radical damage in lipids investigated with the fragment molecular orbital method. Chemical Physics Letters, 2016, 651, 56-61. | 2.7 | 8 |
| 43 | Thermal Isomerizations of Diethynyl Cyclobutadienes and Implications for Fullerene Formation. Journal of Organic Chemistry, 2015, 80, 11863-11868. | 3.3 | 5 |
| 44 | 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 |
| 45 | 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 |
| 46 | Introduction: Calculations on Large Systems. Chemical Reviews, 2015, 115, 5605-5606. | 51.4 | 11 |
| 47 | Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215. | 1.7 | 2,647 |
| 48 | Vibronic coupling in asymmetric bichromophores: Experimental investigation of diphenylmethane-d5. Journal of Chemical Physics, 2014, 141, 064316. | 3.1 | 13 |
| 49 | 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 |
| 50 | Vibronic coupling in asymmetric bichromophores: Theory and application to diphenylmethane-d5. Journal of Chemical Physics, 2014, 141, 134119. | 3.1 | 9 |
| 51 | Atmospheric Significance of Water Clusters and Ozoneâ€“Water Complexes. Journal of Physical Chemistry A, 2013, 117, 10381-10396. | 2.6 | 107 |
| 52 | 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 |
| 53 | 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 |
| 54 | Accurate First Principles Model Potentials for Intermolecular Interactions. Annual Review of Physical Chemistry, 2013, 64, 553-578. | 11.3 | 152 |

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| 55 | Interactions between halide anions and a molecular hydrophobic interface. Faraday Discussions, 2013, 160, 255-270. | 3.7 | 48 |
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| 57 | 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 |
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| 59 | Fragmentation Methods: A Route to Accurate Calculations on Large Systems. Chemical Reviews, 2012, 112, 632-672. | 51.4 | 970 |
| 60 | 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 |
| 61 | Effects of Ethynyl Substituents on the Electronic Structure of Cyclobutadiene. Journal of Physical Chemistry A, 2012, 116, 3194-3201. | 2.6 | 6 |
| 62 | 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 |
| 63 | 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 |
| 64 | The dispersion interaction between quantum mechanics and effective fragment potential molecules. Journal of Chemical Physics, 2012, 136, 244107. | 3.1 | 29 |
| 65 | Benzeneâ‹¯Pyridine Interactions Predicted by the Effective Fragment Potential Method. Journal of Physical Chemistry A, 2011, 115, 4598-4609. | 2.6 | 50 |
| 66 | Solvent Effects on the Electronic Transitions ofp-Nitroaniline: A QM/EFP Study. Journal of Physical Chemistry A, 2011, 115, 392-401. | 2.6 | 114 |
| 67 | 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 |
| 68 | Evolution of Amide Stacking in Larger Î³-Peptides: Triamide H-Bonded Cycles. Journal of Physical Chemistry A, 2011, 115, 13783-13798. | 2.6 | 77 |
| 69 | Modeling Solvent Effects on Electronic Excited States. Journal of Physical Chemistry Letters, 2011, 2, 2184-2192. | 4.9 | 109 |
| 70 | Computational Investigation of Amineâ€“Oxygen Exciplex Formation. Journal of Physical Chemistry A, 2011, 115, 10159-10165. | 2.6 | 11 |
| 71 | Effective Fragment Potential Study of the Interaction of DNA Bases. Journal of Physical Chemistry A, 2011, 115, 11269-11276. | 2.6 | 37 |
| 72 | Ï€-Hydrogen Bonding in Liquid Water. Journal of Physical Chemistry Letters, 2011, 2, 2930-2933. | 4.9 | 132 |

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| 73 | 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 |
| 74 | 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 |
| 75 | Systematic Study of the Embedding Potential Description in the Fragment Molecular Orbital Method<sup>â€</sup>. Journal of Physical Chemistry A, 2010, 114, 8742-8753. | 2.6 | 61 |
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| 77 | Damping functions in the effective fragment potential method. Molecular Physics, 2009, 107, 999-1016. | 1.7 | 99 |
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| 80 | Waterâ^'Benzene Interactions: An Effective Fragment Potential and Correlated Quantum Chemistry Study. Journal of Physical Chemistry A, 2009, 113, 2092-2102. | 2.6 | 97 |
| 81 | 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 |
| 82 | The Binding of Ag<sup>+</sup> and Au<sup>+</sup> to Ethene. Journal of Physical Chemistry A, 2009, 113, 7474-7481. | 2.6 | 29 |
| 83 | 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 |
| 84 | 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 |
| 85 | Breaking the Curse of the Non-Dynamical Correlation Problem: The Spin-Flip Method. ACS Symposium Series, 2007, , 89-102. | 0.0 | 11 |
| 86 | 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 |
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| 88 | Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191. | 2.9 | 2,632 |
| 89 | Spin-conserving and spin-flipping equation-of-motion coupled-cluster method with triple excitations. Journal of Chemical Physics, 2005, 123, 084107. | 3.1 | 110 |
| 90 | 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 |

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| 91 | 5-Dehydro-1,3-quinodimethane: A Hydrocarbon with an Open-Shell Doublet Ground State. Angewandte Chemie, 2004, 116, 760-763. | 2.1 | 1 |
| 92 | 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 |
| 93 | Reactivity and Structure of the 5-Dehydro-m-xylylene Anion. Journal of Organic Chemistry, 2004, 69, 5735-5741. | 3.3 | 16 |
| 94 | 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 |
| 95 | 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 |
| 96 | Singlet-triplet gaps in diradicals by the spin-flip approach: A benchmark study. Journal of Chemical Physics, 2002, 117, 4694-4708. | 3.1 | 323 |
| 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 |