

Sylvio Roberto Accioly Canuto

List of Publications by Year in descending order

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263
papers

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94269

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3476
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#	ARTICLE	IF	CITATIONS
1	Free-Energy Landscape of the S_{N2} Reaction $CH_3Br + Cl^- \rightarrow CH_3Cl + Br^-$ in Different Liquid Environments. <i>Journal of Physical Chemistry B</i> , 2022, 126, 3685-3692.	1.2	3
2	New insights on nonlinear solvatochromism in binary mixture of solvents. <i>Advances in Quantum Chemistry</i> , 2022, , .	0.4	0
3	Ultrafast Intersystem Crossing Dynamics of 6-Selenoguanine in Water. <i>Jacs Au</i> , 2022, 2, 1699-1711.	3.6	10
4	Excited-State Properties and Relaxation Pathways of Selenium-Substituted Guanine Nucleobase in Aqueous Solution and DNA Duplex. <i>Journal of Physical Chemistry B</i> , 2021, 125, 1778-1789.	1.2	18
5	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.	2.0	10
6	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.	2.3	5
7	On the population of triplet states of 2-seleno-thymine. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 5447-5454.	1.3	7
8	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.	1.2	3
9	On the spectral line width broadening for simulation of the two-photon absorption cross-section of para-Nitroaniline in liquid environment. <i>Journal of Molecular Liquids</i> , 2020, 301, 112405.	2.3	7
10	A theoretical study of the magnetic shielding of ^{15}N of formamide in liquid water. <i>Journal of Molecular Liquids</i> , 2020, 320, 114415.	2.3	11
11	Free energy gradient for understanding the stability and properties of neutral and charged L-alanine molecule in water. <i>Journal of Molecular Liquids</i> , 2020, 319, 114109.	2.3	4
12	Solvation Structures and Deactivation Pathways of Luminescent Isothiazole-Derived Nucleobases: A , G , and I . <i>Journal of Physical Chemistry A</i> , 2020, 124, 6834-6844.	1.1	8
13	Theoretical analysis of the influence of $C-H \cdots O$ bonds on the NMR constants of uracil in DMSO. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	5
14	Unraveling the Electric Field-Induced Second Harmonic Generation Responses of Stilbazolium Ion Pairs Complexes in Solution Using a Multiscale Simulation Method. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 4817-4826.	2.5	14
15	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.	2.5	42
16	Quantum mechanics meets scaling theory near the critical point. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	0
17	Understanding the absorption spectrum of mesityl oxide dye in solvents of different polarities. <i>Journal of Molecular Liquids</i> , 2020, 307, 112924.	2.3	10
18	A new interpretation of the absorption and the dual fluorescence of Prodan in solution. <i>Journal of Chemical Physics</i> , 2020, 153, 244104.	1.2	10

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19	On the calculation of magnetic properties of nucleic acids in liquid water with the sequential QM/MM method. <i>Journal of Molecular Liquids</i> , 2019, 294, 111611.	2.3	13
20	Photophysics of Emissive tz C[Isythiazoloâ€Cytidine] and tz U[Isythiazoloâ€Uridine] Pyrimidine Analogues. <i>ChemPhotoChem</i> , 2019, 3, 916-924.	1.5	3
21	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
22	NMR spinâ€spin coupling constants in hydrogenâ€bonded glycine clusters. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25608.	1.0	4
23	Theoretical study of the NMR chemical shift of Xe in supercritical condition. <i>Journal of Molecular Modeling</i> , 2018, 24, 62.	0.8	3
24	Oxazole Dyes with Potential for Photoluminescence Bioprobes: A Two-Photon Absorption Study. <i>Journal of Physical Chemistry C</i> , 2018, 122, 10526-10534.	1.5	16
25	Microscopic Origin of Different Hydration Patterns of <i>para</i>-Nitrophenol and Its Anion: A Study Combining Multiconfigurational Calculations and the Free-Energy Gradient Method. <i>Journal of Physical Chemistry B</i> , 2018, 122, 9202-9209.	1.2	4
26	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
27	Electronic structure and absorption spectra of fluorescent nucleoside analogues. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 29354-29363.	1.3	12
28	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
29	A theoretical study of the low-lying excited states and the photophysics of dimethoxy curcumin in cyclohexane and acetonitrile. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	0
30	Solvent Effects on the Dynamic Polarizability and Raman Response of Moleculeâ€Metal Oxide Hybrid Clusters. <i>ChemPhysChem</i> , 2016, 17, 2590-2595.	1.0	4
31	Hydration effects on the electronic properties of eumelanin building blocks. <i>Journal of Chemical Physics</i> , 2016, 145, 084501.	1.2	14
32	A simple model for a theoretical study of the spectral line shifts of alkali atoms attached to helium nanodroplets. <i>Chemical Physics Letters</i> , 2016, 644, 142-146.	1.2	3
33	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
34	An insightful approach for understanding solvatochromic reversal. <i>Chemical Physics Letters</i> , 2016, 655-656, 30-34.	1.2	15
35	A complete basis set study of the lowest nâ€f* and fâ€f* electronic transitions of acrolein in explicit water environment. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	13
36	Free energy barrier for dissociation of the guanosine monophosphate anion in water. <i>European Physical Journal D</i> , 2016, 70, 1.	0.6	11

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37	A CASPT2 study of the spectral shift of the resonance emission lines of Rb and Cs embedded in liquid He. <i>Chemical Physics Letters</i> , 2016, 655-656, 91-95.	1.2	1
38	Theoretical study of the spectral shift of the absorption line of Rb and Cs in liquid helium. <i>Chemical Physics Letters</i> , 2015, 633, 256-260.	1.2	4
39	Electronic Properties in Supercritical Fluids. <i>Advances in Quantum Chemistry</i> , 2015, , 323-339.	0.4	6
40	Experimental and theoretical investigation of the first-order hyperpolarizability of a class of triarylamine derivatives. <i>Journal of Chemical Physics</i> , 2015, 142, 064312.	1.2	25
41	Interpreting the First-Order Electronic Hyperpolarizability for a Series of Octupolar Push-Pull Triarylamine Molecules Containing Trifluoromethyl. <i>Journal of Physical Chemistry C</i> , 2015, 119, 12589-12597.	1.5	16
42	Probing Lewis Acid-Base Interactions with Born-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.	1.2	7
43	Behavior of the dielectric constant of Ar near the critical point. <i>Physical Review E</i> , 2015, 91, 032115.	0.8	4
44	Magnetic dipolar and quadrupolar transitions in two-electron atoms under exponential-cosine-screened Coulomb potential. <i>Physics of Plasmas</i> , 2015, 22, 032902.	0.7	6
45	A first principles approach to the electronic properties of liquid and supercritical CO ₂ . <i>Journal of Chemical Physics</i> , 2015, 142, 024504.	1.2	15
46	Including Thermal Disorder of Hydrogen Bonding to Describe the Vibrational Circular Dichroism Spectrum of Zwitterionic Alanine in Water. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5099-5106.	1.1	6
47	Communication: Transient anion states of phenol (H ₂ O) _n (<i>n</i> = 1, 2) complexes: Search for microsolvation signatures. <i>Journal of Chemical Physics</i> , 2014, 141, 051105.	1.2	13
48	Combining ab initio multiconfigurational and Free Energy Gradient methods to study the $\tilde{\pi}^* \leftarrow \tilde{\pi}$ excited state structure and properties of uracil in water. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 312-320.	1.1	26
49	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
50	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
51	Dynamics of complexation and electronic absorption of calix[4]arene-Ar ₂ . <i>Chemical Physics Letters</i> , 2014, 612, 266-272.	1.2	6
52	Origin of the Red Shift for the Lowest Singlet $\tilde{\pi} \rightarrow \tilde{\pi}^*$ Charge-Transfer Absorption of <i>p</i> -Nitroaniline in Supercritical CO ₂ . <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1554-1562.	2.3	21
53	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
54	Self-Aggregation and Optical Absorption of Stilbazolium Merocyanine in Chloroform. <i>Journal of Physical Chemistry B</i> , 2014, 118, 1715-1725.	1.2	19

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55	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
56	Molecular Structure and Optical Property Relationships for a Series of Non-Centrosymmetric Two-photon Absorbing Push-Pull Triarylamine Molecules. <i>Scientific Reports</i> , 2014, 4, 4447.	1.6	55
57	A simple analysis of the influence of the solvent-induced electronic polarization on the ¹⁵ N magnetic shielding of pyridine in water. <i>Highlights in Theoretical Chemistry</i> , 2014, , 117-124.	0.0	1
58	Solvent effects on the two lowest-lying singlet excited states of 5-fluorouracil. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	25
59	Revealing the Electronic and Molecular Structure of Randomly Oriented Molecules by Polarized Two-Photon Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1753-1759.	2.1	16
60	A theoretical study of the spectral shifts of Xe atom in Ar environment. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2013, 377, 1720-1724.	0.9	4
61	Solvent Effect on the Stokes Shift and on the Nonfluorescent Decay of the Daidzein Molecular System. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4404-4411.	1.1	13
62	Electron collisions with the HCOOH· ⁻ (H ₂ O) _n 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
63	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
64	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
65	Effect of hydrogen bond formation on the elastic molecular scattering: a case study with methanol. <i>Molecular Physics</i> , 2012, 110, 297-306.	0.8	11
66	Electronic Properties of Water in Liquid Environment. A Sequential QM/MM Study Using the Free Energy Gradient Method. <i>Journal of Physical Chemistry B</i> , 2012, 116, 11247-11254.	1.2	43
67	Ionization of chlorophyll-c2 in liquid methanol. <i>Chemical Physics Letters</i> , 2012, 546, 67-73.	1.2	7
68	Structural properties and energetics of diffuse ⁸⁷ Rb clusters in three-dimension. <i>Journal of Chemical Physics</i> , 2012, 137, 014301.	1.2	6
69	Experimental and Theoretical Study on the One- and Two-Photon Absorption Properties of Novel Organic Molecules Based on Phenylacetylene and Azoaromatic Moieties. <i>Journal of Physical Chemistry B</i> , 2012, 116, 14677-14688.	1.2	27
70	A simple analysis of the influence of the solvent-induced electronic polarization on the ¹⁵ N magnetic shielding of pyridine in water. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	18
71	The Role of Molecular Conformation and Polarizable Embedding for One- and Two-Photon Absorption of Disperse Orange 3 in Solution. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8169-8181.	1.2	40
72	Theoretical study of the XP ₃ (X=Al, B, Ga) clusters. <i>Chemical Physics</i> , 2012, 399, 23-27.	0.9	2

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73	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
74	Two-photon absorption in oxazole derivatives: An experimental and quantum chemical study. <i>Optical Materials</i> , 2012, 34, 1013-1018.	1.7	13
75	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
76	CASPT2 Study of the Potential Energy Surface of the HSO ₂ System. <i>Journal of Physical Chemistry A</i> , 2011, 115, 1453-1461.	1.1	30
77	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, .	1.0	6
78	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
79	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
80	Electronic properties of a methane-water solution. <i>Chemical Physics Letters</i> , 2011, 506, 183-189.	1.2	12
81	Experimental and theoretical study of two-photon absorption in nitrofurans derivatives: Promising compounds for photochemotherapy. <i>Journal of Chemical Physics</i> , 2011, 134, 014509.	1.2	23
82	Use of correlated potential harmonic basis functions for the description of the 4He trimer and small clusters. <i>Journal of Chemical Physics</i> , 2011, 134, 164106.	1.2	10
83	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
84	Photophysics and photostability of adenine in aqueous solution: A theoretical study. <i>Chemical Physics Letters</i> , 2010, 492, 164-169.	1.2	29
85	Characterization and spectroscopic analysis of phenol-ethanol hydrogen bonded clusters. <i>Chemical Physics Letters</i> , 2010, 496, 236-242.	1.2	1
86	Thermodynamic stability of hydrogen-bonded systems in polar and nonpolar environments. <i>Journal of Computational Chemistry</i> , 2010, 31, 2046-2055.	1.5	24
87	Many-body energy decomposition of hydrogen-bonded glycine clusters in gas-phase. <i>Chemical Physics Letters</i> , 2010, 491, 86-90.	1.2	9
88	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
89	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
90	Continuum, discrete, and explicit solvation models for describing the low-energy absorption spectrum of the pterin acid in aqueous environment. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2371-2377.	1.0	5

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91	Preface: Proceedings of the XV Brazilian Symposium of Theoretical Chemistry. International Journal of Quantum Chemistry, 2010, 110, 2005-2005.	1.0	0
92	Delocalized water and fluoride contributions to Dyson orbitals for electron detachment from the hydrated fluoride anion. Journal of Chemical Physics, 2010, 132, 214507.	1.2	11
93	Hyperpolarizabilities of the methanol molecule: A CCSD calculation including vibrational corrections. Journal of Chemical Physics, 2010, 132, 034307.	1.2	26
94	Electronic spectroscopy of biomolecules in solution: fluorescein dianion in water. Molecular Physics, 2010, 108, 3125-3130.	0.8	7
95	Study of the optical and magnetic properties of pyrimidine in water combining PCM and QM/MM methodologies. Physical Chemistry Chemical Physics, 2010, 12, 14023.	1.3	47
96	Hydrogen bond interactions between acetone and supercritical water. Physical Chemistry Chemical Physics, 2010, 12, 6660.	1.3	19
97	Dynamic polarizability, Cauchy moments, and the optical absorption spectrum of liquid water: A sequential molecular dynamics/quantum mechanical approach. Journal of Chemical Physics, 2009, 130, 014505.	1.2	24
98	⁸⁵ Rb Bose-Einstein condensate with tunable interaction: A quantum many body approach. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 258-261.	0.9	37
99	Dipole polarizability and Rayleigh light scattering by the hydrated electron. Chemical Physics Letters, 2009, 481, 73-77.	1.2	11
100	Polarization and Spectral Shift of Benzophenone in Supercritical Water. Journal of Physical Chemistry A, 2009, 113, 5112-5118.	1.1	25
101	Solvent Effects on Global Reactivity Properties for Neutral and Charged Systems Using the Sequential Monte Carlo Quantum Mechanics Model. Journal of Physical Chemistry B, 2009, 113, 4314-4322.	1.2	24
102	Combined Monte Carlo and quantum mechanics study of the solvatochromism of phenol in water. The origin of the blue shift of the lowest $\pi \rightarrow \pi^*$ transition. Physical Chemistry Chemical Physics, 2009, 11, 1388.	1.3	43
103	NMR Chemical Shielding and Spin-Spin Coupling Constants of Liquid NH_3 : A Systematic Investigation using the Sequential QM/MM Method. Journal of Physical Chemistry A, 2009, 113, 14936-14942.	1.1	33
104	Solvent Effects in Chemical Processes. Water-Assisted Proton Transfer Reaction of Pterin in Aqueous Environment. Journal of Physical Chemistry A, 2009, 113, 12485-12495.	1.1	62
105	Spectroscopy of Atoms in Liquid Helium Environment: A Theoretical Perspective. Progress in Theoretical Chemistry and Physics, 2009, , 183-200.	0.2	4
106	Spectroscopy of Confined Atomic Systems: Effect of Plasma. Advances in Quantum Chemistry, 2009, , 115-175.	0.4	121
107	Electron collisions with the CH_2^+ ion. Physical Review A, 2009, 80, .	1.0	24
108	Sequential Monte Carlo and Quantum Mechanics Calculation of the Static Dielectric Constant of Liquid Argon. , 2009, , 327-336.		0

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109	Preface: Proceedings of the XIV Brazilian Symposium of Theoretical Chemistry. International Journal of Quantum Chemistry, 2008, 108, 2305-2305.	1.0	0
110	Calculations of vibrational frequencies, Raman activities and degrees of depolarization for complexes involving water, methanol and ethanol. Chemical Physics Letters, 2008, 452, 54-58.	1.2	31
111	2-Aminopurine non-radiative decay and emission in aqueous solution: A theoretical study. Chemical Physics Letters, 2008, 463, 201-205.	1.2	24
112	Polarization and solvatochromic shift of ortho-betaine in water. Chemical Physics, 2008, 349, 109-114.	0.9	26
113	Conformational behavior of different possible ways of oligoglycine formation in a solvent-free environment. Computational and Theoretical Chemistry, 2008, 849, 25-32.	1.5	4
114	The isotropic nuclear magnetic shielding constants of acetone in supercritical water: A sequential Monte Carlo/quantum mechanics study including solute polarization. Journal of Chemical Physics, 2008, 129, 034502.	1.2	30
115	Electronic properties of liquid ammonia: A sequential molecular dynamics/quantum mechanics approach. Journal of Chemical Physics, 2008, 128, 014506.	1.2	36
116	Analyzing the $\pi \rightarrow \pi^*$ electronic transition of formaldehyde in water: a sequential Monte Carlo/time-dependent density functional theory. Journal of the Brazilian Chemical Society, 2008, 19, .	0.6	5
117	The Sequential qm/mm Method and its Applications to Solvent Effects in Electronic and Structural Properties of Solutes. Challenges and Advances in Computational Chemistry and Physics, 2008, , 159-189.	0.6	28
118	Behavior of a Bose-Einstein condensate containing a large number of atoms interacting through a finite-range interatomic interaction. Physical Review A, 2007, 75, .	1.0	44
119	An approximate many-body calculation for trapped bosons with attractive interaction. Journal of Physics B: Atomic, Molecular and Optical Physics, 2007, 40, 2225-2239.	0.6	21
120	A Monte Carlo-quantum mechanics study of the lowest $n \rightarrow \pi^*$ and $\pi \rightarrow \pi^*$ states of uracil in water. Physical Chemistry Chemical Physics, 2007, 9, 4907.	1.3	54
121	Solvent effects on the UV-visible absorption spectrum of benzophenone in water: A combined Monte Carlo quantum mechanics study including solute polarization. Journal of Chemical Physics, 2007, 126, 034507.	1.2	107
122	Probing supercritical water with the $n \rightarrow \pi^*$ transition of acetone: A Monte Carlo/quantum mechanics study. Journal of Chemical Physics, 2007, 126, 034508.	1.2	21
123	Isotropic and anisotropic NMR chemical shifts in liquid water: a sequential QM/MM study. Journal of the Brazilian Chemical Society, 2007, 18, 74-84.	0.6	24
124	An efficient statistically converged average configuration for solvent effects. Chemical Physics Letters, 2007, 437, 148-152.	1.2	168
125	On the relative abundance and interconversion of the two lowest isomers of AIP3. Chemical Physics Letters, 2007, 444, 247-251.	1.2	3
126	Reaction Mechanism and Tautomeric Equilibrium of 2-Mercaptopyrimidine in the Gas Phase and in Aqueous Solution: A Combined Monte Carlo and Quantum Mechanics Study. Journal of Physical Chemistry A, 2006, 110, 7253-7261.	1.1	42

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127	Ab Initio Study of the Isomeric Equilibrium of the HCN $\cdot\cdot$ H ₂ O and H ₂ O $\cdot\cdot$ HCN Hydrogen-Bonded Clusters. Journal of Physical Chemistry A, 2006, 110, 10303-10308.	1.1	27
128	SEQUENTIAL MONTE CARLO/QUANTUM MECHANICS STUDY OF THE DIPOLE POLARIZABILITY OF ATOMIC LIQUIDS: THE ARGON CASE. , 2006, , 405-420.		1
129	Theoretical electronic spectra of 2-aminopurine in vapor and in water. International Journal of Quantum Chemistry, 2006, 106, 2564-2577.	1.0	19
130	Preface: Proceedings of the XIII Brazilian Symposium of Theoretical Chemistry. International Journal of Quantum Chemistry, 2006, 106, 2551-2551.	1.0	0
131	Reply to comment on "The enthalpy of the O-H bond homolytic dissociation: Basis-set extrapolated density functional theory and coupled cluster calculations". Chemical Physics Letters, 2006, 417, 570-572.	1.2	8
132	Electron binding energies of water clusters: Implications for the electronic properties of liquid water. Chemical Physics Letters, 2006, 429, 129-135.	1.2	28
133	Converged electronic polarization of acetone in liquid water and the role in the "n \rightarrow " transition. Chemical Physics Letters, 2006, 429, 119-123.	1.2	83
134	Rayleigh scattering properties of small polyglycine molecules. Computational and Theoretical Chemistry, 2006, 760, 15-20.	1.5	31
135	The Dipole Polarizability of F \cdot in Aqueous Solution. A Sequential Monte Carlo/Quantum Mechanics Study. Advances in Quantum Chemistry, 2005, 48, 141-150.	0.4	9
136	The enthalpy of the O-H bond homolytic dissociation: Basis-set extrapolated density functional theory and coupled cluster calculations. Chemical Physics Letters, 2005, 406, 300-305.	1.2	39
137	Electronic polarization in liquid acetonitrile: A sequential Monte Carlo/quantum mechanics investigation. Chemical Physics Letters, 2005, 407, 13-17.	1.2	48
138	The low-lying electronic states of the GaN molecule. Chemical Physics Letters, 2005, 413, 65-70.	1.2	16
139	The relative stability of the two isomers of AlP ₃ . Chemical Physics Letters, 2005, 411, 14-17.	1.2	6
140	A look inside the cavity of hydrated β -cyclodextrin: A computer simulation study. Chemical Physics Letters, 2005, 413, 16-21.	1.2	32
141	Ab initio NMR study of the isomeric hydrogen-bonded methanol-water complexes. International Journal of Quantum Chemistry, 2005, 102, 554-564.	1.0	15
142	Theoretical investigation of hydrogen bonding in lactonitrile-water complexes. International Journal of Quantum Chemistry, 2005, 103, 654-658.	1.0	2
143	Preface proceedings of the XII Brazilian Symposium of Theoretical Chemistry. International Journal of Quantum Chemistry, 2005, 103, 471-471.	1.0	0
144	Calculated infrared spectra of hydrogen-bonded methanol-water, water-methanol, and methanol-methanol complexes. International Journal of Quantum Chemistry, 2005, 104, 808-815.	1.0	34

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145	A sequential Monte Carlo quantum mechanics study of the hydrogen-bond interaction and the solvatochromic shift of the $\pi^* \leftarrow \pi$ transition of acrolein in water. <i>Journal of Chemical Physics</i> , 2005, 123, 124307.	1.2	42
146	Spectral shift of sodium in a liquid-helium environment: A sequential Monte Carlo time-dependent density-functional-theory study. <i>Physical Review A</i> , 2005, 72, .	1.0	16
147	Conformational stability of furfural in aqueous solution: the role of hydrogen bonding. <i>Brazilian Journal of Physics</i> , 2004, 34, 84-89.	0.7	28
148	A sequential Monte Carlo/Quantum Mechanics study of the dipole polarizability of liquid benzene. <i>Journal of Computational Methods in Sciences and Engineering</i> , 2004, 4, 559-568.	0.1	2
149	Sequential classical-quantum description of the absorption spectrum of the hydrated electron. <i>Physical Review B</i> , 2004, 70, .	1.1	21
150	Combined Monte Carlo and quantum mechanics study of the hydration of the guanine-cytosine base pair. <i>Physical Review E</i> , 2004, 69, 061902.	0.8	13
151	Is There a Favorite Isomer for Hydrogen-Bonded Methanol in Water?. <i>Advances in Quantum Chemistry</i> , 2004, 47, 51-63.	0.4	12
152	Can larger dipoles solvate less? solute \leftrightarrow solvent hydrogen bond and the differential solvation of phenol and phenoxy. <i>Chemical Physics Letters</i> , 2004, 399, 534-538.	1.2	18
153	Relative strength of hydrogen bond interaction in alcohol \leftrightarrow water complexes. <i>Chemical Physics Letters</i> , 2004, 400, 494-499.	1.2	135
154	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.	1.3	27
155	Conformational Stability of Lactonitrile \leftrightarrow Water Complexes: An ab Initio Study. <i>Journal of Physical Chemistry A</i> , 2004, 108, 1601-1607.	1.1	5
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