

Giacomo Prampolini

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Insights for an Accurate Comparison of Computational Data to Experimental Absorption and Emission Spectra: Beyond the Vertical Transition Approximation. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2072-2082.	2.3	194
2	Parametrization and Validation of Intramolecular Force Fields Derived from DFT Calculations. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1803-1817.	2.3	102
3	Joyce and Ulysses: integrated and user-friendly tools for the parameterization of intramolecular force fields from quantum mechanical data. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 3736.	1.3	89
4	First-principle computation of absorption and fluorescence spectra in solution accounting for vibronic structure, temperature effects and solvent inhomogeneous broadening. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 328-337.	1.1	88
5	Absorption and Emission Spectra of a Flexible Dye in Solution: A Computational Time-Dependent Approach. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4507-4516.	2.3	78
6	Computer Simulation of Solid and Liquid Benzene with an Atomistic Interaction Potential Derived from ab Initio Calculations. <i>Journal of the American Chemical Society</i> , 2004, 126, 14278-14286.	6.6	74
7	Absorption and emission UV-Vis spectra of the TRITC fluorophore molecule in solution: a quantum mechanical study. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 1000-1006.	1.3	67
8	Accuracy of Quantum Mechanically Derived Force-Fields Parameterized from Dispersion-Corrected DFT Data: The Benzene Dimer as a Prototype for Aromatic Interactions. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5182-5196.	2.3	67
9	Modeling Solvent Broadening on the Vibronic Spectra of a Series of Coumarin Dyes. From Implicit to Explicit Solvent Models. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5810-5825.	2.3	66
10	Calculation of the intermolecular energy of large molecules by a fragmentation scheme: Application to the 4-n-pentyl-4'-cyanobiphenyl (5CB) dimer. <i>Journal of Chemical Physics</i> , 2002, 117, 3003-3012.	1.2	65
11	Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	64
12	Exciton Binding Energy in Molecular Triads. <i>Journal of Physical Chemistry C</i> , 2017, 121, 17088-17095.	1.5	64
13	Eumelanin broadband absorption develops from aggregation-modulated chromophore interactions under structural and redox control. <i>Scientific Reports</i> , 2017, 7, 41532.	1.6	63
14	Harmonic Models in Cartesian and Internal Coordinates to Simulate the Absorption Spectra of Carotenoids at Finite Temperatures. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4947-4958.	2.3	62
15	Structure and Dynamics of Ferrocyanide and Ferricyanide Anions in Water and Heavy Water: An Insight by MD Simulations and 2D IR Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2014, 118, 14899-14912.	1.2	59
16	Vibronic Coupling Explains the Different Shape of Electronic Circular Dichroism and of Circularly Polarized Luminescence Spectra of Hexahelicenes. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2799-2819.	2.3	59
17	Fluorescence spectra of organic dyes in solution: a time dependent multilevel approach. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 2160-2166.	1.3	57
18	Realistic Modeling of Fluorescent Dye-Doped Silica Nanoparticles: A Step Toward the Understanding of their Enhanced Photophysical Properties.. <i>Chemistry of Materials</i> , 2011, 23, 5016-5023.	3.2	57

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19	Absorption and Emission Spectral Shapes of a Prototype Dye in Water by Combining Classical/Dynamical and Quantum/Static Approaches. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5426-5438.	1.1	50
20	Adiabatic-Molecular Dynamics Generalized Vertical Hessian Approach: A Mixed Quantum Classical Method To Compute Electronic Spectra of Flexible Molecules in the Condensed Phase. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1215-1231.	2.3	50
21	Liquid Crystal Properties of then-Alkyl-cyanobiphenyl Series from Atomistic Simulations with Ab Initio Derived Force Fields. <i>Journal of Physical Chemistry B</i> , 2007, 111, 2130-2137.	1.2	49
22	Atomistic Simulation of a Nematogen Using a Force Field Derived from Quantum Chemical Calculations. <i>Journal of Physical Chemistry B</i> , 2005, 109, 3531-3538.	1.2	46
23	An automated approach for the parameterization of accurate intermolecular force fields: Pyridine as a case study. <i>Journal of Computational Chemistry</i> , 2012, 33, 1055-1067.	1.5	46
24	Classical Force Fields Tailored for QM Applications: Is It Really a Feasible Strategy?. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4636-4648.	2.3	45
25	Theoretical multilevel approach for studying the photophysical properties of organic dyes in solution. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 10550.	1.3	43
26	Computational Design, Synthesis, and Mechanochromic Properties of New Thiophene-Based π -Conjugated Chromophores. <i>Chemistry - A European Journal</i> , 2013, 19, 1996-2004.	1.7	43
27	Oligomers based on weak hydrogen bond networks: a rotational study of the tetramer of difluoromethane. <i>Chemical Communications</i> , 2014, 50, 171-173.	2.2	43
28	Revisiting Vertical Models To Simulate the Line Shape of Electronic Spectra Adopting Cartesian and Internal Coordinates. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4970-4985.	2.3	41
29	Deuterium and Carbon-13 NMR Study of a Banana Mesogen: A Molecular Structure and Order. <i>Journal of Physical Chemistry B</i> , 2004, 108, 7694-7701.	1.2	40
30	Torsional Barriers and Correlations between Dihedrals in p-Polyphenyls. <i>Journal of Physical Chemistry A</i> , 2003, 107, 8665-8670.	1.1	37
31	Force field modeling through quantum mechanical calculations: Molecular dynamics simulations of a nematogenic molecule in its condensed phases. <i>Journal of Computational Chemistry</i> , 2009, 30, 366-378.	1.5	37
32	Intermolecular interactions in eumelanins: a computational bottom-up approach. I. small building blocks. <i>RSC Advances</i> , 2015, 5, 38513-38526.	1.7	37
33	Absorption and emission spectra of fluorescent silica nanoparticles from TD-DFT/MM/PCM calculations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 16689.	1.3	36
34	Systematic and Automated Development of Quantum Mechanically Derived Force Fields: The Challenging Case of Halogenated Hydrocarbons. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5525-5540.	2.3	35
35	Developing accurate intramolecular force fields for conjugated systems through explicit coupling terms. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	35
36	Predicting fluorescence quantum yields for molecules in solution: A critical assessment of the harmonic approximation and the choice of the lineshape function. <i>Journal of Chemical Physics</i> , 2020, 152, 054107.	1.2	35

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37	An Integrated Protocol for the Accurate Calculation of Magnetic Interactions in Organic Magnets. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 699-706.	2.3	32
38	Mixed Quantum/Classical Method for Nonadiabatic Quantum Dynamics in Explicit Solvent Models: The Decay of Thymine in Water as a Test Case. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 820-832.	2.3	31
39	DFT Study of the Torsional Potential in Ethylbenzene and Ethoxybenzene: The Smallest Prototypes of Alkyl and Alkoxy Aryl Mesogens. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5228-5232.	1.1	30
40	Vibrationally resolved electronic spectra including vibrational pre-excitation: Theory and application to VIPER spectroscopy. <i>Journal of Chemical Physics</i> , 2017, 147, 164116.	1.2	29
41	Disentangling vibronic and solvent broadening effects in the absorption spectra of coumarin derivatives for dye sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 11401-11411.	1.3	28
42	Intermolecular Force Fields of Large Molecules by the Fragmentation Reconstruction Method (FRM): Application to a Nematic Liquid Crystal. <i>Journal of Physical Chemistry A</i> , 2004, 108, 10336-10341.	1.1	27
43	Computational study through atomistic potentials of a partial bilayer liquid crystal: structure and dynamics. <i>Soft Matter</i> , 2009, 5, 3517.	1.2	27
44	Unraveling the interplay of different contributions to the stability of the quinhydrone dimer. <i>RSC Advances</i> , 2014, 4, 876-885.	1.7	26
45	Development and Validation of Quantum Mechanically Derived Force-Fields: Thermodynamic, Structural, and Vibrational Properties of Aromatic Heterocycles. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4884-4900.	2.3	26
46	Atomistic Computer Simulation and Experimental Study on the Dynamics of the n-Cyanobiphenyls Mesogenic Series. <i>Journal of Physical Chemistry B</i> , 2008, 112, 9777-9786.	1.2	25
47	Magnetic Interactions in Phenyl-Bridged Nitroxide Diradicals: Conformational Effects by Multireference and Broken Symmetry DFT Approaches. <i>Journal of Physical Chemistry A</i> , 2009, 113, 15150-15155.	1.1	25
48	Comparing classical approaches with empirical or quantum-mechanically derived force fields for the simulation electronic lineshapes: application to coumarin dyes. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	25
49	Structure-Properties Relationships in Triplet Ground State Organic Diradicals: A Computational Study. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 300-307.	2.3	24
50	Coupled cluster study of the x-ray absorption spectra of formaldehyde derivatives at the oxygen, carbon, and fluorine K-edges. <i>Journal of Chemical Physics</i> , 2019, 151, 064107.	1.2	24
51	DFT conformational study of banana-shaped mesogens. <i>Chemical Physics</i> , 2005, 314, 283-290.	0.9	23
52	Banana-Shaped Molecules Peculiarly Oriented in a Magnetic Field: ² H NMR Spectroscopy and Quantum Mechanical Calculations. <i>ChemPhysChem</i> , 2007, 8, 2321-2330.	1.0	23
53	Interaction Energy Landscapes of Aromatic Heterocycles through a Reliable yet Affordable Computational Approach. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 543-556.	2.3	23
54	Modeling a Liquid Crystal Dynamics by Atomistic Simulation with an Ab Initio Derived Force Field. <i>Journal of Physical Chemistry B</i> , 2006, 110, 2847-2854.	1.2	22

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55	Quantum and semiclassical dynamical studies of nonadiabatic processes in solution: achievements and perspectives. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 8181-8199.	1.3	22
56	Parametrization and Validation of Coarse Grained Force-Fields Derived from ab Initio Calculations. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 556-567.	2.3	21
57	Conformational changes of β -carotene and zeaxanthin immersed in a model membrane through atomistic molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 6527.	1.3	21
58	Accurate yet feasible post-Hartree-Fock computation of magnetic interactions in large biradicals through a combined variational/perturbative approach: Setup and validation. <i>Journal of Chemical Physics</i> , 2009, 131, 224103.	1.2	20
59	Benchmarking Cation- π Interactions: Assessment of Density Functional Theory and Møller-Plesset Second-Order Perturbation Theory Calculations with Optimized Basis Sets (Na^+ , K^+ , Rb^+ , and Cs^+) for Complexes of Benzene, Phenol, and Catechol with Na^+ , K^+ , Rb^+ , and Cs^+ . <i>Journal of Physical Chemistry A</i> , 2020, 124, 3445-3459.	1.1	20
60	Structure and dynamics of mesogens using intermolecular potentials derived from ab initio calculations. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 885-901.	0.5	19
61	Chemical Detail Force Fields for Mesogenic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1865-1876.	2.3	19
62	Singlet-triplet energy gap of a diarylnitroxide diradical by an accurate many-body perturbative approach. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 4709.	1.3	19
63	Quantum-Classical Calculation of Vibronic Spectra along a Reaction Path: The Case of the ECD of Easily Interconvertible Conformers with Opposite Chiral Responses. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4891-4897.	2.1	19
64	Multistate coupled quantum dynamics of photoexcited cytosine in gas-phase: Nonadiabatic absorption spectrum and ultrafast internal conversions. <i>Chemical Physics</i> , 2018, 515, 452-463.	0.9	19
65	A General Treatment to Study Molecular Complexes Stabilized by Hydrogen-, Halogen-, and Carbon-Bond Networks: Experiment and Theory of $(\text{CH}_2\text{F}_2)_n \cdots (\text{H}_2\text{O})_m$. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 8437-8442.		19
66	Molecular Dynamics Simulations of the Self-Assembly of Tetraphenylporphyrin-Based Monolayers and Bilayers at a Silver Interface. <i>Journal of Physical Chemistry C</i> , 2011, 115, 18434-18444.	1.5	18
67	Conformational Effects on the Magnetic Properties of an Organic Diradical: A Computational Study. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1958-1963.	2.3	18
68	Modeling benzene with single-site potentials from ab initio calculations: A step toward hybrid models of complex molecules. <i>Journal of Chemical Physics</i> , 2004, 120, 3648-3656.	1.2	17
69	Noncovalent Interactions in the Catechol Dimer. <i>Biomimetics</i> , 2017, 2, 18.	1.5	17
70	Short- and Long-Range Solvation Effects on the Transient UV-Vis Absorption Spectra of a Ru(II)-Polypyridine Complex Disentangled by Nonequilibrium Molecular Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2885-2891.	2.1	17
71	Dynamical and Environmental Effects on the Optical Properties of an Heteroleptic Ru(II)-Polypyridine Complex: A Multilevel Approach Combining Accurate Ground and Excited State QM-Derived Force Fields, MD and TD-DFT. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 529-545.	2.3	17
72	Accounting for Vibronic Features through a Mixed Quantum-Classical Scheme: Structure, Dynamics, and Absorption Spectra of a Perylene Diimide Dye in Solution. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7061-7077.	2.3	17

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73	Sensors for DNA detection: theoretical investigation of the conformational properties of immobilized single-strand DNA. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 10644.	1.3	16
74	Predicting light absorption properties of anthocyanidins in solution: a multi-level computational approach. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	16
75	How the Odd-Even Effects on the Inter-Molecular Potentials Propagate to the Order Parameter in the 4-Cyano-4- n -Alkylbiphenyl Series. <i>Molecular Crystals and Liquid Crystals</i> , 2007, 465, 175-186.	0.4	14
76	Subdiffusive dynamics of a liquid crystal in the isotropic phase. <i>Journal of Chemical Physics</i> , 2008, 128, 194501.	1.2	14
77	Modified virtual orbitals for CI calculations of energy splitting in organic diradicals. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 3854.	1.3	14
78	Theoretical investigation of the broad one-photon absorption line-shape of a flexible symmetric carbazole derivative. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 22889-22905.	1.3	14
79	Simulating DNA Hybridization on an Amine-Functionalized Silicon Substrate. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8341-8349.	1.2	13
80	Sequential Bending and Twisting around C-C Single Bonds by Mechanical Lifting of a Pre-Adsorbed Polymer. <i>Nano Letters</i> , 2020, 20, 652-657.	4.5	12
81	Automated parameterization of quantum-mechanically derived force-fields including explicit sigma holes: A pathway to energetic and structural features of halogen bonds in gas and condensed phase. <i>Journal of Chemical Physics</i> , 2020, 153, 044106.	1.2	12
82	The Role of Non-Covalent Interactions on Cluster Formation: Pentamer, Hexamers and Heptamer of Difluoromethane. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 16894-16899.	7.2	12
83	How the Interplay among Conformational Disorder, Solvation, Local, and Charge-Transfer Excitations Affects the Absorption Spectrum and Photoinduced Dynamics of Perylene Diimide Dimers: A Molecular Dynamics/Quantum Vibronic Approach. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3718-3736.	2.3	12
84	Stability of the nematic phase of 4- n -pentyl-4-cyanobiphenyl studied by computer simulation using a hybrid model. <i>Journal of Chemical Physics</i> , 2002, 117, 448-453.	1.2	11
85	Anomalous Diffusion and Cage Effects in the Isotropic Phase of a Liquid Crystal. <i>Journal of Physical Chemistry B</i> , 2007, 111, 7473-7477.	1.2	11
86	Estimate of Benzene-Triphenylene and Triphenylene-Triphenylene Interactions: A Topic Relevant to Columnar Discotic Liquid Crystals. <i>Journal of Physical Chemistry C</i> , 2008, 112, 9501-9509.	1.5	11
87	Parameterization and validation of an accurate force-field for the simulation of alkylamine functionalized silicon (111) surfaces. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 4201.	1.3	11
88	Interactions of Nucleotide Bases with Decorated Si Surfaces from Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2011, 115, 9146-9156.	1.5	11
89	Comparison of the results of a mean-field mixed quantum/classical method with full quantum predictions for nonadiabatic dynamics: application to the π - π^* $\text{I}^{\text{R}}/\text{I}^{\text{A}}$ decay of thymine. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	11
90	Automated Parameterization of Quantum Mechanically Derived Force Fields for Soft Materials and Complex Fluids: Development and Validation. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4449-4464.	2.3	11

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91	The phenoxy group-modulated interplay of cation- π and π - π -type interactions in the alkali metal series. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 27105-27120.	1.3	11
92	Computer Simulation of P-Phenyls with Interaction Potentials from Ab-Initio Calculations. <i>Molecular Crystals and Liquid Crystals</i> , 2003, 395, 171-182.	0.4	10
93	Structural, dynamic and photophysical properties of a fluorescent dye incorporated in an amorphous hydrophobic polymer bundle. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 16573-16587.	1.3	10
94	Perturbative Multireference Configuration Interaction (CI-MRPT2) Calculations in a Focused Dynamical Approach: A Computational Study of Solvatochromism in Pyrimidine. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5250-5259.	1.1	10
95	BALOO: A Fast and Versatile Code for Accurate Multireference Variational/Perturbative Calculations. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2024-2035.	2.3	10
96	Toward a general mixed quantum/classical method for the calculation of the vibronic ECD of a flexible dye molecule with different stable conformers: Revisiting the case of 2,2,2-trifluoroanthrylethanol. <i>Chirality</i> , 2018, 30, 730-743.	1.3	10
97	A computational study of the vibrationally-resolved electronic circular dichroism spectra of single-chain transoid and cisoid oligothiophenes in chiral conformations. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21864-21880.	1.3	10
98	Predicting Spontaneous Orientational Self-Assembly: <i>In Silico</i> Design of Materials with Quantum Mechanically Derived Force Fields. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 243-250.	2.1	10
99	Density Functional Theory Study of the Conformational Space of Phenyl Benzoate, a Common Fragment in Many Mesogenic Molecules. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6290-6293.	1.1	9
100	The Absorption Spectrum of Guanine Based Radicals: a Comparative Computational Analysis. <i>ChemPhotoChem</i> , 2019, 3, 846-855.	1.5	9
101	Extension of the AMBER Force Field for Nitroxide Radicals and Combined QM/MM/PCM Approach to the Accurate Determination of EPR Parameters of DMPO-H in Solution. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3626-3636.	2.3	8
102	Proton and Electron Transfer Mechanisms in the Formation of Neutral and Charged Quinhydrone-Like Complexes: A Multilayered Computational Study. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4883-4895.	2.3	8
103	Computational Screening of Weak Hydrogen Bond Networks: Predicting Stable Structures for Difluoromethane Oligomers. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2204-2211.	2.3	8
104	Accurate interaction energies by spin component scaled Møller-Plesset second order perturbation theory calculations with optimized basis sets (SCS-MP2 mod): Development and application to aromatic heterocycles. <i>Journal of Chemical Physics</i> , 2019, 150, 234113.	1.2	8
105	The Intriguing Case of the One-Photon and Two-Photon Absorption of a Prototypical Symmetric Squaraine: Comparison of TDDFT and Wavefunction Methods. <i>ChemPhotoChem</i> , 2019, 3, 778-793.	1.5	8
106	Iron's Wake: The Performance of Quantum Mechanical-Derived Versus General-Purpose Force Fields Tested on a Luminescent Iron Complex. <i>Molecules</i> , 2020, 25, 3084.	1.7	8
107	DNA hybridization mechanism on silicon nanowires: a molecular dynamics approach. <i>Molecular BioSystems</i> , 2010, 6, 2230.	2.9	7
108	Theoretical study of the conformational and optical properties of a fluorescent dye. A step toward modeling sensors grafted on polymer structures. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 21471.	1.3	7

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109	Evidences of long lived cages in functionalized polymers: Effects on chromophore dynamic and spectroscopic properties. <i>Chemical Physics Letters</i> , 2014, 601, 134-138.	1.2	7
110	Electronic spectroscopy of a solvatochromic dye in water: comparison of static cluster/implicit and dynamical/explicit solvent models on structures and energies. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	7
111	The shape of the electronic circular dichroism spectrum of (2,6-dimethylphenyl)(phenyl)methanol: interplay between conformational equilibria and vibronic effects. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 32349-32360.	1.3	7
112	Structural and morphological aspects of small 3,5-disubstituted isoxazoles. <i>Journal of Fluorine Chemistry</i> , 2018, 211, 24-36.	0.9	7
113	Geometry Optimization of Large and Flexible van der Waals Dimers: A Fragmentation~Reconstruction Approach. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2536-2546.	2.3	6
114	Organic Functionalization and Optimal Coverage of a Silicon(111) Surface in Solvent: A Computational Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 4145-4154.	1.5	6
115	Magnetic gaps in organic tri-radicals: From a simple model to accurate estimates. <i>Journal of Chemical Physics</i> , 2017, 146, 104103.	1.2	5
116	Flexible Superlubricity Unveiled in Sidewinding Motion of Individual Polymeric Chains. <i>Physical Review Letters</i> , 2022, 128, .	2.9	5
117	Complementary and partially complementary DNA duplexes tethered to a functionalized substrate: a molecular dynamics approach to biosensing. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 12478.	1.3	4
118	Vibronic approach to the calculation of the decay rate of the photoexcited charge-transfer state of Guanine~Cytosine stacked dimer in water solution. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	4
119	Quantitative prediction and interpretation of spin energy gaps in polyradicals: the virtual magnetic balance. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 9039-9044.	1.3	4
120	Solvent effect on the energetics of proton coupled electron transfer in guanine-cytosine pair in chloroform by mixed explicit and implicit solvation models. <i>Chemical Physics</i> , 2018, 515, 493-501.	0.9	4
121	A General Treatment to Study Molecular Complexes Stabilized by Hydrogen~, Halogen~, and Carbon~Bond Networks: Experiment and Theory of (CH ₂ F ₂) _n ...~... (H ₂ O) _m . <i>Angewandte Chemie</i> , 2019, 131, 8525-8530.	1.6	4
122	Noncovalent interactions in catechol/ammonium-rich adhesive motifs: Reassessing the role of cation~ complexes?. <i>Chemical Physics Letters</i> , 2021, 779, 138815.	1.2	4
123	Solvent-Induced Stereochemical Behavior of a Bile Acid-Based Biphenyl Phosphite: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 14930-14935.	1.1	1
124	Complexes of Alkaline and Ammonium Cations with Dopamine and Eumelanin Precursors: Dissecting the Role of Noncovalent Cation~ and Cation~ Lone Pair (f-Type) Interactions. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2330-2341.	1.1	1
125	The Role of Non~Covalent Interactions on Cluster Formation: Pentamer, Hexamers and Heptamer of Difluoromethane. <i>Angewandte Chemie</i> , 2021, 133, 17031-17036.	1.6	0
126	Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case. <i>Highlights in Theoretical Chemistry</i> , 2013, , 319-337.	0.0	0