

Kaline Coutinho

List of Publications by Year in descending order

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138
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175258

52
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141
all docs

141
docs citations

141
times ranked

2375
citing authors

#	ARTICLE	IF	CITATIONS
1	Solvent effects in emission spectroscopy: A Monte Carlo quantum mechanics study of the n π^* shift of formaldehyde in water. <i>Journal of Chemical Physics</i> , 2000, 113, 9132-9139.	3.0	173
2	An efficient statistically converged average configuration for solvent effects. <i>Chemical Physics Letters</i> , 2007, 437, 148-152.	2.6	168
3	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.	3.0	152
4	Solvent Effects from a Sequential Monte Carlo - Quantum Mechanical Approach. <i>Advances in Quantum Chemistry</i> , 1997, 28, 89-105.	0.8	150
5	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.	3.0	107
6	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.	3.0	95
7	From hydrogen bond to bulk: Solvation analysis of the n π^* transition of formaldehyde in water. , 2000, 77, 192-198.		90
8	The sequential Monte Carlo-quantum mechanics methodology. Application to the solvent effects in the Stokes shift of acetone in water. <i>Computational and Theoretical Chemistry</i> , 2003, 632, 235-246.	1.5	84
9	Converged electronic polarization of acetone in liquid water and the role in the n π^* transition. <i>Chemical Physics Letters</i> , 2006, 429, 119-123.	2.6	83
10	Electronic polarization of liquid water: converged Monte Carlo-quantum mechanics results for the multipole moments. <i>Chemical Physics Letters</i> , 2003, 369, 345-353.	2.6	67
11	Theoretical analysis of the hydrogen bond interaction between acetone and water. <i>Computational and Theoretical Chemistry</i> , 1999, 466, 69-75.	1.5	66
12	New developments in Monte Carlo/quantum mechanics methodology. The solvatochromism of β -carotene in different solvents. <i>Advances in Quantum Chemistry</i> , 2002, 41, 161-183.	0.8	66
13	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.	2.5	62
14	Sampling configurations in Monte Carlo simulations for quantum mechanical studies of solvent effects. <i>International Journal of Quantum Chemistry</i> , 1998, 66, 249-253.	2.0	55
15	A Monte Carlo-quantum mechanics study of the lowest n π^* and $\pi\pi^*$ states of uracil in water. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 4907.	2.8	54
16	Including dispersion in configuration interaction-singles calculations for the spectroscopy of chromophores in solution. <i>Journal of Chemical Physics</i> , 2000, 112, 7293-7299.	3.0	49
17	Electronic changes due to thermal disorder of hydrogen bonds in liquids: Pyridine in an aqueous environment. <i>Physical Review E</i> , 2003, 67, 061504.	2.1	48
18	Electronic polarization in liquid acetonitrile: A sequential Monte Carlo/quantum mechanics investigation. <i>Chemical Physics Letters</i> , 2005, 407, 13-17.	2.6	48

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19	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.	2.8	47
20	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.	2.8	43
21	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.	2.8	42
22	An efficient quantum mechanical/molecular mechanics Monte Carlo simulation of liquid water. <i>Chemical Physics Letters</i> , 2001, 335, 127-133.	2.6	42
23	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.	2.6	42
24	A sequential Monte Carlo quantum mechanics study of the hydrogen-bond interaction and the solvatochromic shift of the $n\pi^*$ transition of acrolein in water. <i>Journal of Chemical Physics</i> , 2005, 123, 124307.	3.0	42
25	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.	2.5	42
26	DICE: A Monte Carlo Code for Molecular Simulation Including the Configurational Bias Monte Carlo Method. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3472-3488.	5.4	42
27	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.	1.4	39
28	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.	1.9	39
29	Solvent Effects on the Energetics of the Phenol O-H Bond: Differential Solvation of Phenol and Phenoxy Radical in Benzene and Acetonitrile. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9197-9207.	2.5	36
30	Electronic properties of liquid ammonia: A sequential molecular dynamics/quantum mechanics approach. <i>Journal of Chemical Physics</i> , 2008, 128, 014506.	3.0	36
31	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.	2.6	35
32	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.	2.6	35
33	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.	3.0	35
34	Synthesis, mechanism of formation, and molecular orbital calculations of arylamidoximes. <i>Monatshefte für Chemie</i> , 2009, 140, 1319-1324.	1.8	34
35	A look inside the cavity of hydrated β -cyclodextrin: A computer simulation study. <i>Chemical Physics Letters</i> , 2005, 413, 16-21.	2.6	32
36	Calculation of the absorption spectrum of benzene in condensed phase. A study of the solvent effects. <i>International Journal of Quantum Chemistry</i> , 1997, 65, 885-891.	2.0	31

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37	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.	3.0	30
38	New Insights on the Fluorescent Emission Spectra of Prodan and Laurdan. <i>Journal of Fluorescence</i> , 2015, 25, 621-629.	2.5	29
39	Conformational stability of furfural in aqueous solution: the role of hydrogen bonding. <i>Brazilian Journal of Physics</i> , 2004, 34, 84-89.	1.4	28
40	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
41	Solute relaxation on the solvatochromism of ortho-betaine dyes. A sequential Monte Carlo/quantum mechanics study. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 2088.	2.8	27
42	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.	5.3	27
43	Partial and random lattice covering times in two dimensions. <i>Physical Review Letters</i> , 1994, 72, 3745-3749.	7.8	26
44	Polarization and solvatochromic shift of ortho-betaine in water. <i>Chemical Physics</i> , 2008, 349, 109-114.	1.9	26
45	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.	3.0	26
46	Molecular Dynamics Investigations of PRODAN in a DLPC Bilayer. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2713-2721.	2.6	26
47	Polarization and Spectral Shift of Benzophenone in Supercritical Water. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5112-5118.	2.5	25
48	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
49	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.	3.0	24
50	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.	2.6	24
51	Thermodynamic stability of hydrogen-bonded systems in polar and nonpolar environments. <i>Journal of Computational Chemistry</i> , 2010, 31, 2046-2055.	3.3	24
52	Electric dipole moments of the fluorescent probes Prodan and Laurdan: experimental and theoretical evaluations. <i>Biophysical Reviews</i> , 2014, 6, 63-74.	3.2	24
53	SuAVE: A Tool for Analyzing Curvature-Dependent Properties in Chemical Interfaces. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 473-484.	5.4	24
54	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.	2.5	23

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55	A Monte Carlo quantum mechanics study of the spectroscopic properties of molecules in solution. Computational and Theoretical Chemistry, 2001, 539, 171-179.	1.5	22
56	Solvent effects on the electronic absorption spectrum of camphor using continuum, discrete or explicit approaches. Chemical Physics Letters, 2010, 484, 185-191.	2.6	22
57	Electron collisions with the HCOOH·(H ₂ O) _n complexes (n = 1, 2) in liquid phase: The influence of microsolvation on the n-π* resonance of formic acid. Journal of Chemical Physics, 2013, 138, 174307.	3.0	22
58	Sequential classical-quantum description of the absorption spectrum of the hydrated electron. Physical Review B, 2004, 70, .	3.2	21
59	Probing supercritical water with the n-π* transition of acetone: A Monte Carlo/quantum mechanics study. Journal of Chemical Physics, 2007, 126, 034508.	3.0	21
60	Isotropic magnetic shielding constants of retinal derivatives in aprotic and protic solvents. Journal of Chemical Physics, 2013, 139, 094502.	3.0	20
61	Solvent effect on the <i>syn/anti</i> conformational stability: A comparison between conformational bias Monte Carlo and molecular dynamics methods. International Journal of Quantum Chemistry, 2019, 119, e25688.	2.0	20
62	Theoretical electronic spectra of 2-aminopurine in vapor and in water. International Journal of Quantum Chemistry, 2006, 106, 2564-2577.	2.0	19
63	Hydrogen bond interactions between acetone and supercritical water. Physical Chemistry Chemical Physics, 2010, 12, 6660.	2.8	19
64	Explicit solvent effects on the visible absorption spectrum of a photosynthetic pigment: Chlorophyll-c2 in methanol. Chemical Physics Letters, 2011, 516, 250-253.	2.6	19
65	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.	1.7	18
66	Hydrophobic interaction and solvatochromic shift of benzene in water. Chemical Physics Letters, 1997, 274, 269-274.	2.6	18
67	Can larger dipoles solvate less? solute-solvent hydrogen bond and the differential solvation of phenol and phenoxy. Chemical Physics Letters, 2004, 399, 534-538.	2.6	18
68	Spectral shift of sodium in a liquid-helium environment: A sequential Monte Carlo time-dependent density-functional-theory study. Physical Review A, 2005, 72, .	2.5	16
69	Monte Carlo Quantum Mechanics Study of Magnetic Properties of Hydrogen Peroxide in Liquid Water. Journal of Physical Chemistry A, 2014, 118, 6239-6247.	2.5	16
70	Robust Scaling in Fragmentation from d = 1 to 5. Europhysics Letters, 1992, 18, 119-124.	2.0	15
71	Theoretical study of the hydrogen bond interaction between methylene blue and water and possible role on energy transfer for photodynamics. International Journal of Quantum Chemistry, 2002, 90, 634-640.	2.0	15
72	Optical characterization of Prodan aggregates in water medium. Physical Chemistry Chemical Physics, 2013, 15, 11800.	2.8	15

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73	A first principles approach to the electronic properties of liquid and supercritical CO ₂ . Journal of Chemical Physics, 2015, 142, 024504.	3.0	15
74	An insightful approach for understanding solvatochromic reversal. Chemical Physics Letters, 2016, 655-656, 30-34.	2.6	15
75	Computational Prediction of ¹ H and ¹³ C NMR Chemical Shifts for Protonated Alkylpyrroles: Electron Correlation and Not Solvation is the Salvation. ChemPhysChem, 2019, 20, 78-91.	2.1	15
76	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. Chemical Physics Letters, 2011, 514, 251-256.	2.6	14
77	Theoretically describing the 17O magnetic shielding constant of biomolecular systems: uracil and 5-fluorouracil in water environment. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	14
78	Hydration effects on the electronic properties of eumelanin building blocks. Journal of Chemical Physics, 2016, 145, 084501.	3.0	14
79	Combined Monte Carlo and quantum mechanics study of the hydration of the guanine-cytosine base pair. Physical Review E, 2004, 69, 061902.	2.1	13
80	Communication: Transient anion states of phenolâ€¦(H ₂ O) _n (n = 1, 2) complexes: Search for microsolvation signatures. Journal of Chemical Physics, 2014, 141, 051105.	3.0	13
81	Binding and Flip as Initial Steps for BP-100 Antimicrobial Actions. Scientific Reports, 2019, 9, 8622.	3.3	13
82	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.	4.9	13
83	Is There a Favorite Isomer for Hydrogen-Bonded Methanol in Water?. Advances in Quantum Chemistry, 2004, 47, 51-63.	0.8	12
84	Electronic properties of a methaneâ€¦water solution. Chemical Physics Letters, 2011, 506, 183-189.	2.6	12
85	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.	5.3	12
86	Dipole polarizability and Rayleigh light scattering by the hydrated electron. Chemical Physics Letters, 2009, 481, 73-77.	2.6	11
87	Delocalized water and fluoride contributions to Dyson orbitals for electron detachment from the hydrated fluoride anion. Journal of Chemical Physics, 2010, 132, 214507.	3.0	11
88	Different structures give similar vibrational spectra: The case of OH ⁺ in aqueous solution. Journal of Chemical Physics, 2013, 138, 064503.	3.0	11
89	Free energy barrier for dissociation of the guanosine monophosphate anion in water. European Physical Journal D, 2016, 70, 1.	1.3	11
90	Solvent effects on the $\tilde{\nu}^*$ shape resonances of uracil. Journal of Chemical Physics, 2020, 152, 084301.	3.0	11

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91	Understanding the absorption spectrum of mesityl oxide dye in solvents of different polarities. <i>Journal of Molecular Liquids</i> , 2020, 307, 112924.	4.9	10
92	A QM/MM study of the conformation stability and electronic structure of the photochromic switches derivatives of DHA/VHF in acetonitrile solution. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 251, 119434.	3.9	10
93	A new interpretation of the absorption and the dual fluorescence of Prodan in solution. <i>Journal of Chemical Physics</i> , 2020, 153, 244104.	3.0	10
94	Electronic polarization of 1H-benzotriazole in water: Ground and first excited-state dipole moments. <i>International Journal of Quantum Chemistry</i> , 2003, 95, 572-579.	2.0	9
95	The Dipole Polarizability of Fã ⁺ in Aqueous Solution. A Sequential Monte Carlo/Quantum Mechanics Study. <i>Advances in Quantum Chemistry</i> , 2005, 48, 141-150.	0.8	9
96	Structure and electronic properties of hydrated mesityl oxide: a sequential quantum mechanics/molecular mechanics approach. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	9
97	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.	2.7	9
98	Dynamical scaling in fragmentation. <i>Journal of Applied Physics</i> , 1993, 74, 7577-7587.	2.5	8
99	Excited state electronic polarization and reappraisal of the n ã ⁺ ã ⁻ emission of acetone in water. <i>Chemical Physics Letters</i> , 2010, 499, 108-112.	2.6	8
100	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.	2.6	8
101	Born-Oppenheimer molecular dynamics and electronic properties of chlorophyll-c2 in liquid methanol. <i>Journal of Chemical Physics</i> , 2013, 138, 225102.	3.0	8
102	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.	3.9	8
103	Electronic spectroscopy of biomolecules in solution: fluorescein dianion in water. <i>Molecular Physics</i> , 2010, 108, 3125-3130.	1.7	7
104	Ionization of chlorophyll-c2 in liquid methanol. <i>Chemical Physics Letters</i> , 2012, 546, 67-73.	2.6	7
105	Probing Lewis Acidã€“Base Interactions with Bornã€“Oppenheimer Molecular Dynamics: The Electronic Absorption Spectrum of <i>p</i> -Nitroaniline in Supercritical CO ₂ . <i>Journal of Physical Chemistry B</i> , 2015, 119, 8397-8405.	2.6	7
106	The relative stability of the two isomers of AIP3. <i>Chemical Physics Letters</i> , 2005, 411, 14-17.	2.6	6
107	Electronic properties of liquid hydrogen fluoride: A sequential quantum mechanical/Bornã€“Oppenheimer molecular dynamics approach. <i>Chemical Physics Letters</i> , 2010, 495, 40-45.	2.6	6
108	Combining Monte Carlo simulation and density-functional theory to describe the spectral changes of Na ₂ in liquid helium. <i>Physical Review A</i> , 2011, 83, .	2.5	6

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109	Free base phthalocyanine: Influence of thermal effects and dimerization on the electronic absorption spectrum. <i>Chemical Physics Letters</i> , 2014, 595-596, 97-102.	2.6	6
110	Dynamics of complexation and electronic absorption of calix[4]arene-Ar ₂ . <i>Chemical Physics Letters</i> , 2014, 612, 266-272.	2.6	6
111	Electronic Properties in Supercritical Fluids. <i>Advances in Quantum Chemistry</i> , 2015, , 323-339.	0.8	6
112	Experimental and theoretical studies of emodin interacting with a lipid bilayer of DMPC. <i>Biophysical Reviews</i> , 2017, 9, 729-745.	3.2	6
113	X-ray Photoelectron Fingerprints of High-Valence Ruthenium Oxo Complexes along the Oxidation Reaction Pathway in an Aqueous Environment. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 7636-7643.	4.6	6
114	Theoretical description of the absorption spectra of solid and liquid benzene. <i>Computational and Theoretical Chemistry</i> , 1993, 287, 99-106.	1.5	5
115	Continuum, discrete, and explicit solvation models for describing the low-frequency absorption spectrum of the pterin acid in aqueous environment. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2371-2377.	2.0	5
116	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. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5885-5895.	5.3	5
117	CLUSTER CALCULATION OF THE ELECTRONIC STRUCTURE OF K ₃ C ₆₀ . <i>Modern Physics Letters B</i> , 1995, 09, 95-101.	1.9	4
118	Spectroscopy of Atoms in Liquid Helium Environment: A Theoretical Perspective. <i>Progress in Theoretical Chemistry and Physics</i> , 2009, , 183-200.	0.2	4
119	Behavior of the dielectric constant of Ar near the critical point. <i>Physical Review E</i> , 2015, 91, 032115.	2.1	4
120	Simulations reveal that antimicrobial BP100 induces local membrane thinning, slows lipid dynamics and favors water penetration. <i>RSC Advances</i> , 2022, 12, 4573-4588.	3.6	4
121	Unraveling the acid-base characterization and solvent effects on structural and electronic properties of a bis-bidentated bridging ligand. <i>Physical Chemistry Chemical Physics</i> , 2022, , .	2.8	4
122	Theoretical study of the NMR chemical shift of Xe in supercritical condition. <i>Journal of Molecular Modeling</i> , 2018, 24, 62.	1.8	3
123	Preferential solvation and optical properties of eumelanin building blocks in binary mixture of methanol and water. <i>Journal of Chemical Physics</i> , 2021, 155, 174504.	3.0	3
124	Spectrophotometric studies of charge-transfer complexes formed with ions N,N'-alkyldiyl-bis(pyridinium) derivatives and iodide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, , 120664.	3.9	3
125	SEQUENTIAL MONTE CARLO/QUANTUM MECHANICS STUDY OF THE DIPOLE POLARIZABILITY OF ATOMIC LIQUIDS: THE ARGON CASE. , 2006, , 405-420.		1
126	Calculation of the absorption spectrum of benzene in condensed phase. A study of the solvent effects. , 1997, 65, 885.		1

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127	Sampling configurations in Monte Carlo simulations for quantum mechanical studies of solvent effects. , 1998, 66, 249.		1
128	Van der Waals Interaction Probed by Solvatochromic Shifts. , 2002, , 127-133.		1
129	Molecular Polarization in Liquid Environment. , 2006, , 80-90.		1
130	Electron collisions with the HCOOH... H ₂ O complex. Journal of Physics: Conference Series, 2012, 388, 052024.	0.4	0
131	Quantum Chemistry with Thermodynamic Condition. A Journey into the Supercritical Region and Approaching the Critical Point. Advances in Quantum Chemistry, 2017, 74, 253-265.	0.8	0
132	Quantum mechanics meets scaling theory near the critical point. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	0
133	Hydrogen Bonding and the Energetics of Homolytic Dissociation in Solution. , 2004, , 581-599.		0
134	Sequential Monte Carlo and Quantum Mechanics Calculation of the Static Dielectric Constant of Liquid Argon. , 2009, , 327-336.		0
135	Structure and electronic properties of hydrated mesityl oxide: a sequential quantum mechanics/molecular mechanics approach. Highlights in Theoretical Chemistry, 2014, , 49-62.	0.0	0
136	Structure and Electronic Properties of Liquids and Complex Molecular Systems in Solution: Coupling Many-Body Energy Decomposition Schemes to Born-Oppenheimer Molecular Dynamics. Challenges and Advances in Computational Chemistry and Physics, 2015, , 197-217.	0.6	0
137	Multicomponent Quantum Mechanics/Molecular Mechanics Study of Hydrated Positronium. Journal of Physical Chemistry B, 2022, , .	2.6	0
138	New insights on nonlinear solvatochromism in binary mixture of solvents. Advances in Quantum Chemistry, 2022, , .	0.8	0