Giacomo Prampolini

List of Publications by Year
in descending order

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126 papers	3,398 citations	126708 33 h-index	189595 50 g-index
127 all docs	127 docs citations	127 times ranked	2974 citing authors

#	Article	IF	Citations
1	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. Journal of Chemical Theory and Computation, 2022, 18, 3718-3736.	2.3	12
2	Complexes of Alkaline and Ammonium Cations with Dopamine and Eumelanin Precursors: Dissecting the Role of Noncovalent Cationâ˜Ï€ and Cationâ€“Lone Pair (Ïƒ-Type) Interactions. Journal of Physical Chemistry A, 2022, 126, 2330-2341.	1.1	1
3	Predicting Spontaneous Orientational Self-Assembly: In Silico Design of Materials with Quantum Mechanically Derived Force Fields. Journal of Physical Chemistry Letters, 2022, 13, 243-250.	2.1	10
4	Flexible Superlubricity Unveiled in Sidewinding Motion of Individual Polymeric Chains. Physical Review Letters, 2022, 128, .	2.9	5
5	The Role of Nonâ€Covalent Interactions on Cluster Formation: Pentamer, Hexamers and Heptamer of Difluoromethane. Angewandte Chemie, 2021, 133, 17031-17036.	1.6	0
6	Automated Parameterization of Quantum Mechanically Derived Force Fields for Soft Materials and Complex Fluids: Development and Validation. Journal of Chemical Theory and Computation, 2021, 17, 4449-4464.	2.3	11
7	The Role of Nonâ€Covalent Interactions on Cluster Formation: Pentamer, Hexamers and Heptamer of Difluoromethane. Angewandte Chemie - International Edition, 2021, 60, 16894-16899.	7.2	12
8	Noncovalent interactions in catechol/ammonium-rich adhesive motifs: Reassessing the role of cation-Ïƒ complexes?. Chemical Physics Letters, 2021, 779, 138815.	1.2	4
9	Quantum and semiclassical dynamical studies of nonadiabatic processes in solution: achievements and perspectives. Physical Chemistry Chemical Physics, 2021, 23, 8181-8199.	1.3	22
10	Adiabatic-Molecular Dynamics Generalized Vertical Hessian Approach: A Mixed Quantum Classical Method To Compute Electronic Spectra of Flexible Molecules in the Condensed Phase. Journal of Chemical Theory and Computation, 2020, 16, 1215-1231.	2.3	50
11	Sequential Bending and Twisting around Câ€“C Single Bonds by Mechanical Lifting of a Pre-Adsorbed Polymer. Nano Letters, 2020, 20, 652-657.	4.5	12
12	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. Journal of Chemical Physics, 2020, 153, 044106.	1.2	12
13	Accounting for Vibronic Features through a Mixed Quantum-Classical Scheme: Structure, Dynamics, and Absorption Spectra of a Perylene Diimide Dye in Solution. Journal of Chemical Theory and Computation, 2020, 16, 7061-7077.	2.3	17
14	Ironâ€™s Wake: The Performance of Quantum Mechanical-Derived Versus General-Purpose Force Fields Tested on a Luminescent Iron Complex. Molecules, 2020, 25, 3084.	1.7	8
15	Predicting fluorescence quantum yields for molecules in solution: A critical assessment of the harmonic approximation and the choice of the lineshape function. Journal of Chemical Physics, 2020, 152, 054107.	1.2	35
16	Benchmarking Cationâ˜Ï€ Interactions: Assessment of Density Functional Theory and MÃ¶llerâ€“Plesset Second-Order Perturbation Theory Calculations with Optimized Basis Sets (<scp>mp</scp>2^{mod}) for Complexes of Benzene, Phenol, and Catechol with Na⁺, K⁺, Rb⁺, and Cs⁺. Journal of Physical Chemistry A, 2020, 124, 3445-3459.	1.1	20
17	The phenoxyl group-modulated interplay of cationâ€Ï€ and Ïƒ-type interactions in the alkali metal series. Physical Chemistry Chemical Physics, 2020, 22, 27105-27120.	1.3	11
18	Coupled cluster study of the x-ray absorption spectra of formaldehyde derivatives at the oxygen, carbon, and fluorine K-edges. Journal of Chemical Physics, 2019, 151, 064107.	1.2	24

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19	Accurate interaction energies by spin component scaled MÃ¶ller-Plesset second order perturbation theory calculations with optimized basis sets (SCS-MP2 mod): Development and application to aromatic heterocycles. Journal of Chemical Physics, 2019, 150, 234113.	1.2	8
20	The Absorption Spectrum of Guanine Based Radicals: a Comparative Computational Analysis. ChemPhotoChem, 2019, 3, 846-855.	1.5	9
21	A General Treatment to Study Molecular Complexes Stabilized by Hydrogenâ€, Halogenâ€, and Carbonâ€Bond Networks: Experiment and Theory of (CH₂F₂)_nâ‹…â‹…â‹…(H₂O)_m. Angewandte Chemie, 2019, 131, 8525-8530.	1.6	4
22	The Intriguing Case of the Oneâ€Photon and Twoâ€Photon Absorption of a Prototypical Symmetric Squaraine: Comparison of TDDFT and Waveâ€Function Methods. ChemPhotoChem, 2019, 3, 778-793.	1.5	8
23	Short- and Long-Range Solvation Effects on the Transient UVâ€“Vis Absorption Spectra of a Ru(II)â€“Polypyridine Complex Disentangled by Nonequilibrium Molecular Dynamics. Journal of Physical Chemistry Letters, 2019, 10, 2885-2891.	2.1	17
24	A General Treatment to Study Molecular Complexes Stabilized by Hydrogenâ€, Halogenâ€, and Carbonâ€Bond Networks: Experiment and Theory of (CH 2 F 2) n â‹…â‹…â‹…(H 2 O) m. Angewandte Chemie - International Edition, 2019, 58, 8437-8442.	7.2	19
25	Dynamical and Environmental Effects on the Optical Properties of an Heteroleptic Ru(II)â€“Polypyridine Complex: A Multilevel Approach Combining Accurate Ground and Excited State QM-Derived Force Fields, MD and TD-DFT. Journal of Chemical Theory and Computation, 2019, 15, 529-545.	2.3	17
26	Comparison of the results of a mean-field mixed quantum/classical method with full quantum predictions for nonadiabatic dynamics: application to the $$pi pi ^*/npi ^*$$ Ï€ Ï€ â^— / n Ï€ â^— decay of thymine. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	11
27	Structural and morphological aspects of small 3,5-disubstituted isoxazoles. Journal of Fluorine Chemistry, 2018, 211, 24-36.	0.9	7
28	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 2,2,2â€trifluoroâ€anthrylethanol. Chirality, 2018, 30, 730-743.	1.3	10
29	Interaction Energy Landscapes of Aromatic Heterocycles through a Reliable yet Affordable Computational Approach. Journal of Chemical Theory and Computation, 2018, 14, 543-556.	2.3	23
30	Developing accurate intramolecular force fields for conjugated systems through explicit coupling terms. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	35
31	A computational study of the vibrationally-resolved electronic circular dichroism spectra of single-chain transoid and cisoid oligothiophenes in chiral conformations. Physical Chemistry Chemical Physics, 2018, 20, 21864-21880.	1.3	10
32	Development and Validation of Quantum Mechanically Derived Force-Fields: Thermodynamic, Structural, and Vibrational Properties of Aromatic Heterocycles. Journal of Chemical Theory and Computation, 2018, 14, 4884-4900.	2.3	26
33	Solvent effect on the energetics of proton coupled electron transfer in guanine-cytosine pair in chloroform by mixed explicit and implicit solvation models. Chemical Physics, 2018, 515, 493-501.	0.9	4
34	Multistate coupled quantum dynamics of photoexcited cytosine in gas-phase: Nonadiabatic absorption spectrum and ultrafast internal conversions. Chemical Physics, 2018, 515, 452-463.	0.9	19
35	Mixed Quantum/Classical Method for Nonadiabatic Quantum Dynamics in Explicit Solvent Models: The Ï€Ï€*/nÏ€* Decay of Thymine in Water as a Test Case. Journal of Chemical Theory and Computation, 2018, 14, 820-832.	2.3	31
36	Quantitative prediction and interpretation of spin energy gaps in polyradicals: the virtual magnetic balance. Physical Chemistry Chemical Physics, 2017, 19, 9039-9044.	1.3	4

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37	Eumelanin broadband absorption develops from aggregation-modulated chromophore interactions under structural and redox control. Scientific Reports, 2017, 7, 41532.	1.6	63
38	Magnetic gaps in organic tri-radicals: From a simple model to accurate estimates. Journal of Chemical Physics, 2017, 146, 104103.	1.2	5
39	Classical Force Fields Tailored for QM Applications: Is It Really a Feasible Strategy?. Journal of Chemical Theory and Computation, 2017, 13, 4636-4648.	2.3	45
40	Exciton Binding Energy in Molecular Triads. Journal of Physical Chemistry C, 2017, 121, 17088-17095.	1.5	64
41	The shape of the electronic circular dichroism spectrum of (2,6-dimethylphenyl)(phenyl)methanol: interplay between conformational equilibria and vibronic effects. Physical Chemistry Chemical Physics, 2017, 19, 32349-32360.	1.3	7
42	Vibrationally resolved electronic spectra including vibrational pre-excitation: Theory and application to VIPER spectroscopy. Journal of Chemical Physics, 2017, 147, 164116.	1.2	29
43	Noncovalent Interactions in the Catechol Dimer. Biomimetics, 2017, 2, 18.	1.5	17
44	Comparing classical approaches with empirical or quantum-mechanically derived force fields for the simulation electronic lineshapes: application to coumarin dyes. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	25
45	Vibronic Coupling Explains the Different Shape of Electronic Circular Dichroism and of Circularly Polarized Luminescence Spectra of Hexahelicenes. Journal of Chemical Theory and Computation, 2016, 12, 2799-2819.	2.3	59
46	Revisiting Vertical Models To Simulate the Line Shape of Electronic Spectra Adopting Cartesian and Internal Coordinates. Journal of Chemical Theory and Computation, 2016, 12, 4970-4985.	2.3	41
47	Systematic and Automated Development of Quantum Mechanically Derived Force Fields: The Challenging Case of Halogenated Hydrocarbons. Journal of Chemical Theory and Computation, 2016, 12, 5525-5540.	2.3	35
48	Vibronic approach to the calculation of the decay rate of the photoexcited charge-transfer state of Guanineâ€“Cytosine stacked dimer in water solution. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	4
49	Theoretical investigation of the broad one-photon absorption line-shape of a flexible symmetric carbazole derivative. Physical Chemistry Chemical Physics, 2016, 18, 22889-22905.	1.3	14
50	Quantum-Classical Calculation of Vibronic Spectra along a Reaction Path: The Case of the ECD of Easily Interconvertible Conformers with Opposite Chiral Responses. Journal of Physical Chemistry Letters, 2016, 7, 4891-4897.	2.1	19
51	Electronic spectroscopy of a solvatochromic dye in water: comparison of static cluster/implicit and dynamical/explicit solvent models on structures and energies. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	7
52	Predicting light absorption properties of anthocyanidins in solution: a multi-level computational approach. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	16
53	Perturbative Multireference Configuration Interaction (CI-MRPT2) Calculations in a Focused Dynamical Approach: A Computational Study of Solvatochromism in Pyrimidine. Journal of Physical Chemistry A, 2015, 119, 5250-5259.	1.1	10
54	Disentangling vibronic and solvent broadening effects in the absorption spectra of coumarin derivatives for dye sensitized solar cells. Physical Chemistry Chemical Physics, 2015, 17, 11401-11411.	1.3	28

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55	Absorption and Emission Spectral Shapes of a Prototype Dye in Water by Combining Classical/Dynamical and Quantum/Static Approaches. Journal of Physical Chemistry A, 2015, 119, 5426-5438.	1.1	50
56	BALOO: A Fast and Versatile Code for Accurate Multireference Variational/Perturbative Calculations. Journal of Chemical Theory and Computation, 2015, 11, 2024-2035.	2.3	10
57	Accuracy of Quantum Mechanically Derived Force-Fields Parameterized from Dispersion-Corrected DFT Data: The Benzene Dimer as a Prototype for Aromatic Interactions. Journal of Chemical Theory and Computation, 2015, 11, 5182-5196.	2.3	67
58	Intermolecular interactions in eumelanins: a computational bottom-up approach. I. small building blocks. RSC Advances, 2015, 5, 38513-38526.	1.7	37
59	Modeling Solvent Broadening on the Vibronic Spectra of a Series of Coumarin Dyes. From Implicit to Explicit Solvent Models. Journal of Chemical Theory and Computation, 2015, 11, 5810-5825.	2.3	66
60	Structure and Dynamics of Ferrocyanide and Ferricyanide Anions in Water and Heavy Water: An Insight by MD Simulations and 2D IR Spectroscopy. Journal of Physical Chemistry B, 2014, 118, 14899-14912.	1.2	59
61	Evidences of long lived cages in functionalized polymers: Effects on chromophore dynamic and spectroscopic properties. Chemical Physics Letters, 2014, 601, 134-138.	1.2	7
62	First-principle computation of absorption and fluorescence spectra in solution accounting for vibronic structure, temperature effects and solvent inhomogenous broadening. Computational and Theoretical Chemistry, 2014, 1040-1041, 328-337.	1.1	88
63	Unraveling the interplay of different contributions to the stability of the quinhydrone dimer. RSC Advances, 2014, 4, 876-885.	1.7	26
64	Proton and Electron Transfer Mechanisms in the Formation of Neutral and Charged Quinhydrone-Like Complexes: A Multilayered Computational Study. Journal of Chemical Theory and Computation, 2014, 10, 4883-4895.	2.3	8
65	Oligomers based on weak hydrogen bond networks: a rotational study of the tetramer of difluoromethane. Chemical Communications, 2014, 50, 171-173.	2.2	43
66	Structural, dynamic and photophysical properties of a fluorescent dye incorporated in an amorphous hydrophobic polymer bundle. Physical Chemistry Chemical Physics, 2014, 16, 16573-16587.	1.3	10
67	Computational Screening of Weak Hydrogen Bond Networks: Predicting Stable Structures for Difluoromethane Oligomers. Journal of Chemical Theory and Computation, 2014, 10, 2204-2211.	2.3	8
68	Harmonic Models in Cartesian and Internal Coordinates to Simulate the Absorption Spectra of Carotenoids at Finite Temperatures. Journal of Chemical Theory and Computation, 2013, 9, 4947-4958.	2.3	62
69	Absorption and Emission Spectra of a Flexible Dye in Solution: A Computational Time-Dependent Approach. Journal of Chemical Theory and Computation, 2013, 9, 4507-4516.	2.3	78
70	Computational Design, Synthesis, and Mechanochromic Properties of New Thiopheneâ€Based Ï€â€Conjugated Chromophores. Chemistry - A European Journal, 2013, 19, 1996-2004.	1.7	43
71	Insights for an Accurate Comparison of Computational Data to Experimental Absorption and Emission Spectra: Beyond the Vertical Transition Approximation. Journal of Chemical Theory and Computation, 2013, 9, 2072-2082.	2.3	194
72	Joyce and Ulysses: integrated and user-friendly tools for the parameterization of intramolecular force fields from quantum mechanical data. Physical Chemistry Chemical Physics, 2013, 15, 3736.	1.3	89

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73	Conformational changes of Î²-carotene and zeaxanthin immersed in a model membrane through atomistic molecular dynamics simulations. Physical Chemistry Chemical Physics, 2013, 15, 6527.	1.3	21
74	Conformational Effects on the Magnetic Properties of an Organic Diradical: A Computational Study. Journal of Chemical Theory and Computation, 2013, 9, 1958-1963.	2.3	18
75	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. Journal of Chemical Theory and Computation, 2013, 9, 3626-3636.	2.3	8
76	Structureâ€“Properties Relationships in Triplet Ground State Organic Diradicals: A Computational Study. Journal of Chemical Theory and Computation, 2013, 9, 300-307.	2.3	24
77	Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case. Highlights in Theoretical Chemistry, 2013, , 319-337.	0.0	0
78	Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	64
79	An automated approach for the parameterization of accurate intermolecular forceâ€fields: Pyridine as a case study. Journal of Computational Chemistry, 2012, 33, 1055-1067.	1.5	46
80	Organic Functionalization and Optimal Coverage of a Silicon(111) Surface in Solvent: A Computational Study. Journal of Physical Chemistry C, 2011, 115, 4145-4154.	1.5	6
81	Singletâ€“triplet energy gap of a diarylnitroxide diradical by an accurate many-body perturbative approach. Physical Chemistry Chemical Physics, 2011, 13, 4709.	1.3	19
82	Molecular Dynamics Simulations of the Self-Assembly of Tetraphenylporphyrin-Based Monolayers and Bilayers at a Silver Interface. Journal of Physical Chemistry C, 2011, 115, 18434-18444.	1.5	18
83	Theoretical study of the conformational and optical properties of a fluorescent dye. A step toward modeling sensors grafted on polymer structures. Physical Chemistry Chemical Physics, 2011, 13, 21471.	1.3	7
84	Interactions of Nucleotide Bases with Decorated Si Surfaces from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2011, 115, 9146-9156.	1.5	11
85	An Integrated Protocol for the Accurate Calculation of Magnetic Interactions in Organic Magnets. Journal of Chemical Theory and Computation, 2011, 7, 699-706.	2.3	32
86	Absorption and emission spectra of fluorescent silica nanoparticles from TD-DFT/MM/PCM calculations. Physical Chemistry Chemical Physics, 2011, 13, 16689.	1.3	36
87	Fluorescence spectra of organic dyes in solution: a time dependent multilevel approach. Physical Chemistry Chemical Physics, 2011, 13, 2160-2166.	1.3	57
88	Realistic Modeling of Fluorescent Dye-Doped Silica Nanoparticles: A Step Toward the Understanding of their Enhanced Photophysical Properties.. Chemistry of Materials, 2011, 23, 5016-5023.	3.2	57
89	Complementary and partially complementary DNA duplexes tethered to a functionalized substrate: a molecular dynamics approach to biosensing. Physical Chemistry Chemical Physics, 2011, 13, 12478.	1.3	4
90	Geometry Optimization of Large and Flexible van der Waals Dimers: A Fragmentationâ^'Reconstruction Approach. Journal of Chemical Theory and Computation, 2010, 6, 2536-2546.	2.3	6

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91	Simulating DNA Hybridization on an Amine-Functionalized Silicon Substrate. Journal of Physical Chemistry B, 2010, 114, 8341-8349.	1.2	13
92	Absorption and emission UV-Vis spectra of the TRITC fluorophore molecule in solution: a quantum mechanical study. Physical Chemistry Chemical Physics, 2010, 12, 1000-1006.	1.3	67
93	Theoretical multilevel approach for studying the photophysical properties of organic dyes in solution. Physical Chemistry Chemical Physics, 2010, 12, 10550.	1.3	43
94	Parameterization and validation of an accurate force-field for the simulation of alkylamine functionalized silicon (111) surfaces. Physical Chemistry Chemical Physics, 2010, 12, 4201.	1.3	11
95	DNA hybridization mechanism on silicon nanowires: a molecular dynamics approach. Molecular BioSystems, 2010, 6, 2230.	2.9	7
96	Accurate yet feasible post-Hartreeâ€“Fock computation of magnetic interactions in large biradicals through a combined variational/perturbative approach: Setup and validation. Journal of Chemical Physics, 2009, 131, 224103.	1.2	20
97	Forceâ€field modeling through quantum mechanical calculations: Molecular dynamics simulations of a nematogenic molecule in its condensed phases. Journal of Computational Chemistry, 2009, 30, 366-378.	1.5	37
98	Chemical Detail Force Fields for Mesogenic Molecules. Journal of Chemical Theory and Computation, 2009, 5, 1865-1876.	2.3	19
99	Sensors for DNA detection: theoretical investigation of the conformational properties of immobilized single-strand DNA. Physical Chemistry Chemical Physics, 2009, 11, 10644.	1.3	16
100	Modified virtual orbitals for CI calculations of energy splitting in organic diradicals. Physical Chemistry Chemical Physics, 2009, 11, 3854.	1.3	14
101	Computational study through atomistic potentials of a partial bilayer liquid crystal: structure and dynamics. Soft Matter, 2009, 5, 3517.	1.2	27
102	Solvent-Induced Stereochemical Behavior of a Bile Acid-Based Biphenyl Phosphite: A Computational Study. Journal of Physical Chemistry A, 2009, 113, 14930-14935.	1.1	1
103	Magnetic Interactions in Phenyl-Bridged Nitroxide Diradicals: Conformational Effects by Multireference and Broken Symmetry DFT Approaches. Journal of Physical Chemistry A, 2009, 113, 15150-15155.	1.1	25
104	Estimate of Benzeneâ^'Triphenylene and Triphenyleneâ^'Triphenylene Interactions: A Topic Relevant to Columnar Discotic Liquid Crystals. Journal of Physical Chemistry C, 2008, 112, 9501-9509.	1.5	11
105	Atomistic Computer Simulation and Experimental Study on the Dynamics of the n-Cyanobiphenyls Mesogenic Series. Journal of Physical Chemistry B, 2008, 112, 9777-9786.	1.2	25
106	Subdiffusive dynamics of a liquid crystal in the isotropic phase. Journal of Chemical Physics, 2008, 128, 194501.	1.2	14
107	How the Odd-Even Effects on the Inter-Molecular Potentials Propagate to the Order Parameter in the 4-Cyano-4â€²n-Alkylbiphenyl Series. Molecular Crystals and Liquid Crystals, 2007, 465, 175-186.	0.4	14
108	Anomalous Diffusion and Cage Effects in the Isotropic Phase of a Liquid Crystal. Journal of Physical Chemistry B, 2007, 111, 7473-7477.	1.2	11

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109	Parametrization and Validation of Intramolecular Force Fields Derived from DFT Calculations. Journal of Chemical Theory and Computation, 2007, 3, 1803-1817.	2.3	102
110	Liquid Crystal Properties of then-Alkyl-cyanobiphenyl Series from Atomistic Simulations withAb InitioDerived Force Fields. Journal of Physical Chemistry B, 2007, 111, 2130-2137.	1.2	49
111	Bananaâ€Shaped Molecules Peculiarly Oriented in a Magnetic Field: ²H NMR Spectroscopy and Quantum Mechanical Calculations. ChemPhysChem, 2007, 8, 2321-2330.	1.0	23
112	Structure and dynamics of mesogens using intermolecular potentials derived from ab initio calculations. Theoretical Chemistry Accounts, 2007, 117, 885-901.	0.5	19
113	Modeling a Liquid Crystal Dynamics by Atomistic Simulation with an Ab Initio Derived Force Field. Journal of Physical Chemistry B, 2006, 110, 2847-2854.	1.2	22
114	Parametrization and Validation of Coarse Grained Force-Fields Derived from ab Initio Calculations. Journal of Chemical Theory and Computation, 2006, 2, 556-567.	2.3	21
115	DFT conformational study of banana-shaped mesogens. Chemical Physics, 2005, 314, 283-290.	0.9	23
116	Density Functional Theory Study of the Conformational Space of Phenyl Benzoate, a Common Fragment in Many Mesogenic Molecules. Journal of Physical Chemistry A, 2005, 109, 6290-6293.	1.1	9
117	Atomistic Simulation of a Nematogen Using a Force Field Derived from Quantum Chemical Calculations. Journal of Physical Chemistry B, 2005, 109, 3531-3538.	1.2	46
118	Modeling benzene with single-site potentials fromab initiocalculations: A step toward hybrid models of complex molecules. Journal of Chemical Physics, 2004, 120, 3648-3656.	1.2	17
119	Deuterium and Carbon-13 NMR Study of a Banana Mesogen:Â Molecular Structure and Order. Journal of Physical Chemistry B, 2004, 108, 7694-7701.	1.2	40
120	Intermolecular Force Fields of Large Molecules by the Fragmentation Reconstruction Method (FRM):Â Application to a Nematic Liquid Crystal. Journal of Physical Chemistry A, 2004, 108, 10336-10341.	1.1	27
121	Computer Simulation of Solid and Liquid Benzene with an Atomistic Interaction Potential Derived from ab Initio Calculations. Journal of the American Chemical Society, 2004, 126, 14278-14286.	6.6	74
122	DFT Study of the Torsional Potential in Ethylbenzene and Ethoxybenzene:â€‰ The Smallest Prototypes of Alkylâ^' and Alkoxyâ^'Aryl Mesogens. Journal of Physical Chemistry A, 2003, 107, 5228-5232.	1.1	30
123	Torsional Barriers and Correlations between Dihedrals inp-Polyphenyls. Journal of Physical Chemistry A, 2003, 107, 8665-8670.	1.1	37
124	Computer Simulation of P-Phenyls with Interaction Potentials from Ab-Initio Calculations. Molecular Crystals and Liquid Crystals, 2003, 395, 171-182.	0.4	10
125	Calculation of the intermolecular energy of large molecules by a fragmentation scheme: Application to the 4-n-pentyl-4â€²- cyanobiphenyl (5CB) dimer. Journal of Chemical Physics, 2002, 117, 3003-3012.	1.2	65
126	Stability of the nematic phase of 4-n-pentyl-4â€²-cyanobiphenyl studied by computer simulation using a hybrid model. Journal of Chemical Physics, 2002, 117, 448-453.	1.2	11