Giacomo Prampolini

List of Publications by Year in Descending Order

123 papers	2,781 citations	31 h-index	44 g-index
127 ext. papers	3,098 ext. citations	4.4 avg, IF	5.37 L-index

#	Paper	IF	Citations
123	The Role of Non-Covalent Interactions on Cluster Formation: Pentamer, Hexamers and Heptamer of Difluoromethane. *Angewandte Chemie*, **2021**, 133, 17031-17036	3.6	
122	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	6.4	2
121	The Role of Non-Covalent Interactions on Cluster Formation: Pentamer, Hexamers and Heptamer of Difluoromethane. *Angewandte Chemie - International Edition*, **2021**, 60, 16894-16899	16.4	6
120	Noncovalent interactions in catechol/ammonium-rich adhesive motifs: Reassessing the role of cation-□complexes?. *Chemical Physics Letters*, **2021**, 779, 138815	2.5	1
119	Quantum and semiclassical dynamical studies of nonadiabatic processes in solution: achievements and perspectives. *Physical Chemistry Chemical Physics*, **2021**, 23, 8181-8199	3.6	7
118	Predicting Spontaneous Orientational Self-Assembly: Design of Materials with Quantum Mechanically Derived Force Fields.. *Journal of Physical Chemistry Letters*, **2021**, 243-250	6.4	1
117	Iron□s Wake: The Performance of Quantum Mechanical-Derived Versus General-Purpose Force Fields Tested on a Luminescent Iron Complex. *Molecules*, **2020**, 25,	4.8	3
116	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	3.9	18
115	The phenoxyl group-modulated interplay of cation-□and □-type interactions in the alkali metal series. *Physical Chemistry Chemical Physics*, **2020**, 22, 27105-27120	3.6	5
114	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	6.4	23
113	Sequential Bending and Twisting around C-C Single Bonds by Mechanical Lifting of a Pre-Adsorbed Polymer. *Nano Letters*, **2020**, 20, 652-657	11.5	6
112	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	3.9	7
111	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	6.4	7
110	Benchmarking Cation-□Interactions: Assessment of Density Functional Theory and M□ller-Plesset Second-Order Perturbation Theory Calculations with Optimized Basis Sets (mp2) for Complexes of Benzene, Phenol, and Catechol with Na, K, Rb, and Cs. *Journal of Physical Chemistry A*, **2020**, 124, 3445-3459	2.8	12
109	Accurate interaction energies by spin component scaled M□ller-Plesset second order perturbation theory calculations with optimized basis sets (SCS-MP2): Development and application to aromatic heterocycles. *Journal of Chemical Physics*, **2019**, 150, 234113	3.9	6
108	The Absorption Spectrum of Guanine Based Radicals: a Comparative Computational Analysis. *ChemPhotoChem*, **2019**, 3, 846-855	3.3	6
107	A General Treatment to Study Molecular Complexes Stabilized by Hydrogen-, Halogen-, and Carbon-Bond Networks: Experiment and Theory of (CH2F2)n???(H2O)m. *Angewandte Chemie*, **2019**, 131, 8525	3.6	

106	The Intriguing Case of the One-Photon and Two-Photon Absorption of a Prototypical Symmetric Squaraine: Comparison of TDDFT and Wave-Function Methods. *ChemPhotoChem*, **2019**, 3, 778-793	3.3	5
105	Short- and Long-Range Solvation Effects on the Transient UV-Vis Absorption Spectra of a Ru(II)-Polypyridine Complex Disentangled by Nonequilibrium Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2019**, 10, 2885-2891	6.4	8
104	A General Treatment to Study Molecular Complexes Stabilized by Hydrogen-, Halogen-, and Carbon-Bond Networks: Experiment and Theory of (CH F) ???(H O). *Angewandte Chemie - International Edition*, **2019**, 58, 8437-8442	16.4	17
103	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	3.9	18
102	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. *Journal of Chemical Theory and Computation*, **2019**, 15, 529-545	6.4	9
101	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 ^*) decay of thymine. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	10
100	Structural and morphological aspects of small 3,5-disubstituted isoxazoles. *Journal of Fluorine Chemistry*, **2018**, 211, 24-36	2.1	7
99	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-trifluoro-anthrylethanol. *Chirality*, **2018**, 30, 730-743	2.1	7
98	Interaction Energy Landscapes of Aromatic Heterocycles through a Reliable yet Affordable Computational Approach. *Journal of Chemical Theory and Computation*, **2018**, 14, 543-556	6.4	17
97	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	3.6	9
96	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	6.4	16
95	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	2.3	2
94	Multistate coupled quantum dynamics of photoexcited cytosine in gas-phase: Nonadiabatic absorption spectrum and ultrafast internal conversions. *Chemical Physics*, **2018**, 515, 452-463	2.3	15
93	Mixed Quantum/Classical Method for Nonadiabatic Quantum Dynamics in Explicit Solvent Models: The □/n□ Decay of Thymine in Water as a Test Case. *Journal of Chemical Theory and Computation* , **2018**, 14, 820-832	6.4	20
92	Developing accurate intramolecular force fields for conjugated systems through explicit coupling terms. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	20
91	Quantitative prediction and interpretation of spin energy gaps in polyradicals: the virtual magnetic balance. *Physical Chemistry Chemical Physics*, **2017**, 19, 9039-9044	3.6	3
90	Eumelanin broadband absorption develops from aggregation-modulated chromophore interactions under structural and redox control. *Scientific Reports*, **2017**, 7, 41532	4.9	45
89	Magnetic gaps in organic tri-radicals: From a simple model to accurate estimates. *Journal of Chemical Physics*, **2017**, 146, 104103	3.9	3

88	Classical Force Fields Tailored for QM Applications: Is It Really a Feasible Strategy?. *Journal of Chemical Theory and Computation*, **2017**, 13, 4636-4648	6.4	41
87	Exciton Binding Energy in Molecular Triads. *Journal of Physical Chemistry C*, **2017**, 121, 17088-17095	3.8	31
86	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	3.6	6
85	Vibrationally resolved electronic spectra including vibrational pre-excitation: Theory and application to VIPER spectroscopy. *Journal of Chemical Physics*, **2017**, 147, 164116	3.9	17
84	Noncovalent Interactions in the Catechol Dimer. *Biomimetics*, **2017**, 2,	3.7	7
83	Vibronic approach to the calculation of the decay rate of the photoexcited charge-transfer state of Guanine□Cytosine stacked dimer in water solution. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	2
82	Theoretical investigation of the broad one-photon absorption line-shape of a flexible symmetric carbazole derivative. *Physical Chemistry Chemical Physics*, **2016**, 18, 22889-905	3.6	13
81	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	6.4	15
80	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	1.9	7
79	Predicting light absorption properties of anthocyanidins in solution: a multi-level computational approach. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	13
78	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	1.9	18
77	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, 2799-819	6.4	40
76	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	6.4	26
75	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	6.4	30
74	Disentangling vibronic and solvent broadening effects in the absorption spectra of coumarin derivatives for dye sensitized solar cells. *Physical Chemistry Chemical Physics*, **2015**, 17, 11401-11	3.6	25
73	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, 5426-38	2.8	45
72	BALOO: A Fast and Versatile Code for Accurate Multireference Variational/Perturbative Calculations. *Journal of Chemical Theory and Computation*, **2015**, 11, 2024-35	6.4	10
71	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, 5182-96	6.4	53

70	Intermolecular interactions in eumelanins: a computational bottom-up approach. I. small building blocks. *RSC Advances*, **2015**, 5, 38513-38526	3.7	31
69	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, 5810-25	6.4	54
68	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, 5250-9	2.8	9
67	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	2	77
66	Unraveling the interplay of different contributions to the stability of the quinhydrone dimer. *RSC Advances*, **2014**, 4, 876-885	3.7	22
65	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, 4883-95	6.4	6
64	Oligomers based on weak hydrogen bond networks: a rotational study of the tetramer of difluoromethane. *Chemical Communications*, **2014**, 50, 171-3	5.8	41
63	Structural, dynamic and photophysical properties of a fluorescent dye incorporated in an amorphous hydrophobic polymer bundle. *Physical Chemistry Chemical Physics*, **2014**, 16, 16573-87	3.6	10
62	Computational Screening of Weak Hydrogen Bond Networks: Predicting Stable Structures for Difluoromethane Oligomers. *Journal of Chemical Theory and Computation*, **2014**, 10, 2204-11	6.4	7
61	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, 14899-912	3.4	48
60	Evidences of long lived cages in functionalized polymers: Effects on chromophore dynamic and spectroscopic properties. *Chemical Physics Letters*, **2014**, 601, 134-138	2.5	7
59	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, 4947-58	6.4	47
58	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	6.4	66
57	Computational design, synthesis, and mechanochromic properties of new thiophene-based π-conjugated chromophores. *Chemistry - A European Journal*, **2013**, 19, 1996-2004	4.8	41
56	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, 2072-82	6.4	166
55	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, 3736-51	3.6	69
54	Conformational changes of β-carotene and zeaxanthin immersed in a model membrane through atomistic molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2013**, 15, 6527-38	3.6	17
53	Conformational Effects on the Magnetic Properties of an Organic Diradical: A Computational Study. *Journal of Chemical Theory and Computation*, **2013**, 9, 1958-63	6.4	16

52	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, 3626-36	6.4	6
51	Structure-Properties Relationships in Triplet Ground State Organic Diradicals: A Computational Study. *Journal of Chemical Theory and Computation*, **2013**, 9, 300-7	6.4	24
50	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		
49	An automated approach for the parameterization of accurate intermolecular force-fields: pyridine as a case study. *Journal of Computational Chemistry*, **2012**, 33, 1055-67	3.5	39
48	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	1.9	63
47	An Integrated Protocol for the Accurate Calculation of Magnetic Interactions in Organic Magnets. *Journal of Chemical Theory and Computation*, **2011**, 7, 699-706	6.4	30
46	Absorption and emission spectra of fluorescent silica nanoparticles from TD-DFT/MM/PCM calculations. *Physical Chemistry Chemical Physics*, **2011**, 13, 16689-97	3.6	34
45	Fluorescence spectra of organic dyes in solution: a time dependent multilevel approach. *Physical Chemistry Chemical Physics*, **2011**, 13, 2160-6	3.6	51
44	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	9.6	56
43	Complementary and partially complementary DNA duplexes tethered to a functionalized substrate: a molecular dynamics approach to biosensing. *Physical Chemistry Chemical Physics*, **2011**, 13, 12478-87	3.6	4
42	Organic Functionalization and Optimal Coverage of a Silicon(111) Surface in Solvent: A Computational Study. *Journal of Physical Chemistry C*, **2011**, 115, 4145-4154	3.8	6
41	Singlet-triplet energy gap of a diarylnitroxide diradical by an accurate many-body perturbative approach. *Physical Chemistry Chemical Physics*, **2011**, 13, 4709-14	3.6	18
40	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	3.8	17
39	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, 21471-8	3.6	7
38	Interactions of Nucleotide Bases with Decorated Si Surfaces from Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2011**, 115, 9146-9156	3.8	10
37	Geometry Optimization of Large and Flexible van der Waals Dimers: A Fragmentation-Reconstruction Approach. *Journal of Chemical Theory and Computation*, **2010**, 6, 2536-46	6.4	6
36	Simulating DNA hybridization on an amine-functionalized silicon substrate. *Journal of Physical Chemistry B*, **2010**, 114, 8341-9	3.4	12
35	Absorption and emission UV-Vis spectra of the TRITC fluorophore molecule in solution: a quantum mechanical study. *Physical Chemistry Chemical Physics*, **2010**, 12, 1000-6	3.6	64

34	Theoretical multilevel approach for studying the photophysical properties of organic dyes in solution. *Physical Chemistry Chemical Physics*, **2010**, 12, 10550-61	3.6	41
33	Parameterization and validation of an accurate force-field for the simulation of alkylamine functionalized silicon (111) surfaces. *Physical Chemistry Chemical Physics*, **2010**, 12, 4201-9	3.6	10
32	DNA hybridization mechanism on silicon nanowires: A molecular dynamics approach. *Molecular BioSystems*, **2010**, 6, 2230-40		6
31	Accurate yet feasible post-Hartree-Fock computation of magnetic interactions in large biradicals through a combined variational/perturbative approach: Setup and validation. *Journal of Chemical Physics*, **2009**, 131, 224103	3.9	19
30	Force-field modeling through quantum mechanical calculations: molecular dynamics simulations of a nematogenic molecule in its condensed phases. *Journal of Computational Chemistry*, **2009**, 30, 366-78	3.5	36
29	Chemical Detail Force Fields for Mesogenic Molecules. *Journal of Chemical Theory and Computation*, **2009**, 5, 1865-76	6.4	18
28	Sensors for DNA detection: theoretical investigation of the conformational properties of immobilized single-strand DNA. *Physical Chemistry Chemical Physics*, **2009**, 11, 10644-56	3.6	15
27	Modified virtual orbitals for CI calculations of energy splitting in organic diradicals. *Physical Chemistry Chemical Physics*, **2009**, 11, 3854-60	3.6	14
26	Computational study through atomistic potentials of a partial bilayer liquid crystal: structure and dynamics. *Soft Matter*, **2009**, 5, 3517	3.6	26
25	Solvent-induced stereochemical behavior of a bile acid-based biphenyl phosphite: a computational study. *Journal of Physical Chemistry A*, **2009**, 113, 14930-5	2.8	1
24	Magnetic interactions in phenyl-bridged nitroxide diradicals: conformational effects by multireference and broken symmetry DFT approaches. *Journal of Physical Chemistry A*, **2009**, 113, 15150-5	2.8	24
23	Estimate of Benzene□riphenylene and Triphenylene□riphenylene Interactions: A Topic Relevant to Columnar Discotic Liquid Crystals. *Journal of Physical Chemistry C*, **2008**, 112, 9501-9509	3.8	11
22	Atomistic computer simulation and experimental study on the dynamics of the n-cyanobiphenyls mesogenic series. *Journal of Physical Chemistry B*, **2008**, 112, 9777-86	3.4	25
21	Subdiffusive dynamics of a liquid crystal in the isotropic phase. *Journal of Chemical Physics*, **2008**, 128, 194501	3.9	12
20	Liquid crystal properties of the n-alkyl-cyanobiphenyl series from atomistic simulations with ab initio derived force fields. *Journal of Physical Chemistry B*, **2007**, 111, 2130-7	3.4	46
19	Banana-shaped molecules peculiarly oriented in a magnetic field: (2)H NMR spectroscopy and quantum mechanical calculations. *ChemPhysChem*, **2007**, 8, 2321-30	3.2	23
18	Structure and dynamics of mesogens using intermolecular potentials derived from ab initio calculations. *Theoretical Chemistry Accounts*, **2007**, 117, 885-901	1.9	18
17	How the Odd-Even Effects on the Inter-Molecular Potentials Propagate to the Order Parameter in the 4-Cyano-4?n-Alkylbiphenyl Series. *Molecular Crystals and Liquid Crystals*, **2007**, 465, 175-186	0.5	13

16	Anomalous diffusion and cage effects in the isotropic phase of a liquid crystal. *Journal of Physical Chemistry B*, **2007**, 111, 7473-7	3.4	11
15	Parametrization and Validation of Intramolecular Force Fields Derived from DFT Calculations. *Journal of Chemical Theory and Computation*, **2007**, 3, 1803-17	6.4	75
14	Modeling a liquid crystal dynamics by atomistic simulation with an ab initio derived force field. *Journal of Physical Chemistry B*, **2006**, 110, 2847-54	3.4	20
13	Parametrization and Validation of Coarse Grained Force-Fields Derived from ab Initio Calculations. *Journal of Chemical Theory and Computation*, **2006**, 2, 556-67	6.4	19
12	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, 6290-3	2.8	9
11	Atomistic simulation of a nematogen using a force field derived from quantum chemical calculations. *Journal of Physical Chemistry B*, **2005**, 109, 3531-8	3.4	45
10	DFT conformational study of banana-shaped mesogens. *Chemical Physics*, **2005**, 314, 283-290	2.3	21
9	Modeling benzene with single-site potentials from ab initio calculations: a step toward hybrid models of complex molecules. *Journal of Chemical Physics*, **2004**, 120, 3648-56	3.9	16
8	Deuterium and Carbon-13 NMR Study of a Banana Mesogen:Molecular Structure and Order. *Journal of Physical Chemistry B*, **2004**, 108, 7694-7701	3.4	38
7	Intermolecular Force Fields of Large Molecules by the Fragmentation Reconstruction Method (FRM): Application to a Nematic Liquid Crystal. *Journal of Physical Chemistry A*, **2004**, 108, 10336-10341	2.8	26
6	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, 14278-86	16.4	69
5	DFT Study of the Torsional Potential in Ethylbenzene and Ethoxybenzene: The Smallest Prototypes of Alkyl and Alkoxy Aryl Mesogens. *Journal of Physical Chemistry A*, **2003**, 107, 5228-5232	2.8	26
4	Torsional Barriers and Correlations between Dihedrals inp-Polyphenyls. *Journal of Physical Chemistry A*, **2003**, 107, 8665-8670	2.8	37
3	Computer Simulation of P-Phenyls with Interaction Potentials from Ab-Initio Calculations. *Molecular Crystals and Liquid Crystals*, **2003**, 395, 171-182	0.5	10
2	Calculation of the intermolecular energy of large molecules by a fragmentation scheme: Application to the 4-n-pentyl-4?- cyanobiphenyl (5CB) dimer. *Journal of Chemical Physics*, **2002**, 117, 3003-3012	3.9	62
1	Stability of the nematic phase of 4-n-pentyl-4?-cyanobiphenyl studied by computer simulation using a hybrid model. *Journal of Chemical Physics*, **2002**, 117, 448-453	3.9	11