

# Kaline Coutinho

## List of Publications by Year in descending order

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138  
papers

3,568  
citations

136740

32  
h-index

182168

51  
g-index

141  
all docs

141  
docs citations

141  
times ranked

2375  
citing authors

#	ARTICLE	IF	CITATIONS
1	Simulations reveal that antimicrobial BP100 induces local membrane thinning, slows lipid dynamics and favors water penetration. RSC Advances, 2022, 12, 4573-4588.	1.7	4
2	Unraveling the acid-base characterization and solvent effects on structural and electronic properties of a bis-bidentated bridging ligand. Physical Chemistry Chemical Physics, 2022, , .	1.3	4
3	Multicomponent Quantum Mechanics/Molecular Mechanics Study of Hydrated Positronium. Journal of Physical Chemistry B, 2022, , .	1.2	0
4	New insights on nonlinear solvatochromism in binary mixture of solvents. Advances in Quantum Chemistry, 2022, , .	0.4	0
5	A QM/MM study of the conformation stability and electronic structure of the photochromic switches derivatives of DHA/VHF in acetonitrile solution. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 251, 119434.	2.0	10
6	Molecular Dynamics Approach to Calculate the Thermodiffusion (Soret and Seebeck) Coefficients of Salts in Aqueous Solutions. Journal of Chemical Theory and Computation, 2021, 17, 3539-3553.	2.3	12
7	Free Energy Computation for an Isomerizing Chromophore in a Molecular Cavity via the Average Solvent Electrostatic Configuration Model: Applications in Rhodopsin and Rhodopsin-Mimicking Systems. Journal of Chemical Theory and Computation, 2021, 17, 5885-5895.	2.3	5
8	Preferential solvation and optical properties of eumelanin building blocks in binary mixture of methanol and water. Journal of Chemical Physics, 2021, 155, 174504.	1.2	3
9	Spectrophotometric studies of charge-transfer complexes formed with ions N,Nâ€™-alkyldiyl-bis(pyridinium) derivatives and iodide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, , 120664.	2.0	3
10	SuAVE: A Tool for Analyzing Curvature-Dependent Properties in Chemical Interfaces. Journal of Chemical Information and Modeling, 2020, 60, 473-484.	2.5	24
11	DICE: A Monte Carlo Code for Molecular Simulation Including the Configurational Bias Monte Carlo Method. Journal of Chemical Information and Modeling, 2020, 60, 3472-3488.	2.5	42
12	Solvent effects on the $\pi^*$ shape resonances of uracil. Journal of Chemical Physics, 2020, 152, 084301.	1.2	11
13	Quantum mechanics meets scaling theory near the critical point. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	0
14	Understanding the absorption spectrum of mesityl oxide dye in solvents of different polarities. Journal of Molecular Liquids, 2020, 307, 112924.	2.3	10
15	A new interpretation of the absorption and the dual fluorescence of Prodan in solution. Journal of Chemical Physics, 2020, 153, 244104.	1.2	10
16	Computational Prediction of $^1\text{H}$ and $^{13}\text{C}$ NMR Chemical Shifts for Protonated Alkylpyrroles: Electron Correlation and Not Solvation is the Salvation. ChemPhysChem, 2019, 20, 78-91.	1.0	15
17	Binding and Flip as Initial Steps for BP-100 Antimicrobial Actions. Scientific Reports, 2019, 9, 8622.	1.6	13
18	On the calculation of magnetic properties of nucleic acids in liquid water with the sequential QM/MM method. Journal of Molecular Liquids, 2019, 294, 111611.	2.3	13

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19	X-ray Photoelectron Fingerprints of High-Valence Ruthenium <sup>II</sup> Oxo Complexes along the Oxidation Reaction Pathway in an Aqueous Environment. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 7636-7643.	2.1	6
20	Solvent effect on the <i>syn/anti</i> conformational stability: A comparison between conformational bias Monte Carlo and molecular dynamics methods. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25688.	1.0	20
21	Theoretical study of the NMR chemical shift of Xe in supercritical condition. <i>Journal of Molecular Modeling</i> , 2018, 24, 62.	0.8	3
22	Quantum Chemistry with Thermodynamic Condition. A Journey into the Supercritical Region and Approaching the Critical Point. <i>Advances in Quantum Chemistry</i> , 2017, 74, 253-265.	0.4	0
23	Experimental and theoretical studies of emodin interacting with a lipid bilayer of DMPC. <i>Biophysical Reviews</i> , 2017, 9, 729-745.	1.5	6
24	An Average Solvent Electrostatic Configuration Protocol for QM/MM Free Energy Optimization: Implementation and Application to Rhodopsin Systems. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 6391-6404.	2.3	27
25	Hydration effects on the electronic properties of eumelanin building blocks. <i>Journal of Chemical Physics</i> , 2016, 145, 084501.	1.2	14
26	A First-Principles Approach to the Dynamics and Electronic Properties of <i>p</i> -Nitroaniline in Water. <i>Journal of Physical Chemistry A</i> , 2016, 120, 3878-3887.	1.1	23
27	An insightful approach for understanding solvatochromic reversal. <i>Chemical Physics Letters</i> , 2016, 655-656, 30-34.	1.2	15
28	Free energy barrier for dissociation of the guanosine monophosphate anion in water. <i>European Physical Journal D</i> , 2016, 70, 1.	0.6	11
29	Membrane negative curvature induced by a hybrid peptide from pediocin PA-1 and plantaricin 149 as revealed by atomistic molecular dynamics simulations. <i>Soft Matter</i> , 2016, 12, 8884-8898.	1.2	9
30	Electronic Properties in Supercritical Fluids. <i>Advances in Quantum Chemistry</i> , 2015, , 323-339.	0.4	6
31	Probing Lewis Acid-Base Interactions with Born-Oppenheimer Molecular Dynamics: The Electronic Absorption Spectrum of <i>p</i> -Nitroaniline in Supercritical CO <sub>2</sub> . <i>Journal of Physical Chemistry B</i> , 2015, 119, 8397-8405.	1.2	7
32	Behavior of the dielectric constant of Ar near the critical point. <i>Physical Review E</i> , 2015, 91, 032115.	0.8	4
33	New Insights on the Fluorescent Emission Spectra of Prodan and Laurdan. <i>Journal of Fluorescence</i> , 2015, 25, 621-629.	1.3	29
34	A first principles approach to the electronic properties of liquid and supercritical CO <sub>2</sub> . <i>Journal of Chemical Physics</i> , 2015, 142, 024504.	1.2	15
35	Structure and Electronic Properties of Liquids and Complex Molecular Systems in Solution: Coupling Many-Body Energy Decomposition Schemes to Born-Oppenheimer Molecular Dynamics. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2015, , 197-217.	0.6	0
36	Communication: Transient anion states of phenol <sup>-</sup> (H <sub>2</sub> O) <sub><i>n</i></sub> ( <i>n</i> = 1, 2) complexes: Search for microsolvation signatures. <i>Journal of Chemical Physics</i> , 2014, 141, 051105.	1.2	13

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37	Free base phthalocyanine: Influence of thermal effects and dimerization on the electronic absorption spectrum. <i>Chemical Physics Letters</i> , 2014, 595-596, 97-102.	1.2	6
38	Electric dipole moments of the fluorescent probes Prodan and Laurdan: experimental and theoretical evaluations. <i>Biophysical Reviews</i> , 2014, 6, 63-74.	1.5	24
39	Theoretically describing the 17O magnetic shielding constant of biomolecular systems: uracil and 5-fluorouracil in water environment. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	14
40	Dynamics of complexation and electronic absorption of calix[4]arene-Ar2. <i>Chemical Physics Letters</i> , 2014, 612, 266-272.	1.2	6
41	Protonation/deprotonation process of Emodin in aqueous solution and pKa determination: UV/Visible spectrophotometric titration and quantum/molecular mechanics calculations. <i>Chemical Physics</i> , 2014, 440, 69-79.	0.9	39
42	Monte Carlo "Quantum Mechanics Study of Magnetic Properties of Hydrogen Peroxide in Liquid Water. <i>Journal of Physical Chemistry A</i> , 2014, 118, 6239-6247.	1.1	16
43	One- and two-photon absorption of fluorescein dianion in water: A study using S-QM/MM methodology and ZINDO method. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 119, 63-75.	2.0	8
44	Structure and electronic properties of hydrated mesityl oxide: a sequential quantum mechanics/molecular mechanics approach. <i>Highlights in Theoretical Chemistry</i> , 2014, , 49-62.	0.0	0
45	Optical characterization of Prodan aggregates in water medium. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 11800.	1.3	15
46	Isotropic magnetic shielding constants of retinal derivatives in aprotic and protic solvents. <i>Journal of Chemical Physics</i> , 2013, 139, 094502.	1.2	20
47	Different structures give similar vibrational spectra: The case of OH <sup>+</sup> in aqueous solution. <i>Journal of Chemical Physics</i> , 2013, 138, 064503.	1.2	11
48	Electron collisions with the HCOOH <sup>-</sup> (H <sub>2</sub> O) <sub>n</sub> complexes (n = 1, 2) in liquid phase: The influence of microsolvation on the $\tilde{\nu}^*$ resonance of formic acid. <i>Journal of Chemical Physics</i> , 2013, 138, 174307.	1.2	22
49	Born-Oppenheimer molecular dynamics and electronic properties of chlorophyll-c2 in liquid methanol. <i>Journal of Chemical Physics</i> , 2013, 138, 225102.	1.2	8
50	Theoretical study of the absorption and nonradiative deactivation of 1-nitronaphthalene in the low-lying singlet and triplet excited states including methanol and ethanol solvent effects. <i>Journal of Chemical Physics</i> , 2012, 137, 054307.	1.2	35
51	Electron collisions with the HCOOH... H <sub>2</sub> O complex. <i>Journal of Physics: Conference Series</i> , 2012, 388, 052024.	0.3	0
52	Molecular Dynamics Investigations of PRODAN in a DLPC Bilayer. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2713-2721.	1.2	26
53	Ionization of chlorophyll-c2 in liquid methanol. <i>Chemical Physics Letters</i> , 2012, 546, 67-73.	1.2	7
54	Structure and electronic properties of hydrated mesityl oxide: a sequential quantum mechanics/molecular mechanics approach. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	9

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55	Calculations of the spectral shifts and line profiles of alkaline earth atoms in liquid helium environment. <i>Chemical Physics Letters</i> , 2012, 533, 25-29.	1.2	8
56	Comparison of polarizable continuum model and quantum mechanics/molecular mechanics solute electronic polarization: Study of the optical and magnetic properties of diazines in water. <i>Journal of Chemical Physics</i> , 2011, 135, 144103.	1.2	26
57	Combining Monte Carlo simulation and density-functional theory to describe the spectral changes of Na <sub>2</sub> In liquid helium. <i>Physical Review A</i> , 2011, 83, .	1.0	6
58	A sequential MC/TD-DFT study of the solvatochromic shift of the pyridinium-N-phenoxide betaine dye in water using standard and long-range corrected functionals. <i>Chemical Physics Letters</i> , 2011, 514, 251-256.	1.2	14
59	Explicit solvent effects on the visible absorption spectrum of a photosynthetic pigment: Chlorophyll-c2 in methanol. <i>Chemical Physics Letters</i> , 2011, 516, 250-253.	1.2	19
60	Electronic properties of a methane-water solution. <i>Chemical Physics Letters</i> , 2011, 506, 183-189.	1.2	12
61	Solvent effects on the electronic absorption spectrum of camphor using continuum, discrete or explicit approaches. <i>Chemical Physics Letters</i> , 2010, 484, 185-191.	1.2	22
62	Thermodynamic stability of hydrogen-bonded systems in polar and nonpolar environments. <i>Journal of Computational Chemistry</i> , 2010, 31, 2046-2055.	1.5	24
63	Electronic properties of liquid hydrogen fluoride: A sequential quantum mechanical/Born-Oppenheimer molecular dynamics approach. <i>Chemical Physics Letters</i> , 2010, 495, 40-45.	1.2	6
64	Excited state electronic polarization and reappraisal of the n → π* emission of acetone in water. <i>Chemical Physics Letters</i> , 2010, 499, 108-112.	1.2	8
65	Continuum, discrete, and explicit solvation models for describing the low-lying absorption spectrum of the pterin acid in aqueous environment. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2371-2377.	1.0	5
66	Delocalized water and fluoride contributions to Dyson orbitals for electron detachment from the hydrated fluoride anion. <i>Journal of Chemical Physics</i> , 2010, 132, 214507.	1.2	11
67	Electronic spectroscopy of biomolecules in solution: fluorescein dianion in water. <i>Molecular Physics</i> , 2010, 108, 3125-3130.	0.8	7
68	Study of the optical and magnetic properties of pyrimidine in water combining PCM and QM/MM methodologies. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 14023.	1.3	47
69	Hydrogen bond interactions between acetone and supercritical water. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6660.	1.3	19
70	Dynamic polarizability, Cauchy moments, and the optical absorption spectrum of liquid water: A sequential molecular dynamics/quantum mechanical approach. <i>Journal of Chemical Physics</i> , 2009, 130, 014505.	1.2	24
71	Synthesis, mechanism of formation, and molecular orbital calculations of arylamidoximes. <i>Monatshefte für Chemie</i> , 2009, 140, 1319-1324.	0.9	34
72	Dipole polarizability and Rayleigh light scattering by the hydrated electron. <i>Chemical Physics Letters</i> , 2009, 481, 73-77.	1.2	11

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73	Polarization and Spectral Shift of Benzophenone in Supercritical Water. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5112-5118.	1.1	25
74	Solvent Effects on Global Reactivity Properties for Neutral and Charged Systems Using the Sequential Monte Carlo Quantum Mechanics Model. <i>Journal of Physical Chemistry B</i> , 2009, 113, 4314-4322.	1.2	24
75	Combined Monte Carlo and quantum mechanics study of the solvatochromism of phenol in water. The origin of the blue shift of the lowest $\pi\pi^*$ transition. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 1388.	1.3	43
76	Solvent Effects in Chemical Processes. Water-Assisted Proton Transfer Reaction of Pterin in Aqueous Environment. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12485-12495.	1.1	62
77	Spectroscopy of Atoms in Liquid Helium Environment: A Theoretical Perspective. <i>Progress in Theoretical Chemistry and Physics</i> , 2009, , 183-200.	0.2	4
78	Sequential Monte Carlo and Quantum Mechanics Calculation of the Static Dielectric Constant of Liquid Argon. , 2009, , 327-336.		0
79	Polarization and solvatochromic shift of ortho-betaine in water. <i>Chemical Physics</i> , 2008, 349, 109-114.	0.9	26
80	The isotropic nuclear magnetic shielding constants of acetone in supercritical water: A sequential Monte Carlo/quantum mechanics study including solute polarization. <i>Journal of Chemical Physics</i> , 2008, 129, 034502.	1.2	30
81	Electronic properties of liquid ammonia: A sequential molecular dynamics/quantum mechanics approach. <i>Journal of Chemical Physics</i> , 2008, 128, 014506.	1.2	36
82	The Sequential qm/mm Method and its Applications to Solvent Effects in Electronic and Structural Properties of Solutes. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2008, , 159-189.	0.6	28
83	A Monte Carlo-quantum mechanics study of the lowest $n\pi^*$ and $\pi\pi^*$ states of uracil in water. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 4907.	1.3	54
84	Solvent effects on the UV-visible absorption spectrum of benzophenone in water: A combined Monte Carlo quantum mechanics study including solute polarization. <i>Journal of Chemical Physics</i> , 2007, 126, 034507.	1.2	107
85	Probing supercritical water with the $n\pi^*$ transition of acetone: A Monte Carlo/quantum mechanics study. <i>Journal of Chemical Physics</i> , 2007, 126, 034508.	1.2	21
86	Isotropic and anisotropic NMR chemical shifts in liquid water: a sequential QM/MM study. <i>Journal of the Brazilian Chemical Society</i> , 2007, 18, 74-84.	0.6	24
87	An efficient statistically converged average configuration for solvent effects. <i>Chemical Physics Letters</i> , 2007, 437, 148-152.	1.2	168
88	Reaction Mechanism and Tautomeric Equilibrium of 2-Mercaptopyrimidine in the Gas Phase and in Aqueous Solution: A Combined Monte Carlo and Quantum Mechanics Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7253-7261.	1.1	42
89	SEQUENTIAL MONTE CARLO/QUANTUM MECHANICS STUDY OF THE DIPOLE POLARIZABILITY OF ATOMIC LIQUIDS: THE ARGON CASE. , 2006, , 405-420.		1
90	Theoretical electronic spectra of 2-aminopurine in vapor and in water. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2564-2577.	1.0	19

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91	Converged electronic polarization of acetone in liquid water and the role in the $\pi \rightarrow \pi^*$ transition. Chemical Physics Letters, 2006, 429, 119-123.	1.2	83
92	Molecular Polarization in Liquid Environment. , 2006, , 80-90.		1
93	The Dipole Polarizability of $\tilde{F}_2$ in Aqueous Solution. A Sequential Monte Carlo/Quantum Mechanics Study. Advances in Quantum Chemistry, 2005, 48, 141-150.	0.4	9
94	Electronic polarization in liquid acetonitrile: A sequential Monte Carlo/quantum mechanics investigation. Chemical Physics Letters, 2005, 407, 13-17.	1.2	48
95	The relative stability of the two isomers of AlP3. Chemical Physics Letters, 2005, 411, 14-17.	1.2	6
96	A look inside the cavity of hydrated $\beta$ -cyclodextrin: A computer simulation study. Chemical Physics Letters, 2005, 413, 16-21.	1.2	32
97	A sequential Monte Carlo quantum mechanics study of the hydrogen-bond interaction and the solvatochromic shift of the $\pi \rightarrow \pi^*$ transition of acrolein in water. Journal of Chemical Physics, 2005, 123, 124307.	1.2	42
98	Spectral shift of sodium in a liquid-helium environment: A sequential Monte Carlo time-dependent density-functional-theory study. Physical Review A, 2005, 72, .	1.0	16
99	Conformational stability of furfural in aqueous solution: the role of hydrogen bonding. Brazilian Journal of Physics, 2004, 34, 84-89.	0.7	28
100	Sequential classical-quantum description of the absorption spectrum of the hydrated electron. Physical Review B, 2004, 70, .	1.1	21
101	Combined Monte Carlo and quantum mechanics study of the hydration of the guanine-cytosine base pair. Physical Review E, 2004, 69, 061902.	0.8	13
102	Is There a Favorite Isomer for Hydrogen-Bonded Methanol in Water?. Advances in Quantum Chemistry, 2004, 47, 51-63.	0.4	12
103	Can larger dipoles solvate less? solute $\rightarrow$ solvent hydrogen bond and the differential solvation of phenol and phenoxy. Chemical Physics Letters, 2004, 399, 534-538.	1.2	18
104	Solute relaxation on the solvatochromism of ortho-betaine dyes. A sequential Monte Carlo/quantum mechanics study. Physical Chemistry Chemical Physics, 2004, 6, 2088.	1.3	27
105	Hydrogen Bonding and the Energetics of Homolytic Dissociation in Solution. , 2004, , 581-599.		0
106	Electronic polarization of liquid water: converged Monte Carlo-quantum mechanics results for the multipole moments. Chemical Physics Letters, 2003, 369, 345-353.	1.2	67
107	The sequential Monte Carlo-quantum mechanics methodology. Application to the solvent effects in the Stokes shift of acetone in water. Computational and Theoretical Chemistry, 2003, 632, 235-246.	1.5	84
108	Electronic polarization of 1H-benzotriazole in water: Ground and first excited-state dipole moments. International Journal of Quantum Chemistry, 2003, 95, 572-579.	1.0	9

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109	Solvent Effects on the Energetics of the Phenol O-H Bond: A Differential Solvation of Phenol and Phenoxy Radical in Benzene and Acetonitrile. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9197-9207.	1.1	36
110	Differential Hydration of Phenol and Phenoxy Radical and the Energetics of the Phenol O-H Bond in Solution. <i>Journal of Physical Chemistry B</i> , 2003, 107, 4304-4310.	1.2	35
111	Electronic changes due to thermal disorder of hydrogen bonds in liquids: Pyridine in an aqueous environment. <i>Physical Review E</i> , 2003, 67, 061504.	0.8	48
112	Ab initio calculation of hydrogen bonds in liquids: A sequential Monte Carlo quantum mechanics study of pyridine in water. <i>Journal of Chemical Physics</i> , 2002, 117, 1692-1699.	1.2	95
113	New developments in Monte Carlo/quantum mechanics methodology. The solvatochromism of $\beta$ -carotene in different solvents. <i>Advances in Quantum Chemistry</i> , 2002, 41, 161-183.	0.4	66
114	A Monte Carlo-Quantum Mechanics Study of the Solvent-Induced Spectral Shift and the Specific Role of Hydrogen Bonds in the Conformational Equilibrium of Furfural in Water. <i>Journal of Physical Chemistry B</i> , 2002, 106, 12317-12322.	1.2	42
115	Solvent effects on the electronic absorption spectrum of formamide studied by a sequential Monte Carlo/quantum mechanical approach. <i>Theoretical Chemistry Accounts</i> , 2002, 108, 31-37.	0.5	39
116	Theoretical study of the hydrogen bond interaction between methylene blue and water and possible role on energy transfer for photodynamics. <i>International Journal of Quantum Chemistry</i> , 2002, 90, 634-640.	1.0	15
117	Van der Waals Interaction Probed by Solvatochromic Shifts. , 2002, , 127-133.		1
118	A Monte Carlo quantum mechanical study of the solvatochromism of pyrimidine in water and in carbon tetrachloride. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 1583-1587.	1.3	42
119	An efficient quantum mechanical/molecular mechanics Monte Carlo simulation of liquid water. <i>Chemical Physics Letters</i> , 2001, 335, 127-133.	1.2	42
120	The electronic spectrum of N-methylacetamide in aqueous solution: a sequential Monte Carlo/quantum mechanical study. <i>Chemical Physics Letters</i> , 2001, 345, 171-178.	1.2	35
121	A Monte Carlo quantum mechanics study of the spectroscopic properties of molecules in solution. <i>Computational and Theoretical Chemistry</i> , 2001, 539, 171-179.	1.5	22
122	From hydrogen bond to bulk: Solvation analysis of the n $\rightarrow$ * transition of formaldehyde in water. , 2000, 77, 192-198.		90
123	Including dispersion in configuration interaction-singles calculations for the spectroscopy of chromophores in solution. <i>Journal of Chemical Physics</i> , 2000, 112, 7293-7299.	1.2	49
124	Solvent effects in emission spectroscopy: A Monte Carlo quantum mechanics study of the n $\rightarrow$ * shift of formaldehyde in water. <i>Journal of Chemical Physics</i> , 2000, 113, 9132-9139.	1.2	173
125	A Monte Carlo-quantum mechanics study of the solvatochromic shifts of the lowest transition of benzene. <i>Journal of Chemical Physics</i> , 2000, 112, 9874-9880.	1.2	152
126	Theoretical analysis of the hydrogen bond interaction between acetone and water. <i>Computational and Theoretical Chemistry</i> , 1999, 466, 69-75.	1.5	66



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127	Sampling configurations in Monte Carlo simulations for quantum mechanical studies of solvent effects. , 1998, 66, 249-253.		55
128	Sampling configurations in Monte Carlo simulations for quantum mechanical studies of solvent effects. , 1998, 66, 249.		1
129	Solvent Effects from a Sequential Monte Carlo - Quantum Mechanical Approach. Advances in Quantum Chemistry, 1997, 28, 89-105.	0.4	150
130	Calculation of the absorption spectrum of benzene in condensed phase. A study of the solvent effects. , 1997, 65, 885-891.		31
131	Hydrophobic interaction and solvatochromic shift of benzene in water. Chemical Physics Letters, 1997, 274, 269-274.	1.2	18
132	Calculation of the absorption spectrum of benzene in condensed phase. A study of the solvent effects. , 1997, 65, 885.		1
133	CLUSTER CALCULATION OF THE ELECTRONIC STRUCTURE OF K3C60. Modern Physics Letters B, 1995, 09, 95-101.	1.0	4
134	Partial and random lattice covering times in two dimensions. Physical Review Letters, 1994, 72, 3745-3749.	2.9	26
135	Simulation Studies of Self-replicating Oligoribotides, with a Proposal for the Transition to a Peptide-assisted Stage. Journal of Theoretical Biology, 1993, 164, 291-305.	0.8	18
136	Theoretical description of the absorption spectra of solid and liquid benzene. Computational and Theoretical Chemistry, 1993, 287, 99-106.	1.5	5
137	Dynamical scaling in fragmentation. Journal of Applied Physics, 1993, 74, 7577-7587.	1.1	8
138	Robust Scaling in Fragmentation from $d = 1$ to 5. Europhysics Letters, 1992, 18, 119-124.	0.7	15