Sylvio Roberto Accioly Canuto

List of Publications by Year
in descending order

263 papers	5,591 citations	94433 37 h-index	144013 57 g-index
271 all docs	271 docs citations	271 times ranked	3476 citing authors

#	Article	IF	Citations
1	Solvent effects in emission spectroscopy: A Monte Carlo quantum mechanics study of the nâ†Ï€* shift of formaldehyde in water. Journal of Chemical Physics, 2000, 113, 9132-9139.	3.0	173
2	An efficient statistically converged average configuration for solvent effects. Chemical Physics Letters, 2007, 437, 148-152.	2.6	168
3	A Monte Carlo-quantum mechanics study of the solvatochromic shifts of the lowest transition of benzene. Journal of Chemical Physics, 2000, 112, 9874-9880.	3.0	152
4	Solvent Effects from a Sequential Monte Carlo - Quantum Mechanical Approach. Advances in Quantum Chemistry, 1997, 28, 89-105.	0.8	150
5	Relative strength of hydrogen bond interaction in alcoholâ€“water complexes. Chemical Physics Letters, 2004, 400, 494-499.	2.6	135
6	Spectroscopy of Confined Atomic Systems: Effect of Plasma. Advances in Quantum Chemistry, 2009, , 115-175.	0.8	121
7	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.	3.0	107
8	Ab initiocalculation of hydrogen bonds in liquids: A sequential Monte Carlo quantum mechanics study of pyridine in water. Journal of Chemical Physics, 2002, 117, 1692-1699.	3.0	95
9	From hydrogen bond to bulk: Solvation analysis of then-?* transition of formaldehyde in water. , 2000, 77, 192-198.		90
10	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
11	Converged electronic polarization of acetone in liquid water and the role in the nâ€“Ï€â^— transition. Chemical Physics Letters, 2006, 429, 119-123.	2.6	83
12	Electronic polarization of liquid water: converged Monte Carlo-quantum mechanics results for the multipole moments. Chemical Physics Letters, 2003, 369, 345-353.	2.6	67
13	Quantifying multiple-body interaction terms in H-bonded HCN chains with many-body perturbation/coupled-cluster theories. Journal of Chemical Physics, 2003, 118, 10593-10601.	3.0	67
14	Theoretical analysis of the hydrogen bond interaction between acetone and water. Computational and Theoretical Chemistry, 1999, 466, 69-75.	1.5	66
15	New developments in Monte Carlo/quantum mechanics methodology. The solvatochromism of Î²-carotene in different solvents. Advances in Quantum Chemistry, 2002, 41, 161-183.	0.8	66
16	Solvent Effects in Chemical Processes. Water-Assisted Proton Transfer Reaction of Pterin in Aqueous Environment. Journal of Physical Chemistry A, 2009, 113, 12485-12495.	2.5	62
17	Sampling configurations in Monte Carlo simulations for quantum mechanical studies of solvent effects. International Journal of Quantum Chemistry, 1998, 66, 249-253.	2.0	55
18	Molecular Structure â€“ Optical Property Relationships for a Series of Non-Centrosymmetric Two-photon Absorbing Push-Pull Triarylamine Molecules. Scientific Reports, 2014, 4, 4447.	3.3	55

#	Article	IF	Citations
19	Theoretical interpretation of the absorption and ionization spectra of the paracyclophanes. Journal of the American Chemical Society, 1990, 112, 2114-2120.	13.7	54
20	A Monte Carlo-quantum mechanics study of the lowest nâ€“Ï€* and Ï€â€“Ï€* states of uracil in water. Physical Chemistry Chemical Physics, 2007, 9, 4907.	2.8	54
21	Including dispersion in configuration interaction-singles calculations for the spectroscopy of chromophores in solution. Journal of Chemical Physics, 2000, 112, 7293-7299.	3.0	49
22	Electronic changes due to thermal disorder of hydrogen bonds in liquids: Pyridine in an aqueous environment. Physical Review E, 2003, 67, 061504.	2.1	48
23	Electronic polarization in liquid acetonitrile: A sequential Monte Carlo/quantum mechanics investigation. Chemical Physics Letters, 2005, 407, 13-17.	2.6	48
24	Study of the optical and magnetic properties of pyrimidine in water combining PCM and QM/MM methodologies. Physical Chemistry Chemical Physics, 2010, 12, 14023.	2.8	47
25	Behavior of a Bose-Einstein condensate containing a large number of atoms interacting through a finite-range interatomic interaction. Physical Review A, 2007, 75, .	2.5	44
26	Combined Monte Carlo and quantum mechanics study of the solvatochromism of phenol in water. The origin of the blue shift of the lowest Ï€â€“Ï€* transition. Physical Chemistry Chemical Physics, 2009, 11, 1388.	2.8	43
27	Electronic Properties of Water in Liquid Environment. A Sequential QM/MM Study Using the Free Energy Gradient Method. Journal of Physical Chemistry B, 2012, 116, 11247-11254.	2.6	43
28	A Monte Carloâ€“quantum mechanical study of the solvatochromism of pyrimidine in water and in carbon tetrachloride. Physical Chemistry Chemical Physics, 2001, 3, 1583-1587.	2.8	42
29	An efficient quantum mechanical/molecular mechanics Monte Carlo simulation of liquid water. Chemical Physics Letters, 2001, 335, 127-133.	2.6	42
30	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. Journal of Physical Chemistry B, 2002, 106, 12317-12322.	2.6	42
31	A sequential Monte Carlo quantum mechanics study of the hydrogen-bond interaction and the solvatochromic shift of the nâ€“Ï€* transition of acrolein in water. Journal of Chemical Physics, 2005, 123, 124307.	3.0	42
32	Reaction Mechanism and Tautomeric Equilibrium of 2-Mercaptopyrimidine in the Gas Phase and in Aqueous Solution:Â A Combined Monte Carlo and Quantum Mechanics Study. Journal of Physical Chemistry A, 2006, 110, 7253-7261.	2.5	42
33	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.	5.4	42
34	The dipole polarizability of Liâ˜. Chemical Physics Letters, 1988, 147, 435-442.	2.6	41
35	Theoretical Study of Mixed Hydrogen-Bonded Complexes:Â H2OÂ·Â·Â·HCNÂ·Â·Â·H2O and H2OÂ·Â·Â·HCNÂ·Â·Â·HCNÂ·Â·Â·H2O. Journal of Physical Chemistry A, 2001, 105, 11260-11265.	2.5	41
36	Rayleigh light scattering of hydrogen bonded clusters investigated by means ofab initiocalculations. Journal of Physics B: Atomic, Molecular and Optical Physics, 2003, 36, 399-408.	1.5	41

#	Article	IF	Citations
37	The Role of Molecular Conformation and Polarizable Embedding for One- and Two-Photon Absorption of Disperse Orange 3 in Solution. Journal of Physical Chemistry B, 2012, 116, 8169-8181.	2.6	40
38	Solvent effects on the electronic absorption spectrum of formamide studied by a sequential Monte Carlo/quantum mechanical approach. Theoretical Chemistry Accounts, 2002, 108, 31-37.	1.4	39
39	The enthalpy of the Oâ€“H bond homolytic dissociation: Basis-set extrapolated density functional theory and coupled cluster calculations. Chemical Physics Letters, 2005, 406, 300-305.	2.6	39
40	85Rb Boseâ€“Einstein condensate with tunable interaction: A quantum many body approach. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 258-261.	2.1	37
41	Electronic and structural trends in small GaAs clusters. Scripta Materialia, 1998, 10, 635-647.	0.5	36
42	Solvent Effects on the Energetics of the Phenol Oâ˜H Bond:Â Differential Solvation of Phenol and Phenoxy Radical in Benzene and Acetonitrile. Journal of Physical Chemistry A, 2003, 107, 9197-9207.	2.5	36
43	Electronic properties of liquid ammonia: A sequential molecular dynamics/quantum mechanics approach. Journal of Chemical Physics, 2008, 128, 014506.	3.0	36
44	The electronic spectrum of N-methylacetamide in aqueous solution: a sequential Monte Carlo/quantum mechanical study. Chemical Physics Letters, 2001, 345, 171-178.	2.6	35
45	Differential Hydration of Phenol and Phenoxy Radical and the Energetics of the Phenol Oâ˜H Bond in Solution. Journal of Physical Chemistry B, 2003, 107, 4304-4310.	2.6	35
46	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. Journal of Chemical Physics, 2012, 137, 054307.	3.0	35
47	Calculated infrared spectra of hydrogen-bonded methanol-water, water-methanol, and methanol-methanol complexes. International Journal of Quantum Chemistry, 2005, 104, 808-815.	2.0	34
48	NMR Chemical Shielding and Spinâ˜Spin Coupling Constants of Liquid NH₃: A Systematic Investigation using the Sequential QM/MM Method. Journal of Physical Chemistry A, 2009, 113, 14936-14942.	2.5	33
49	Theoretical studies of photodissociation and rydbergization in the first triplet state (3s3Aâ€³2) of ammonia. Chemical Physics Letters, 1980, 70, 236-240.	2.6	32
50	A look inside the cavity of hydrated Î±-cyclodextrin: A computer simulation study. Chemical Physics Letters, 2005, 413, 16-21.	2.6	32
51	Calculation of the absorption spectrum of benzene in condensed phase. A study of the solvent effects. International Journal of Quantum Chemistry, 1997, 65, 885-891.	2.0	31
52	An ab initio study of the hydrogen-bonded H2O:HCN and HCN:H2O isomers. Chemical Physics Letters, 2000, 322, 207-212.	2.6	31
53	Rayleigh scattering properties of small polyglycine molecules. Computational and Theoretical Chemistry, 2006, 760, 15-20.	1.5	31
54	Calculations of vibrational frequencies, Raman activities and degrees of depolarization for complexes involving water, methanol and ethanol. Chemical Physics Letters, 2008, 452, 54-58.	2.6	31

#	Article	IF	Citations
55	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.	3.0	30
56	CASPT2 Study of the Potential Energy Surface of the HSO₂ System. Journal of Physical Chemistry A, 2011, 115, 1453-1461.	2.5	30
57	Broken orbital symmetry study of low-lying excited and N15 ionized states of pyrazine. Chemical Physics Letters, 1979, 68, 232-236.	2.6	29
58	Photophysics and photostability of adenine in aqueous solution: A theoretical study. Chemical Physics Letters, 2010, 492, 164-169.	2.6	29
59	Theoretical study on the electronic spectra of model compound II complexes of peroxidases. Journal of the American Chemical Society, 1991, 113, 8614-8621.	13.7	28
60	Conformational stability of furfural in aqueous solution: the role of hydrogen bonding. Brazilian Journal of Physics, 2004, 34, 84-89.	1.4	28
61	Electron binding energies of water clusters: Implications for the electronic properties of liquid water. Chemical Physics Letters, 2006, 429, 129-135.	2.6	28
62	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
63	Role played by N and N-N impurities in type-IV semiconductors. Physical Review B, 1993, 48, 17806-17810.	3.2	27
64	An ab initio study of the peptide bond formation between alanine and glycine: electron correlation effects on the structure and binding energy. Computational and Theoretical Chemistry, 2002, 577, 267-279.	1.5	27
65	Solute relaxation on the solvatochromism of ortho-betaine dyes. A sequential Monte Carlo/quantum mechanics study. Physical Chemistry Chemical Physics, 2004, 6, 2088.	2.8	27
66	Ab Initio Study of the Isomeric Equilibrium of the HCNÂ·Â·Â·H2O and H2OÂ·Â·Â·HCN Hydrogen-Bonded Clusters. Journal of Physical Chemistry A, 2006, 110, 10303-10308.	2.5	27
67	Experimental and Theoretical Study on the One- and Two-Photon Absorption Properties of Novel Organic Molecules Based on Phenylacetylene and Azoaromatic Moieties. Journal of Physical Chemistry B, 2012, 116, 14677-14688.	2.6	27
68	An Average Solvent Electrostatic Configuration Protocol for QM/MM Free Energy Optimization: Implementation and Application to Rhodopsin Systems. Journal of Chemical Theory and Computation, 2017, 13, 6391-6404.	5.3	27
69	Polarization and solvatochromic shift of ortho-betaine in water. Chemical Physics, 2008, 349, 109-114.	1.9	26
70	Hyperpolarizabilities of the methanol molecule: A CCSD calculation including vibrational corrections. Journal of Chemical Physics, 2010, 132, 034307.	3.0	26
71	Comparison of polarizable continuum model and quantum mechanics/molecular mechanics solute electronic polarization: Study of the optical and magnetic properties of diazines in water. Journal of Chemical Physics, 2011, 135, 144103.	3.0	26
72	Combining ab initio multiconfigurational and Free Energy Gradient methods to study the Ï€â€“Ï€* excited state structure and properties of uracil in water. Computational and Theoretical Chemistry, 2014, 1040-1041, 312-320.	2.5	26

#	Article	IF	Citations
73	Monte Carlo study of the temperature dependence of the hydrophobic hydration of benzene. Chemical Physics Letters, 1999, 313, 235-240.	2.6	25
74	Theoretical absorption and emission spectra of 1H- and 2H-benzotriazole. Physical Chemistry Chemical Physics, 2003, 5, 5001-5009.	2.8	25
75	Polarization and Spectral Shift of Benzophenone in Supercritical Water. Journal of Physical Chemistry A, 2009, 113, 5112-5118.	2.5	25
76	Solvent effects on the two lowest-lying singlet excited states of 5-fluorouracil. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	25
77	Experimental and theoretical investigation of the first-order hyperpolarizability of a class of triarylamine derivatives. Journal of Chemical Physics, 2015, 142, 064312.	3.0	25
78	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
79	2-Aminopurine non-radiative decay and emission in aqueous solution: A theoretical study. Chemical Physics Letters, 2008, 463, 201-205.	2.6	24
80	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.	3.0	24
81	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.	2.6	24
82	Electron collisions with the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CH</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub> Physical Review A, 2009, 80, .	2.5	24
83	Thermodynamic stability of hydrogenâ€bonded systems in polar and nonpolar environments. Journal of Computational Chemistry, 2010, 31, 2046-2055.	3.3	24
84	Ab initio studies of the photodissociation in the first excited states of Ã¹ 1A1 and Ã£ 3A1 of PH3. Journal of Chemical Physics, 1982, 76, 5060-5068.	3.0	23
85	Experimental and theoretical study of two-photon absorption in nitrofuran derivatives: Promising compounds for photochemotherapy. Journal of Chemical Physics, 2011, 134, 014509.	3.0	23
86	A First-Principles Approach to the Dynamics and Electronic Properties of p-Nitroaniline in Water. Journal of Physical Chemistry A, 2016, 120, 3878-3887.	2.5	23
87	Theoretical determination of the spectroscopic constants of the MgC molecule. Astrophysical Journal, 1991, 367, L69.	4.5	23
88	A Monte Carloâ€“quantum mechanics study of the spectroscopic properties of molecules in solution. Computational and Theoretical Chemistry, 2001, 539, 171-179.	1.5	22
89	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
90	Electron collisions with the HCOOHâ‹¯(H2O)n complexes (n = 1, 2) in liquid phase: The influence of microsolvation on the Ï€* resonance of formic acid. Journal of Chemical Physics, 2013, 138, 174307.	3.0	22

#	Article	IF	Citations
91	Alternating polarity and Friedel oscillations. Journal of Physics B: Atomic and Molecular Physics, 1981, 14, 1409-1422.	1.6	21
92	Sequential classical-quantum description of the absorption spectrum of the hydrated electron. Physical Review B, 2004, 70, .	3.2	21
93	An approximate many-body calculation for trapped bosons with attractive interaction. Journal of Physics B: Atomic, Molecular and Optical Physics, 2007, 40, 2225-2239.	1.5	21
94	Probing supercritical water with the n-Ï€* transition of acetone: A Monte Carlo/quantum mechanics study. Journal of Chemical Physics, 2007, 126, 034508.	3.0	21
95	Origin of the Red Shift for the Lowest Singlet Ï€ â†' Ï€* Charge-Transfer Absorption of p-Nitroaniline in Supercritical CO₂. Journal of Chemical Theory and Computation, 2014, 10, 1554-1562.	5.3	21
96	Solvent effect on the syn/anti conformational stability: A comparison between conformational bias Monte Carlo and molecular dynamics methods. International Journal of Quantum Chemistry, 2019, 119, e25688.	2.0	20
97	On the inter-ring separation of the lowest excited and ionized states of [2.2]paracyclophane. Chemical Physics Letters, 1989, 157, 353-358.	2.6	19
98	Theoretical determination of the spectroscopic constants ofCaH+. Physical Review A, 1993, 48, 2461-2463.	2.5	19
99	Theoretical electronic spectra of 2-aminopurine in vapor and in water. International Journal of Quantum Chemistry, 2006, 106, 2564-2577.	2.0	19
100	Hydrogen bond interactions between acetone and supercritical water. Physical Chemistry Chemical Physics, 2010, 12, 6660.	2.8	19
101	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
102	Self-Aggregation and Optical Absorption of Stilbazolium Merocyanine in Chloroform. Journal of Physical Chemistry B, 2014, 118, 1715-1725.	2.6	19
103	On the spherical quadratic Zeeman problem in hydrogen. Physics Letters, Section A: General, Atomic and Solid State Physics, 1984, 101, 326-330.	2.1	18
104	Quest for the ground state characterization of CaC. Chemical Physics Letters, 1997, 269, 193-198.	2.6	18
105	Hydrophobic interaction and solvatochromic shift of benzene in water. Chemical Physics Letters, 1997, 274, 269-274.	2.6	18
106	Rayleigh and Raman light scattering in hydrogen-bonded acetonitrile?water. Theoretical Chemistry Accounts, 2003, 110, 360-366.	1.4	18
107	Can larger dipoles solvate less? soluteâ€“solvent hydrogen bond and the differential solvation of phenol and phenoxy. Chemical Physics Letters, 2004, 399, 534-538.	2.6	18
108	A simple analysis of the influence of the solvent-induced electronic polarization on the 15N magnetic shielding of pyridine in water. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	18

#	Article	IF	Citations
109	Excited-State Properties and Relaxation Pathways of Selenium-Substituted Guanine Nucleobase in Aqueous Solution and DNA Duplex. Journal of Physical Chemistry B, 2021, 125, 1778-1789.	2.6	18
110	Dynamic polarizabilities and Rydberg states of the argon isoelectronic sequence. Physical Review A, 1993, 48, 2686-2695.	2.5	17
111	Monte Carlo-quantum mechanics study of the UV-visible spectrum of benzophenone in water. International Journal of Quantum Chemistry, 2000, 80, 1062-1067.	2.0	17
112	The low-lying electronic states of the GaN molecule. Chemical Physics Letters, 2005, 413, 65-70.	2.6	16
113	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
114	Revealing the Electronic and Molecular Structure of Randomly Oriented Molecules by Polarized Two-Photon Spectroscopy. Journal of Physical Chemistry Letters, 2013, 4, 1753-1759.	4.6	16
115	Monte Carloâ€“Quantum Mechanics Study of Magnetic Properties of Hydrogen Peroxide in Liquid Water. Journal of Physical Chemistry A, 2014, 118, 6239-6247.	2.5	16
116	Interpreting the First-Order Electronic Hyperpolarizability for a Series of Octupolar Pushâ€“Pull Triarylamine Molecules Containing Trifluoromethyl. Journal of Physical Chemistry C, 2015, 119, 12589-12597.	3.1	16
117	Oxazole Dyes with Potential for Photoluminescence Bioprobes: A Two-Photon Absorption Study. Journal of Physical Chemistry C, 2018, 122, 10526-10534.	3.1	16
118	Theoretical studies of the absorption spectra of polycyclic aromatic hydrocarbons. Astrophysical Journal, 1991, 377, 150.	4.5	16
119	Structure dependence of the low-lying excited states and the first dipole hyperpolarizability of phenol blue. International Journal of Quantum Chemistry, 1998, 70, 745-750.	2.0	15
120	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
121	Theoretical studies of hydrogen bonding in waterâ€“cyanides and in the base pair Guâ€“Cy. Journal of Molecular Structure, 2002, 615, 257-266.	3.6	15
122	Ab initio NMR study of the isomeric hydrogen-bonded methanol-water complexes. International Journal of Quantum Chemistry, 2005, 102, 554-564.	2.0	15
123	A first principles approach to the electronic properties of liquid and supercritical CO2. Journal of Chemical Physics, 2015, 142, 024504.	3.0	15
124	An insightful approach for understanding solvatochromic reversal. Chemical Physics Letters, 2016, 655-656, 30-34.	2.6	15
125	Study of the predissociation of NH3in the 3sA"2state from ab initio UHF calculations. Journal of Physics B: Atomic and Molecular Physics, 1979, 12, 3149-3156.	1.6	14
126	Many-electron treatment of the off-center substitutional O in Si. Physical Review B, 1986, 33, 4432-4435.	3.2	14

#	Article	IF	Citations
127	Many-body perturbation theory and coupled-cluster calculations of the ground-state structure of CO3. Chemical Physics Letters, 1991, 177, 98-102.	2.6	14
128	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
129	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
130	Hydration effects on the electronic properties of eumelanin building blocks. Journal of Chemical Physics, 2016, 145, 084501.	3.0	14
131	Unraveling the Electric Field-Induced Second Harmonic Generation Responses of Stilbazolium Ion Pairs Complexes in Solution Using a Multiscale Simulation Method. Journal of Chemical Information and Modeling, 2020, 60, 4817-4826.	5.4	14
132	A comparison of theoretical models for interpreting the photoelectron spectrum of borazine. Chemical Physics Letters, 1982, 88, 185-192.	2.6	13
133	Many-body-perturbation-theory calculations of the microwave and vibrational constants of CaC. Physical Review A, 1992, 46, 4415-4417.	2.5	13
134	Coupled-cluster calculation of the static polarisabilities and hyperpolarisabilities of magnesium. Physics Letters, Section A: General, Atomic and Solid State Physics, 1993, 176, 105-108.	2.1	13
135	Isotropic and anisotropic static dipole polarizabilities of the first-row stable atomic anions. Physical Review A, 1994, 49, 3515-3518.	2.5	13
136	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
137	Two-photon absorption in oxazole derivatives: An experimental and quantum chemical study. Optical Materials, 2012, 34, 1013-1018.	3.6	13
138	Solvent Effect on the Stokes Shift and on the Nonfluorescent Decay of the Daidzein Molecular System. Journal of Physical Chemistry A, 2013, 117, 4404-4411.	2.5	13
139	Communication: Transient anion states of phenolâ€¦(H2O)n (n = 1, 2) complexes: Search for microsolvation signatures. Journal of Chemical Physics, 2014, 141, 051105.	3.0	13
140	A complete basis set study of the lowest nâ€“Ï€* and Ï€â€“Ï€* electronic transitions of acrolein in explicit water environment. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	13
141	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
142	Another approach to the spherical Stark problem in hydrogen. Physics Letters, Section A: General, Atomic and Solid State Physics, 1982, 88, 282-284.	2.1	12
143	Is There a Favorite Isomer for Hydrogen-Bonded Methanol in Water?. Advances in Quantum Chemistry, 2004, 47, 51-63.	0.8	12
144	Electronic properties of a methaneâ€“water solution. Chemical Physics Letters, 2011, 506, 183-189.	2.6	12

#	Article	IF	Citations
145	Electronic structure and absorption spectra of fluorescent nucleoside analogues. Physical Chemistry Chemical Physics, 2017, 19, 29354-29363.	2.8	12
146	Stationarity of resonant pole trajectories in complex scaling. International Journal of Quantum Chemistry, 1978, 14, 383-391.	2.0	11
147	Many-body perturbation theory and polarization propagator studies of the structure, energetics and excitation spectrum of CO3. Chemical Physics, 1988, 120, 375-381.	1.9	11
148	Coupled cluster polarisation propagator study of the photodetachment cross section of Li-. Journal of Physics B: Atomic, Molecular and Optical Physics, 1988, 21, 3891-3897.	1.5	11
149	Dipole polarizability and Rayleigh light scattering by the hydrated electron. Chemical Physics Letters, 2009, 481, 73-77.	2.6	11
150	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
151	Effect of hydrogen bond formation on the elastic molecular scattering: a case study with methanol. Molecular Physics, 2012, 110, 297-306.	1.7	11
152	Free energy barrier for dissociation of the guanosine monophosphate anion in water. European Physical Journal D, 2016, 70, 1.	1.3	11
153	A theoretical study of the magnetic shielding of 15N of formamide in liquid water. Journal of Molecular Liquids, 2020, 320, 114415.	4.9	11
154	The virial theorem and the factorized wavefunction approach to perturbation theory. Application to the spherical Stark and spherical quadratic Zeeman problems in hydrogen. Physics Letters, Section A: General, Atomic and Solid State Physics, 1984, 106, 1-4.	2.1	10
155	Extreme electron correlation effects on the electric properties of atomic anions. International Journal of Quantum Chemistry, 1994, 52, 265-270.	2.0	10
156	Effect of bond-length alternation on the dipole hyperpolarizability of phenol blue. International Journal of Quantum Chemistry, 2002, 87, 275-279.	2.0	10
157	Applications of density functional theory methods in millimeter-wave spectroscopy. International Journal of Quantum Chemistry, 2003, 91, 575-585.	2.0	10
158	Use of correlated potential harmonic basis functions for the description of the 4He trimer and small clusters. Journal of Chemical Physics, 2011, 134, 164106.	3.0	10
159	Understanding the absorption spectrum of mesityl oxide dye in solvents of different polarities. Journal of Molecular Liquids, 2020, 307, 112924.	4.9	10
160	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.	3.9	10
161	A new interpretation of the absorption and the dual fluorescence of Prodan in solution. Journal of Chemical Physics, 2020, 153, 244104.	3.0	10
162	Ultrafast Intersystem Crossing Dynamics of 6-Selenoguanine in Water. Jacs Au, 2022, 2, 1699-1711.	7.9	10

#	Article	IF	Citations
163	Ground state structure of C 5 H 5 and van der Waals interaction with He and Ne. Computational and Theoretical Chemistry, 1999, 464, 73-77.	1.5	9
164	Electronic polarization of 1H-benzotriazole in water: Ground and first excited-state dipole moments. International Journal of Quantum Chemistry, 2003, 95, 572-579.	2.0	9
165	The Dipole Polarizability of Fâ¯ in Aqueous Solution. A Sequential Monte Carlo/Quantum Mechanics Study. Advances in Quantum Chemistry, 2005, 48, 141-150.	0.8	9
166	Many-body energy decomposition of hydrogen-bonded glycine clusters in gas-phase. Chemical Physics Letters, 2010, 491, 86-90.	2.6	9
167	Reply to comment on â€˜The enthalpy of the Oâ€“H bond homolytic dissociation: Basis-set extrapolated density functional theory and coupled cluster calculationsâ€™. Chemical Physics Letters, 2006, 417, 570-572.	2.6	8
168	Excited state electronic polarization and reappraisal of the n â†•Ï€â* emission of acetone in water. Chemical Physics Letters, 2010, 499, 108-112.	2.6	8
169	Calculations of the spectral shifts and line profiles of alkaline earth atoms in liquid helium environment. Chemical Physics Letters, 2012, 533, 25-29.	2.6	8
170	Born-Oppenheimer molecular dynamics and electronic properties of chlorophyll-c2 in liquid methanol. Journal of Chemical Physics, 2013, 138, 225102.	3.0	8
171	One- and two-photon absorption of fluorescein dianion in water: A study using S-QM/MM methodology and ZINDO method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 63-75.	3.9	8
172	Solvation Structures and Deactivation Pathways of Luminescent Isothiazole-Derived Nucleobases: ^{tz}A, ^{tz}G, and ^{tz}I. Journal of Physical Chemistry A, 2020, 124, 6834-6844.	2.5	8
173	The equation of state of hard-spherocylinder fluid mixturesElectronic Supplementary Information available. See http://www.rsc.org/suppdata/cp/b1/b109010k/. Physical Chemistry Chemical Physics, 2002, 4, 922-925.	2.8	7
174	Electronic spectroscopy of biomolecules in solution: fluorescein dianion in water. Molecular Physics, 2010, 108, 3125-3130.	1.7	7
175	Ionization of chlorophyll-c2 in liquid methanol. Chemical Physics Letters, 2012, 546, 67-73.	2.6	7
176	Probing Lewis Acidâ€“Base Interactions with Bornâ€“Oppenheimer Molecular Dynamics: The Electronic Absorption Spectrum of p-Nitroaniline in Supercritical CO₂. Journal of Physical Chemistry B, 2015, 119, 8397-8405.	2.6	7
177	On the spectral line width broadening for simulation of the two-photon absorption cross-section of para-Nitroaniline in liquid environment. Journal of Molecular Liquids, 2020, 301, 112405.	4.9	7
178	On the population of triplet states of 2-seleno-thymine. Physical Chemistry Chemical Physics, 2021, 23, 5447-5454.	2.8	7
179	Electronic states of silabenzene. Computational and Theoretical Chemistry, 1982, 89, 77-81.	1.5	6
180	Calculated dipole moment, static dipole polarizability, infrared intensity and Raman scattering activity for the MgC molecule. Journal of Physics B: Atomic, Molecular and Optical Physics, 1993, 26, 4301-4306.	1.5	6

#	Article	IF	Citations
181	The relative stability of the two isomers of AlP3. Chemical Physics Letters, 2005, 411, 14-17.	2.6	6
182	Electronic properties of liquid hydrogen fluoride: A sequential quantum mechanical/Bornâ€“Oppenheimer molecular dynamics approach. Chemical Physics Letters, 2010, 495, 40-45.	2.6	6
183	Combining Monte Carlo simulation and density-functional theory to describe the spectral changes of Na2in liquid helium. Physical Review A, 2011, 83, .	2.5	6
184	Structural properties and energetics of diffuse 87Rb clusters in three-dimension. Journal of Chemical Physics, 2012, 137, 014301.	3.0	6
185	Free base phthalocyanine: Influence of thermal effects and dimerization on the electronic absorption spectrum. Chemical Physics Letters, 2014, 595-596, 97-102.	2.6	6
186	Dynamics of complexation and electronic absorption of calix[4]arene-Ar2. Chemical Physics Letters, 2014, 612, 266-272.	2.6	6
187	Electronic Properties in Supercritical Fluids. Advances in Quantum Chemistry, 2015, , 323-339.	0.8	6
188	Magnetic dipolar and quadrupolar transitions in two-electron atoms under exponential-cosine-screened Coulomb potential. Physics of Plasmas, 2015, 22, 032902.	1.9	6
189	Including Thermal Disorder of Hydrogen Bonding to Describe the Vibrational Circular Dichroism Spectrum of Zwitterionic <scp>l</scp>-Alanine in Water. Journal of Physical Chemistry A, 2015, 119, 5099-5106.	2.5	6
190	Structural phase transitions in molecules. Journal of Physics B: Atomic and Molecular Physics, 1982, 15, 1307-1317.	1.6	5
191	Vibrational excitation of triplet core-ionized states of BeF. Chemical Physics, 1984, 87, 17-22.	1.9	5
192	A comparison of different many-body perturbation theory calculations of the ground state of SiS. International Journal of Quantum Chemistry, 1988, 33, 395-401.	2.0	5
193	Correlated calculations of the electron affinity of HC2. International Journal of Quantum Chemistry, 1988, 34, 199-205.	2.0	5
194	Theoretical description of the absorption spectra of solid and liquid benzene. Computational and Theoretical Chemistry, 1993, 287, 99-106.	1.5	5
195	Influence of donor-triad molecules on the optical properties of semiconductors. Physical Review B, 1993, 48, 18261-18263.	3.2	5
196	Dipole moment, polarizability, and their derivatives for the SiC molecule. Physical Review A, 1993, 48, 826-828.	2.5	5
197	Efficient estimation of second virial coefficients of fused hard-sphere molecules by an artificial neural networkElectronic Supplementary Information available. See http://www.rsc.org/suppdata/cp/b1/b105183k/. Physical Chemistry Chemical Physics, 2001, 3, 4762-4768.	2.8	5
198	Conformational Stability of Lactonitrileâ^'Water Complexes:â€‰ An ab Initio Study. Journal of Physical Chemistry A, 2004, 108, 1601-1607.	2.5	5

#	Article	IF	Citations
199	Analyzing the n<FONT FACE=Symbol>Â®p</FONT>* 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
200	Continuum, discrete, and explicit solvation models for describing the lowâ€lying absorption spectrum of the pterin acid in aqueous environment. International Journal of Quantum Chemistry, 2010, 110, 2371-2377.	2.0	5
201	Theoretical analysis of the influence of Câ€“H$$cdots $$O bonds on the NMR constants of uracil in DMSO. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	5
202	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.	5.3	5
203	Renner spliting in the first ionized state of BeF2. Chemical Physics Letters, 1983, 101, 55-58.	2.6	4
204	Vibrational linewidth of F1s core-hole states. Chemical Physics Letters, 1985, 120, 86-92.	2.6	4
205	Intra-dexcitations: Comparison between approaches for impurities in semiconductors. Physical Review B, 1988, 37, 4770-4773.	3.2	4
206	CLUSTER CALCULATION OF THE ELECTRONIC STRUCTURE OF K3C60. Modern Physics Letters B, 1995, 09, 95-101.	1.9	4
207	Calculated polarizabilities and gradients: Rayleigh and Raman scattering activities for the MgH molecule. Computational and Theoretical Chemistry, 1998, 432, 69-74.	1.5	4
208	Calculated Infrared, Raman, and Rayleigh Properties of the CO3 Molecule. Journal of Molecular Spectroscopy, 2000, 202, 281-284.	1.2	4
209	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
210	Spectroscopy of Atoms in Liquid Helium Environment: A Theoretical Perspective. Progress in Theoretical Chemistry and Physics, 2009, , 183-200.	0.2	4
211	A theoretical study of the spectral shifts of Xe atom in Ar environment. Physics Letters, Section A: General, Atomic and Solid State Physics, 2013, 377, 1720-1724.	2.1	4
212	Theoretical study of the spectral shift of the absorption line of Rb and Cs in liquid helium. Chemical Physics Letters, 2015, 633, 256-260.	2.6	4
213	Behavior of the dielectric constant of Ar near the critical point. Physical Review E, 2015, 91, 032115.	2.1	4
214	Solvent Effects on the Dynamic Polarizability and Raman Response of Moleculeâ€“Metal Oxide Hybrid Clusters. ChemPhysChem, 2016, 17, 2590-2595.	2.1	4
215	NMR spinâ€“spin coupling constants in hydrogenâ€bonded glycine clusters. International Journal of Quantum Chemistry, 2018, 118, e25608.	2.0	4
216	Microscopic Origin of Different Hydration Patterns of para-Nitrophenol and Its Anion: A Study Combining Multiconfigurational Calculations and the Free-Energy Gradient Method. Journal of Physical Chemistry B, 2018, 122, 9202-9209.	2.6	4

#	Article	IF	Citations
217	Free energy gradient for understanding the stability and properties of neutral and charged L-alanine molecule in water. Journal of Molecular Liquids, 2020, 319, 114109.	4.9	4
218	Continuum contribution to polarizabilities and scaling. International Journal of Quantum Chemistry, 1979, 16, 985-991.	2.0	3
219	Spin-unrestricted Hartree-Fock study of the ground state of BeF2-. Journal of Physics B: Atomic and Molecular Physics, 1981, 14, 3537-3542.	1.6	3
220	Vibrational excitation following the Sls core ionization of CS. Chemical Physics Letters, 1983, 96, 591-594.	2.6	3
221	Effect of three-donor cluster on infrared absorption of semiconductor systems. Solid State Communications, 1990, 75, 939-941.	1.9	3
222	Structural and electronic studies of Ga3As3, Ga4As3, and Ga3As4. International Journal of Quantum Chemistry, 1994, 52, 571-577.	2.0	3
223	A detailed theoretical analysis of the electron correlation contribution to the static dipole hyperpolarizabilities of atomic anions: Hâ¯, Câ¯ and Fâ¯. Computational and Theoretical Chemistry, 1995, 335, 45-49.	1.5	3
224	Calculated Raman and Rayleigh properties of the CaC molecule. Computational and Theoretical Chemistry, 1999, 489, 29-34.	1.5	3
225	On the relative abundance and interconversion of the two lowest isomers of AlP3. Chemical Physics Letters, 2007, 444, 247-251.	2.6	3
226	A simple model for a theoretical study of the spectral line shifts of alkali atoms attached to helium nanodroplets. Chemical Physics Letters, 2016, 644, 142-146.	2.6	3
227	Theoretical study of the NMR chemical shift of Xe in supercritical condition. Journal of Molecular Modeling, 2018, 24, 62.	1.8	3
228	Photophysics of Emissive tz C[Isothiazoloâ€Cytidine] and tz U[Isothiazoloâ€Uridine] Pyrimidine Analogues. ChemPhotoChem, 2019, 3, 916-924.	3.0	3
229	Preferential solvation and optical properties of eumelanin building blocks in binary mixture of methanol and water. Journal of Chemical Physics, 2021, 155, 174504.	3.0	3
230	Free-Energy Landscape of the S_N2 Reaction CH₃Br + Cl^{â€“} â†’ CH₃Cl + Br^{â€“} in Different Liquid Environments. Journal of Physical Chemistry B, 2022, 126, 3685-3692.	2.6	3
231	New basis set for molecular calculations. I. A study of AHnmolecules using the complete neglect of differential overlap method of Boyd and Whitehead. Journal of Physics B: Atomic and Molecular Physics, 1975, 8, 2987-2994.	1.6	2
232	Electronic splitting between the 3B2 and 3A2 states of BeF2. Computational and Theoretical Chemistry, 1982, 88, 209-211.	1.5	2
233	Infrared intensity and Raman scattering activity for the SiC molecule. Physics Letters, Section A: General, Atomic and Solid State Physics, 1994, 187, 243-246.	2.1	2
234	Impurity states in the narrow band-gap semiconductor n-type InSb. Solid State Communications, 1996, 99, 295-297.	1.9	2

#	Article	IF	Citations
235	Electron correlation effects on the angular momentum anisotropies of the dipole polarizabilities of the first-row stable atomic anions. International Journal of Quantum Chemistry, 1997, 63, 459-463.	2.0	2
236	A sequential Monte Carlo/Quantum Mechanics study of the dipole polarizability of liquid benzene. Journal of Computational Methods in Sciences and Engineering, 2004, 4, 559-568.	0.2	2
237	Theoretical investigation of hydrogen bonding in lactonitrile-water complexes. International Journal of Quantum Chemistry, 2005, 103, 654-658.	2.0	2
238	Theoretical study of the XP3 (X=Al, B, Ga) clusters. Chemical Physics, 2012, 399, 23-27.	1.9	2
239	Macroscopic description of molecular structural changes. Journal of Physics B: Atomic and Molecular Physics, 1984, 17, 1711-1725.	1.6	1
240	The frequency dependence of the first dipole hyperpolarizability of dimethylaminoindoaniline. Computational and Theoretical Chemistry, 1997, 394, 181-185.	1.5	1
241	Theoretical analysis of the structure and bonding of the van der Waals cluster N2â€¦C5H5. Physics Letters, Section A: General, Atomic and Solid State Physics, 1998, 241, 90-93.	2.1	1
242	Quantum chemical studies of the spectroscopic properties of the E-64 protease inhibitor. Computational and Theoretical Chemistry, 2002, 585, 129-141.	1.5	1
243	SEQUENTIAL MONTE CARLO/QUANTUM MECHANICS STUDY OF THE DIPOLE POLARIZABILITY OF ATOMIC LIQUIDS: THE ARGON CASE. , 2006, , 405-420.		1
244	Characterization and spectroscopic analysis of phenolâ€“ethanol hydrogen bonded clusters. Chemical Physics Letters, 2010, 496, 236-242.	2.6	1
245	A CASPT2 study of the spectral shift of the resonance emission lines of Rb and Cs embedded in liquid He. Chemical Physics Letters, 2016, 655-656, 91-95.	2.6	1
246	Calculation of the absorption spectrum of benzene in condensed phase. A study of the solvent effects. , 1997, 65, 885.		1
247	Sampling configurations in Monte Carlo simulations for quantum mechanical studies of solvent effects. , 1998, 66, 249.		1
248	Van der Waals Interaction Probed by Solvatochromic Shifts. , 2002, , 127-133.		1
249	A simple analysis of the influence of the solvent-induced electronic polarization on the 15N magnetic shielding of pyridine in water. Highlights in Theoretical Chemistry, 2014, , 117-124.	0.0	1
250	Relaxation and vibration structure in the deepest ionized states of SiS. Computational and Theoretical Chemistry, 1985, 133, 221-226.	1.5	0
251	A core-excited rydberg state of SiF. Computational and Theoretical Chemistry, 1986, 139, 109-112.	1.5	0
252	The structure of HSSi+ as determined by fourth-order many-body perturbation theory. Chemical Physics Letters, 1988, 144, 362-365.	2.6	0

#	Article	IF	Citations
253	Many-electron treatment for chalcogen complexes in silicon. Semiconductor Science and Technology, 1990, 5, 196-199.	2.0	0
254	Preface proceedings of the XII Brazilian Symposium of Theoretical Chemistry. International Journal of Quantum Chemistry, 2005, 103, 471-471.	2.0	0
255	Preface: Proceedings of the XIII Brazilian Symposium of Theoretical Chemistry. International Journal of Quantum Chemistry, 2006, 106, 2551-2551.	2.0	0
256	Preface: Proceedings of the XIV Brazilian Symposium of Theoretical Cchemistry. International Journal of Quantum Chemistry, 2008, 108, 2305-2305.	2.0	0
257	Preface: Proceedings of the XV Brazilian Symposium of Theoretical Chemistry. International Journal of Quantum Chemistry, 2010, 110, 2005-2005.	2.0	0
258	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
259	A theoretical study of the low-lying excited states and the photophysics of dimethoxy curcumin in cyclohexane and acetonitrile. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	0
260	Quantum mechanics meets scaling theory near the critical point. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	0
261	Hydrogen Bonding and the Energetics of Homolytic Dissociation in Solution. , 2004, , 581-599.		0
262	Sequential Monte Carlo and Quantum Mechanics Calculation of the Static Dielectric Constant of Liquid Argon. , 2009, , 327-336.		0
263	New insights on nonlinear solvatochromism in binary mixture of solvents. Advances in Quantum Chemistry, 2022, , .	0.8	0