Vicenzo Barone

List of Publications by Year
in descending order

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782 papers	85,136 citations	2427 97 h-index	460 272 g-index
812 all docs	812 docs citations	812 times ranked	43141 citing authors

#	Article	IF	Citations
1	Toward reliable density functional methods without adjustable parameters: The PBE0 model. Journal of Chemical Physics, 1999, 110, 6158-6170.	3.0	14,178
2	Quantum Calculation of Molecular Energies and Energy Gradients in Solution by a Conductor Solvent Model. Journal of Physical Chemistry A, 1998, 102, 1995-2001.	2.5	7,948
3	Energies, structures, and electronic properties of molecules in solution with the C-PCM solvation model. Journal of Computational Chemistry, 2003, 24, 669-681.	3.3	6,758
4	Ab initio study of solvated molecules: a new implementation of the polarizable continuum model. Chemical Physics Letters, 1996, 255, 327-335.	2.6	3,086
5	Exchange functionals with improved long-range behavior and adiabatic connection methods without adjustable parameters: The mPW and mPW1PW models. Journal of Chemical Physics, 1998, 108, 664-675.	3.0	3,068
6	A new definition of cavities for the computation of solvation free energies by the polarizable continuum model. Journal of Chemical Physics, 1997, 107, 3210-3221.	3.0	2,237
7	New developments in the polarizable continuum model for quantum mechanical and classical calculations on molecules in solution. Journal of Chemical Physics, 2002, 117, 43-54.	3.0	2,235
8	Time-dependent density functional theory for molecules in liquid solutions. Journal of Chemical Physics, 2001, 115, 4708-4717.	3.0	1,853
9	Geometry optimization of molecular structures in solution by the polarizable continuum model. Journal of Computational Chemistry, 1998, 19, 404-417.	3.3	1,602
10	Ab initio study of ionic solutions by a polarizable continuum dielectric model. Chemical Physics Letters, 1998, 286, 253-260.	2.6	1,493
11	Anharmonic vibrational properties by a fully automated second-order perturbative approach. Journal of Chemical Physics, 2005, 122, 014108.	3.0	1,352
12	Geometries and properties of excited states in the gas phase and in solution: Theory and application of a time-dependent density functional theory polarizable continuum model. Journal of Chemical Physics, 2006, 124, 094107.	3.0	1,143
13	A state-specific polarizable continuum model time dependent density functional theory method for excited state calculations in solution. Journal of Chemical Physics, 2006, 125, 054103.	3.0	675
14	Accurate excitation energies from time-dependent density functional theory: Assessing the PBE0 model. Journal of Chemical Physics, 1999, 111, 2889-2899.	3.0	661
15	Role and effective treatment of dispersive forces in materials: Polyethylene and graphite crystals as test cases. Journal of Computational Chemistry, 2009, 30, 934-939.	3.3	653
16	Effective method for the computation of optical spectra of large molecules at finite temperature including the Duschinsky and Herzbergâ€“Teller effect: The Qx band of porphyrin as a case study. Journal of Chemical Physics, 2008, 128, 224311.	3.0	523
17	Vibrational zero-point energies and thermodynamic functions beyond the harmonic approximation. Journal of Chemical Physics, 2004, 120, 3059-3065.	3.0	484
18	Effective method to compute Franck-Condon integrals for optical spectra of large molecules in solution. Journal of Chemical Physics, 2007, 126, 084509.	3.0	445

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19	Toward effective and reliable fluorescence energies in solution by a new state specific polarizable continuum model time dependent density functional theory approach. Journal of Chemical Physics, 2007, 127, 074504.	3.0	437
20	Recent Advances in the Description of Solvent Effects with the Polarizable Continuum Model. Advances in Quantum Chemistry, 1998, 32, 227-261.	0.8	411
21	Fully Integrated Approach to Compute Vibrationally Resolved Optical Spectra: From Small Molecules to Macrosystems. Journal of Chemical Theory and Computation, 2009, 5, 540-554.	5.3	406
22	Solvent effect on vertical electronic transitions by the polarizable continuum model. Journal of Chemical Physics, 2000, 112, 2427-2435.	3.0	390
23	Transverse polarisation of quarks in hadrons. Physics Reports, 2002, 359, 1-168.	25.6	384
24	Fully anharmonic IR and Raman spectra of medium-size molecular systems: accuracy and interpretation. Physical Chemistry Chemical Physics, 2014, 16, 1759-1787.	2.8	363
25	Singlet Excited-State Behavior of Uracil and Thymine in Aqueous Solution:Â A Combined Experimental and Computational Study of 11 Uracil Derivatives. Journal of the American Chemical Society, 2006, 128, 607-619.	13.7	359
26	Polarizable dielectric model of solvation with inclusion of charge penetration effects. Journal of Chemical Physics, 2001, 114, 5691-5701.	3.0	315
27	Interplay of Electronic, Environmental, and Vibrational Effects in Determining the Hyperfine Coupling Constants of Organic Free Radicals. Chemical Reviews, 2004, 104, 1231-1254.	47.7	315
28	General Time Dependent Approach to Vibronic Spectroscopy Including Franckâ€“Condon, Herzbergâ€“Teller, and Duschinsky Effects. Journal of Chemical Theory and Computation, 2013, 9, 4097-4115.	5.3	314
29	A second-order perturbation theory route to vibrational averages and transition properties of molecules: General formulation and application to infrared and vibrational circular dichroism spectroscopies. Journal of Chemical Physics, 2012, 136, 124108.	3.0	311
30	Effective method to compute vibrationally resolved optical spectra of large molecules at finite temperature in the gas phase and in solution. Journal of Chemical Physics, 2007, 126, 184102.	3.0	303
31	Harmonic and Anharmonic Vibrational Frequency Calculations with the Double-Hybrid B2PLYP Method: Analytic Second Derivatives and Benchmark Studies. Journal of Chemical Theory and Computation, 2010, 6, 2115-2125.	5.3	274
32	Magnetic coupling in biradicals, binuclear complexes and wide-gap insulators: a survey of ab initio wave function and density functional theory approaches. Theoretical Chemistry Accounts, 2000, 104, 265-272.	1.4	268
33	Toward chemical accuracy in the computation of NMR shieldings: the PBE0 model. Chemical Physics Letters, 1998, 298, 113-119.	2.6	266
34	General Perturbative Approach for Spectroscopy, Thermodynamics, and Kinetics: Methodological Background and Benchmark Studies. Journal of Chemical Theory and Computation, 2012, 8, 1015-1036.	5.3	256
35	General Approach to Compute Vibrationally Resolved One-Photon Electronic Spectra. Journal of Chemical Theory and Computation, 2010, 6, 1256-1274.	5.3	253
36	Development and Validation of the B3LYP/N07D Computational Model for Structural Parameter and Magnetic Tensors of Large Free Radicals. Journal of Chemical Theory and Computation, 2008, 4, 751-764.	5.3	231

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37	Spin density in a nitronyl nitroxide free radical. Polarized neutron diffraction investigation and ab initio calculations. Journal of the American Chemical Society, 1994, 116, 2019-2027.	13.7	228
38	Density Functional Calculations of Magnetic Exchange Interactions in Polynuclear Transition Metal Complexes. Inorganic Chemistry, 1997, 36, 5022-5030.	4.0	226
39	Analytical second derivatives of the free energy in solution by polarizable continuum models. Journal of Chemical Physics, 1998, 109, 6246-6254.	3.0	220
40	Proton transfer in the ground and lowest excited states of malonaldehyde: A comparative density functional and postâ€Hartreeâ€“Fock study. Journal of Chemical Physics, 1996, 105, 11007-11019.	3.0	215
41	Development and validation of reliable quantum mechanical approaches for the study of free radicals in solution. Journal of Chemical Physics, 1996, 105, 11060-11067.	3.0	206
42	A TDDFT study of the electronic spectrum of s-tetrazine in the gas-phase and in aqueous solution. Chemical Physics Letters, 2000, 330, 152-160.	2.6	205
43	Prediction of the pKa of Carboxylic Acids Using the ab Initio Continuum-Solvation Model PCM-UAHF. Journal of Physical Chemistry A, 1998, 102, 6706-6712.	2.5	204
44	Conformation of pleionomers of .alpha.-aminoisobutyric acid. Macromolecules, 1985, 18, 895-902.	4.8	197
45	Absorption and Fluorescence Spectra of Uracil in the Gas Phase and in Aqueous Solution:Â A TD-DFT Quantum Mechanical Study. Journal of the American Chemical Society, 2004, 126, 14320-14321.	13.7	181
46	Vibrational computations beyond the harmonic approximation: Performances of the B3LYP density functional for semirigid molecules. Journal of Computational Chemistry, 2005, 26, 384-388.	3.3	179
47	Hydrogen and Higher Shell Contributions in Zn2+, Ni2+, and Co2+Aqueous Solutions:Â An X-ray Absorption Fine Structure and Molecular Dynamics Study. Journal of the American Chemical Society, 2002, 124, 1958-1967.	13.7	175
48	A Theoretical Investigation of the Ground and Excited States of Selected Ru and Os Polypyridyl Molecular Dyes. Journal of Physical Chemistry A, 2002, 106, 11354-11360.	2.5	174
49	On the Calculation and Modeling of Magnetic Exchange Interactions in Weakly Bonded Systems:Â The Case of the Ferromagnetic Copper(II) Î¼2-Azido Bridged Complexes. Inorganic Chemistry, 1999, 38, 1996-2004.	4.0	173
50	Absolute pKa determination for carboxylic acids using density functional theory and the polarizable continuum model. Chemical Physics Letters, 2003, 373, 411-415.	2.6	173
51	Conformational behavior of gaseous glycine by a density functional approach. Journal of Chemical Physics, 1995, 102, 364-370.	3.0	171
52	On the Performance of Continuum Solvation Methods. A Comment on â€œUniversal Approaches to Solvation Modelingâ€. Accounts of Chemical Research, 2009, 42, 489-492.	15.6	171
53	Separation between Fast and Slow Polarizations in Continuum Solvation Models. Journal of Physical Chemistry A, 2000, 104, 10614-10622.	2.5	168
54	Accuracy and Interpretability: The Devil and the Holy Grail. New Routes across Old Boundaries in Computational Spectroscopy. Chemical Reviews, 2019, 119, 8131-8191.	47.7	167

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55	Ab Initio Calculations of Absorption Spectra of Large Molecules in Solution: Coumarin C153. Angewandte Chemie - International Edition, 2007, 46, 405-408.	13.8	164
56	Structure, Magnetic Properties and Reactivities of Open-Shell Species From Density Functional and Self-Consistent Hybrid Methods. Recent Advances in Computational, 1995, , 287-334.	0.8	162
57	Integrated computational strategies for UV/vis spectra of large molecules in solution. Chemical Society Reviews, 2007, 36, 1724.	38.1	162
58	Transverse-spin and transverse-momentum effects in high-energy processes. Progress in Particle and Nuclear Physics, 2010, 65, 267-333.	14.4	157
59	Quantum Mechanical Computations and Spectroscopy: From Small Rigid Molecules in the Gas Phase to Large Flexible Molecules in Solution. Accounts of Chemical Research, 2008, 41, 605-616.	15.6	155
60	Semi-Experimental Equilibrium Structure Determinations by Employing B3LYP/SNSD Anharmonic Force Fields: Validation and Application to Semirigid Organic Molecules. Journal of Physical Chemistry A, 2015, 119, 2058-2082.	2.5	155
61	A direct procedure for the evaluation of solvent effects in MC-SCF calculations. Journal of Chemical Physics, 1999, 111, 5295-5302.	3.0	153
62	Inclusion of Hartreeâ€“Fock exchange in density functional methods. Hyperfine structure of second row atoms and hydrides. Journal of Chemical Physics, 1994, 101, 6834-6838.	3.0	149
63	Solvent Effect on the Singlet Excited-State Lifetimes of Nucleic Acid Bases:Â A Computational Study of 5-Fluorouracil and Uracil in Acetonitrile and Water. Journal of the American Chemical Society, 2006, 128, 16312-16322.	13.7	149
64	Hydrogen-Bonding Effects on Infrared Spectra from Anharmonic Computations: Uracilâ€“Water Complexes and Uracil Dimers. Journal of Physical Chemistry A, 2015, 119, 4224-4236.	2.5	142
65	Inexpensive and accurate predictions of optical excitations in transition-metal complexes: the TDDFT/PBE0 route. Theoretical Chemistry Accounts, 2000, 105, 169-172.	1.4	141
66	A fully automated implementation of VPT2 Infrared intensities. Chemical Physics Letters, 2010, 496, 157-161.	2.6	140
67	Validation of selfâ€consistent hybrid density functionals for the study of structural and electronic characteristics of organic Ï€ radicals. Journal of Chemical Physics, 1995, 102, 384-393.	3.0	138
68	Physically motivated density functionals with improved performances: The modified Perdewâ€“Burkeâ€“Ernzerhof model. Journal of Chemical Physics, 2002, 116, 5933-5940.	3.0	138
69	Accurate Vibrational Spectra of Large Molecules by Density Functional Computations beyond the Harmonic Approximation:Â The Case of Azabenzenes. Journal of Physical Chemistry A, 2004, 108, 4146-4150.	2.5	138
70	Polarizable Force Fields and Polarizable Continuum Model: A Fluctuating Charges/PCM Approach. 1. Theory and Implementation. Journal of Chemical Theory and Computation, 2011, 7, 3711-3724.	5.3	135
71	Structural revision of clusianone and 7-epi-clusianone and anti-HIV activity of polyisoprenylated benzophenones. Tetrahedron, 2005, 61, 8206-8211.	1.9	132
72	Gas-phase formation of the prebiotic molecule formamide: insights from new quantum computations. Monthly Notices of the Royal Astronomical Society: Letters, 2015, 453, L31-L35.	3.3	131

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73	Understanding the Role of Stereoelectronic Effects in Determining Collagen Stability. 1. A Quantum Mechanical Study of Proline, Hydroxyproline, and Fluoroproline Dipeptide Analogues in Aqueous Solution. Journal of the American Chemical Society, 2001, 123, 12568-12577.	13.7	129
74	Implementation and validation of a multi-purpose virtual spectrometer for large systems in complex environments. Physical Chemistry Chemical Physics, 2012, 14, 12404.	2.8	128
75	Influence of base stacking on excited-state behavior of polyadenine in water, based on time-dependent density functional calculations. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 9931-9936.	7.1	124
76	Extending the molecular size in accurate quantum-chemical calculations: the equilibrium structure and spectroscopic properties of uracil. Physical Chemistry Chemical Physics, 2011, 13, 7189.	2.8	123
77	Achieving linear-scaling computational cost for the polarizable continuum model of solvation. Theoretical Chemistry Accounts, 2004, 111, 90-100.	1.4	120
78	Accurate Harmonic/Anharmonic Vibrational Frequencies for Open-Shell Systems: Performances of the B3LYP/N07D Model for Semirigid Free Radicals Benchmarked by CCSD(T) Computations. Journal of Chemical Theory and Computation, 2010, 6, 828-838.	5.3	120
79	Structure and Conformational Behavior of Biopolymers by Density Functional Calculations Employing Periodic Boundary Conditions. I. The Case of Polyglycine, Polyalanine, and Poly-Î±-aminoisobutyric Acid in Vacuo. Journal of the American Chemical Society, 2001, 123, 3311-3322.	13.7	117
80	Integrated computational approach to vibrationally resolved electronic spectra: Anisole as a test case. Journal of Chemical Physics, 2008, 128, 244105.	3.0	117
81	Accurate structure, thermodynamic and spectroscopic parameters from CC and CC/DFT schemes: the challenge of the conformational equilibrium in glycine. Physical Chemistry Chemical Physics, 2013, 15, 10094.	2.8	117
82	Accurate excitation energies from time-dependent density functional theory: assessing the PBE0 model for organic free radicals. Chemical Physics Letters, 1999, 314, 152-157.	2.6	116
83	Accurate and feasible computations of structural and magnetic properties of large free radicals: The PBE0/N07D model. Chemical Physics Letters, 2008, 454, 139-143.	2.6	115
84	Accurate Anharmonic Vibrational Frequencies for Uracil: The Performance of Composite Schemes and Hybrid CC/DFT Model. Journal of Chemical Theory and Computation, 2011, 7, 3702-3710.	5.3	113
85	Linear Response Theory and Electronic Transition Energies for a Fully Polarizable QM/Classical Hamiltonian. Journal of Chemical Theory and Computation, 2012, 8, 4153-4165.	5.3	111
86	Exploring the conformational and reactive dynamics of biomolecules in solution using an extended version of the glycine reactive force field. Physical Chemistry Chemical Physics, 2013, 15, 15062.	2.8	111
87	Solvent Effects on the UV (nâ†' Ï€*) and NMR (13C and17O) Spectra of Acetone in Aqueous Solution. An Integrated Carâ^'Parrinello and DFT/PCM Approach. Journal of Physical Chemistry B, 2005, 109, 445-453.	2.6	106
88	Structural versatility of peptides from C?,?-dialkylated glycines. I. A conformational energy computation and x-ray diffraction study of homo-peptides from C?,?-diethylglycine. Biopolymers, 1988, 27, 357-371.	2.4	105
89	Time-Dependent Density Functional Tight Binding: New Formulation and Benchmark of Excited States. Journal of Chemical Theory and Computation, 2011, 7, 3304-3313.	5.3	105
90	Accurate vibrational spectra of large molecules by density functional computations beyond the harmonic approximation: the case of uracil and 2-thiouracil. Chemical Physics Letters, 2004, 388, 279-283.	2.6	104

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91	Short-Lived Quinonoid Species from 5,6-Dihydroxyindole Dimers en Route to Eumelanin Polymers:Â Integrated Chemical, Pulse Radiolytic, and Quantum Mechanical Investigation. Journal of the American Chemical Society, 2006, 128, 15490-15498.	13.7	104
92	TD-DFT Benchmark on Inorganic Pt(II) and Ir(III) Complexes. Journal of Chemical Theory and Computation, 2015, 11, 3281-3289.	5.3	104
93	The Genealogical Tree of Ethanol: Gas-phase Formation of Glycolaldehyde, Acetic Acid, and Formic Acid. Astrophysical Journal, 2018, 854, 135.	4.5	103
94	Conformational Characterization of Lanthanide(III)â^'DOTA Complexes by ab Initio Investigation in Vacuo and in Aqueous Solution. Journal of the American Chemical Society, 2002, 124, 4901-4909.	13.7	102
95	Vibrational spectra of large molecules by density functional computations beyond the harmonic approximation: the case of pyrrole and furan. Chemical Physics Letters, 2004, 383, 528-532.	2.6	102
96	Excited States Decay of the Aâ^'T DNA: A PCM/TD-DFT Study in Aqueous Solution of the (9-Methyl-adenine)2Â·(1-methyl-thymine)2 Stacked Tetramer. Journal of the American Chemical Society, 2009, 131, 15232-15245.	13.7	101
97	Toward anharmonic computations of vibrational spectra for large molecular systems. International Journal of Quantum Chemistry, 2012, 112, 2185-2200.	2.0	101
98	Anharmonic Effects on Vibrational Spectra Intensities: Infrared, Raman, Vibrational Circular Dichroism, and Raman Optical Activity. Journal of Physical Chemistry A, 2015, 119, 11862-11874.	2.5	101
99	Assessment of a Combined QM/MM Approach for the Study of Large Nitroxide Systems in Vacuo and in Condensed Phases. Journal of the American Chemical Society, 1998, 120, 7069-7078.	13.7	100
100	Proton transfer in model hydrogen-bonded systems by a density functional approach. Chemical Physics Letters, 1994, 231, 295-300.	2.6	99
101	Seeds of Life in Space (SOLIS). Astronomy and Astrophysics, 2017, 605, L3.	5.1	98
102	Checking the pH-Induced Conformational Transition of Prion Protein by Molecular Dynamics Simulations: Effect of Protonation of Histidine Residues. Biophysical Journal, 2004, 87, 3623-3632.	0.5	96
103	Folded and extended structures of homooligopeptides from .alpha.,.alpha.-dialkylated glycines. A conformational energy computation and x-ray diffraction study. Journal of the American Chemical Society, 1984, 106, 8146-8152.	13.7	95
104	Generalized vibrational perturbation theory for rotovibrational energies of linear, symmetric and asymmetric tops: Theory, approximations, and automated approaches to deal with mediumâ€toâ€large molecular systems. International Journal of Quantum Chemistry, 2015, 115, 948-982.	2.0	95
105	Semiexperimental Equilibrium Structures for Building Blocks of Organic and Biological Molecules: The B2PLYP Route. Journal of Chemical Theory and Computation, 2015, 11, 4689-4707.	5.3	95
106	Density Functional Study of Intrinsic and Environmental Effects in the Tautomeric Equilibrium of 2-Pyridone. The Journal of Physical Chemistry, 1995, 99, 15062-15068.	2.9	94
107	Characterization of the potential energy surface of the HO2molecular system by a density functional approach. Journal of Chemical Physics, 1994, 101, 10666-10676.	3.0	92
108	Development and Validation of an Integrated Computational Approach for the Study of Ionic Species in Solution by Means of Effective Two-Body Potentials. The Case of Zn2 +, Ni2 +, and Co2 +in Aqueous Solutions. Journal of the American Chemical Society, 2002, 124, 1968-1976.	13.7	92

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109	Dispersion corrected DFT approaches for anharmonic vibrational frequency calculations: nucleobases and their dimers. Physical Chemistry Chemical Physics, 2014, 16, 10112-10128.	2.8	92
110	Implementation and validation of the Lacks-Gordon exchange functional in conventional density functional and adiabatic connection methods. Journal of Computational Chemistry, 1998, 19, 418-429.	3.3	91
111	Computing the inhomogeneous broadening of electronic transitions in solution: a first-principle quantum mechanical approach. Physical Chemistry Chemical Physics, 2011, 13, 17007.	2.8	89
112	Joyce and Ulysses: integrated and user-friendly tools for the parameterization of intramolecular force fields from quantum mechanical data. Physical Chemistry Chemical Physics, 2013, 15, 3736.	2.8	89
113	Structure and Magnetic Properties of Glycine Radical in Aqueous Solution at Different pH Values. Journal of the American Chemical Society, 1998, 120, 5723-5732.	13.7	88
114	A theoretical investigation of valence and Rydberg electronic states of acrolein. Journal of Chemical Physics, 2003, 119, 12323-12334.	3.0	88
115	Intrinsic and Environmental Effects in the Structure and Magnetic Properties of Glycine Radical in Aqueous Solution. Journal of the American Chemical Society, 1997, 119, 12962-12967.	13.7	87
116	Accurate Characterization of the Peptide Linkage in the Gas Phase: A Joint Quantum-Chemical and Rotational Spectroscopy Study of the Glycine Dipeptide Analogue. Journal of Physical Chemistry Letters, 2014, 5, 534-540.	4.6	87
117	Accurate static polarizabilities by density functional theory: assessment of the PBE0 model. Chemical Physics Letters, 1999, 307, 265-271.	2.6	86
118	Performances of different density functionals in the computation of vibrational spectra beyond the harmonic approximation. Chemical Physics Letters, 2004, 399, 226-229.	2.6	86
119	Inclusion of Hartree-Fock exchange in the density functional approach. Benchmark computations for diatomic molecules containing H, B, C, N, O, and F atoms. Chemical Physics Letters, 1994, 226, 392-398.	2.6	84
120	Structure, epr parameters, and reactivity of organic free radicals from a density functional approach. Theoretica Chimica Acta, 1995, 91, 113-128.	0.8	84
121	Solvent Polarity and pH Effects on the Magnetic Properties of Ionizable Nitroxide Radicals:Â A Combined Computational and Experimental Study of 2,2,5,5-Tetramethyl-3-carboxypyrrolidine and 2,2,6,6-Tetramethyl-4-carboxypiperidine Nitroxides. Journal of Physical Chemistry A, 2002, 106, 10700-10706.	2.5	84
122	Implementation of a graphical user interface for the virtual multifrequency spectrometer: The VMSâ€Draw tool. Journal of Computational Chemistry, 2015, 36, 321-334.	3.3	84
123	Exploration of the Conformational and Reactive Dynamics of Glycine and Diglycine on TiO₂: Computational Investigations in the Gas Phase and in Solution. Journal of Physical Chemistry C, 2012, 116, 5141-5150.	3.1	83
124	Quantum Chemistry Meets Spectroscopy for Astrochemistry: Increasing Complexity toward Prebiotic Molecules. Accounts of Chemical Research, 2015, 48, 1413-1422.	15.6	83
125	Theoretical study of direct and water-assisted isomerization of formaldehyde radical cation. A comparison between density functional and post-Hartree-Fock approaches. Chemical Physics Letters, 1994, 224, 432-438.	2.6	82
126	Reliable NMR chemical shifts for molecules in solution by methods rooted in density functional theory. Magnetic Resonance in Chemistry, 2004, 42, S57-S67.	1.9	82

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127	The virtual multifrequency spectrometer: a new paradigm for spectroscopy. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 86-110.	14.6	82
128	Intrinsic and Environmental Effects in the Structure and Magnetic Properties of Organic Molecular Magnets:â€‰ Bis(imino)nitroxide. Journal of the American Chemical Society, 1997, 119, 10831-10837.	13.7	81
129	Quantum mechanical study of the conformational behavior of proline and 4R-hydroxyproline dipeptide analogues in vacuum and in aqueous solution. Journal of Computational Chemistry, 2002, 23, 341-350.	3.3	81
130	Glycine conformers: a never-ending story?. Physical Chemistry Chemical Physics, 2013, 15, 1358-1363.	2.8	81
131	A hybrid explicit/implicit solvation method for first-principle molecular dynamics simulations. Journal of Chemical Physics, 2008, 128, 144501.	3.0	79
132	Validation of the B3LYP/N07D and PBE0/N07D Computational Models for the Calculation of Electronic g-Tensors. Journal of Chemical Theory and Computation, 2009, 5, 192-199.	5.3	79
133	Conformational behavior of Î±,Î±-dialkylated peptides. Biopolymers, 1985, 24, 1759-1767.	2.4	78
134	Electronic, vibrational and environmental effects on the hyperfine coupling constants of nitroside radicals. H2NO as a case study. Chemical Physics Letters, 1996, 262, 201-206.	2.6	78
135	Evidence for Sevenfold Coordination in the First Solvation Shell of Hg(II) Aqua Ion. Journal of the American Chemical Society, 2007, 129, 5430-5436.	13.7	78
136	Vibronically Resolved Electronic Circular Dichroism Spectra of (R)-(+)-3-Methylcyclopentanone: A Theoretical Study. Journal of Physical Chemistry A, 2008, 112, 12401-12411.	2.5	78
137	Absorption and Emission Spectra of a Flexible Dye in Solution: A Computational Time-Dependent Approach. Journal of Chemical Theory and Computation, 2013, 9, 4507-4516.	5.3	78
138	The role of dispersion correction to DFT for modelling weakly bound molecular complexes in the ground and excited electronic states. Chemical Physics, 2008, 346, 247-256.	1.9	77
139	Effective Time-Independent Calculations of Vibrational Resonance Raman Spectra of Isolated and Solvated Molecules Including Duschinsky and Herzbergâ€“Teller Effects. Journal of Chemical Theory and Computation, 2011, 7, 1824-1839.	5.3	77
140	Interplay between â€œNeutralâ€•and â€œChargeâ€•Transferâ€•Excimers Rules the Excited State Decay in Adenineâ€Rich Polynucleotides. Angewandte Chemie - International Edition, 2011, 50, 12016-12019.	13.8	76
141	The Optical Rotation of Methyloxirane in Aqueous Solution: A Never Ending Story?. Journal of Chemical Theory and Computation, 2013, 9, 1880-1884.	5.3	76
142	Dual Fluorescence through Kashaâ€™s Rule Breaking: An Unconventional Photomechanism for Intracellular Probe Design. Journal of Physical Chemistry B, 2015, 119, 6144-6154.	2.6	76
143	Solvent Effect on the Singlet Excited-state Dynamics of 5-Fluorouracil in Acetonitrile as Compared with Water. Journal of Physical Chemistry B, 2006, 110, 12843-12847.	2.6	75
144	CC/DFT Route toward Accurate Structures and Spectroscopic Features for Observed and Elusive Conformers of Flexible Molecules: Pyruvic Acid as a Case Study. Journal of Chemical Theory and Computation, 2015, 11, 4342-4363.	5.3	75

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145	Extension of the AMBER force-field for the study of large nitroxides in condensed phases: an ab initio parameterization. Physical Chemistry Chemical Physics, 2010, 12, 11697.	2.8	74
146	Accurate molecular structure and spectroscopic properties of nucleobases: a combined computationalâ€“microwave investigation of 2-thiouracil as a case study. Physical Chemistry Chemical Physics, 2013, 15, 16965.	2.8	74
147	Diving for Accurate Structures in the Ocean of Molecular Systems with the Help of Spectroscopy and Quantum Chemistry. Accounts of Chemical Research, 2018, 51, 548-556.	15.6	74
148	Toward an integrated computational approach to CW-ESR spectra of free radicals. Physical Chemistry Chemical Physics, 2006, 8, 4609.	2.8	73
149	Boer-Mulders effect in unpolarized SIDIS: An analysis of the COMPASS and HERMES data on the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>cos</mml:mi><mml:mo>ï»¿</mml:mo><mml:mn>2</mml:mn><mml:mi>Ï•</mml:mi></mml:math>asymmetry. Physical Review D, 2010, 81, .	4.7	73
150	Extension of the â€œCheapâ€•Composite Approach to Noncovalent Interactions: The jun-ChS Scheme. Journal of Chemical Theory and Computation, 2020, 16, 988-1006.	5.3	73
151	Computational molecular spectroscopy. Nature Reviews Methods Primers, 2021, 1, .	21.2	73
152	Interplay of Stereoelectronic and Enviromental Effects in Tuning the Structural and Magnetic Properties of a Prototypical Spin Probe:Â Further Insights from a First Principle Dynamical Approach. Journal of the American Chemical Society, 2006, 128, 4338-4347.	13.7	72
153	Anharmonic theoretical simulations of infrared spectra of halogenated organic compounds. Journal of Chemical Physics, 2013, 139, 074310.	3.0	72
154	Characterization of the Elusive Conformers of Glycine from State-of-the-Art Structural, Thermodynamic, and Spectroscopic Computations: Theory Complements Experiment. Journal of Chemical Theory and Computation, 2013, 9, 1533-1547.	5.3	72
155	Structural versatility of peptides from C?,?-dialkylated glycines. II. An IR absorption and1H-nmr study of homo-oligopeptides from C?,?-diethylglycine. Biopolymers, 1988, 27, 373-379.	2.4	71
156	A Robust and Effective Time-Independent Route to the Calculation of Resonance Raman Spectra of Large Molecules in Condensed Phases with the Inclusion of Duschinsky, Herzbergâ€“Teller, Anharmonic, and Environmental Effects. Journal of Chemical Theory and Computation, 2014, 10, 346-363.	5.3	71
157	Structure functions of bound nucleons: From the EMC effect to nuclear shadowing. Zeitschrift FÃ¼r Physik C-Particles and Fields, 1993, 58, 541-558.	1.5	70
158	An improved iterative solution to solve the electrostatic problem in the polarizable continuum model. Theoretical Chemistry Accounts, 2001, 105, 446-451.	1.4	70
159	Unraveling the role of entropy in tuning unimolecular vs. bimolecular reaction rates: The case of olefin polymerization catalyzed by transition metals. Molecular Catalysis, 2018, 452, 138-144.	2.0	70
160	Validation of the DFT/N07D computational model on the magnetic, vibrational and electronic properties of vinyl radical. Physical Chemistry Chemical Physics, 2010, 12, 1092-1101.	2.8	69
161	Analytical First and Second Derivatives for a Fully Polarizable QM/Classical Hamiltonian. Journal of Chemical Theory and Computation, 2012, 8, 4270-4278.	5.3	68
162	Benchmarking TD-DFT against Vibrationally Resolved Absorption Spectra at Room Temperature: 7-Aminocoumarins as Test Cases. Journal of Chemical Theory and Computation, 2015, 11, 5371-5384.	5.3	68

#	Article	IF	Citations
163	Computational approach to the study of the lineshape of absorption and electronic circular dichroism spectra. International Journal of Quantum Chemistry, 2010, 110, 476-486.	2.0	67
164	Absorption and emission UV-Vis spectra of the TRITC fluorophore molecule in solution: a quantum mechanical study. Physical Chemistry Chemical Physics, 2010, 12, 1000-1006.	2.8	67
165	Understanding the Role of Stereoelectronic Effects in Determining Collagen Stability. 2. A Quantum Mechanical/Molecular Mechanical Study of (Proline-Proline-Glycine)n Polypeptides. Journal of the American Chemical Society, 2002, 124, 7857-7865.	13.7	66
166	Quantum Dynamics of the Ultrafast Ï€Ï€*/nÏ€* Population Transfer in Uracil and 5-Fluoro-Uracil in Water and Acetonitrile. Journal of Physical Chemistry B, 2009, 113, 14491-14503.	2.6	66
167	First-row transition-metal hydrides: A challenging playground for new theoretical approaches. International Journal of Quantum Chemistry, 1997, 61, 443-451.	2.0	65
168	Theoretical Study of the Addition of Hydrogen Cyanide to Methanimine in the Gas Phase and in Aqueous Solution. Journal of the American Chemical Society, 2000, 122, 324-330.	13.7	65
169	Complete structural and magnetic characterization of biological radicals in solution by an integrated quantum mechanical approach: Glycyl radical as a case study. Journal of Chemical Physics, 2004, 121, 6710-6718.	3.0	65
170	A quantum mechanical/molecular dynamics/mean field study of acrolein in aqueous solution: Analysis of H bonding and bulk effects on spectroscopic properties. Journal of Chemical Physics, 2006, 125, 164515.	3.0	65
171	Structure, Thermochemistry, and Magnetic Properties of Binary Copper Carbonyls by a Density-Functional Approach. The Journal of Physical Chemistry, 1995, 99, 11659-11666.	2.9	64
172	Thiazolidin-4-one formation. Mechanistic and synthetic aspects of the reaction of imines and mercaptoacetic acid under microwave and conventional heating. Organic and Biomolecular Chemistry, 2004, 2, 2809.	2.8	63
173	Photoinduced symmetry-breaking intramolecular charge transfer in a quadrupolar pyridinium derivative. Physical Chemistry Chemical Physics, 2014, 16, 13984-13994.	2.8	62
174	General formulation of vibronic spectroscopy in internal coordinates. Journal of Chemical Physics, 2016, 144, 084114.	3.0	62
175	The polarizability in solution of tetra-phenyl-porphyrin derivatives in their excited electronic states: a PCM/TD-DFT study. Physical Chemistry Chemical Physics, 2009, 11, 4664.	2.8	61
176	Duschinsky, Herzbergâ€“Teller, and Multiple Electronic Resonance Interferential Effects in Resonance Raman Spectra and Excitation Profiles. The Case of Pyrene. Journal of Chemical Theory and Computation, 2013, 9, 3597-3611.	5.3	60
177	Theory Meets Experiment for Noncovalent Complexes: The Puzzling Case of Pnicogen Interactions. Angewandte Chemie - International Edition, 2018, 57, 13853-13857.	13.8	60
178	Theoretical modeling of spectroscopic properties of molecules in solution: toward an effective dynamical discrete/continuum approach. Theoretical Chemistry Accounts, 2007, 117, 1001-1015.	1.4	59
179	Can TDâ€ÐFT calculations accurately describe the excited states behavior of stacked nucleobases? The cytosine dimer as a test case. Journal of Computational Chemistry, 2008, 29, 957-964.	3.3	59
180	From concepts to algorithms for the characterization of reaction mechanisms. H2CS as a case study. Journal of Chemical Physics, 1994, 100, 3717-3741.	3.0	58

#	Article	IF	Citations
181	Accurate Steady-State and Zero-Time Fluorescence Spectra of Large Molecules in Solution by a First-Principle Computational Method. Journal of Physical Chemistry B, 2007, 111, 14080-14082.	2.6	58
182	Vibrational modulation effects on the hyperfine coupling constants of fluoromethyl radicals. Journal of Chemical Physics, 1993, 99, 6787-6798.	3.0	57
183	From concepts to algorithms for the treatment of large amplitude internal motions and unimolecular reactions. Computational and Theoretical Chemistry, 1995, 330, 365-376.	1.5	57
184	Structure and magnetic properties of benzyl, anilino, and phenoxyl radicals by density functional computations. Journal of Chemical Physics, 1998, 109, 10244-10254.	3.0	57
185	Radical cations of DNA bases: some insights on structure and fragmentation patterns by density functional methods. International Journal of Mass Spectrometry, 2000, 201, 321-336.	1.5	57
186	Fluorescence spectra of organic dyes in solution: a time dependent multilevel approach. Physical Chemistry Chemical Physics, 2011, 13, 2160-2166.	2.8	57
187	Realistic Modeling of Fluorescent Dye-Doped Silica Nanoparticles: A Step Toward the Understanding of their Enhanced Photophysical Properties.. Chemistry of Materials, 2011, 23, 5016-5023.	6.7	57
188	Accurate molecular structures and infrared spectra of trans-2,3-dideuterooxirane, methyloxirane, and trans-2,3-dimethyloxirane. Journal of Chemical Physics, 2014, 141, 034107.	3.0	57
189	Density functional approach to the structures and EPR parameters of open shell systems. The case of fluorovinyl radicals. Chemical Physics Letters, 1993, 212, 5-11.	2.6	56
190	Validation of self-consistent hybrid approaches for the study of transition metal complexes. NiCO and CuCO as case studies. Chemical Physics Letters, 1995, 233, 129-133.	2.6	56
191	Vibronic Model for the Quantum Dynamical Study of the Competition between Bright and Charge-Transfer Excited States in Single-Strand Polynucleotides: The Adenine Dimer Case. Journal of Physical Chemistry A, 2009, 113, 15346-15354.	2.5	56
192	State-of-the-Art Thermochemical and Kinetic Computations for Astrochemical Complex Organic Molecules: Formamide Formation in Cold Interstellar Clouds as a Case Study. Journal of Chemical Theory and Computation, 2016, 12, 5385-5397.	5.3	56
193	Assessing the reliability of density functional methods in the conformational study of polypeptides: The treatment of intraresidue nonbonding interactions. Journal of Computational Chemistry, 2004, 25, 1333-1341.	3.3	55
194	Solvent effects on electron-driven proton-transfer processes: adenineâ€“thymine base pairs. Physical Chemistry Chemical Physics, 2012, 14, 8981.	2.8	55
195	Computation of protein pKâ€™s values by an integrated density functional theory/Polarizable Continuum Model approach. Theoretical Chemistry Accounts, 2004, 111, 237-245.	1.4	54
196	Accessing transversity via J/Ï^ production in polarized pâ†'pÌ„â†'Âinteractions. Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics, 2004, 594, 97-104.	4.1	54
197	Accurate vibrational spectra and magnetic properties of organic free radicals: The case of H2CN. Journal of Chemical Physics, 2005, 122, 224308.	3.0	54
198	Non-periodic boundary conditions for ab initio molecular dynamics in condensed phase using localized basis functions. Chemical Physics Letters, 2006, 422, 367-371.	2.6	54

#	Article	IF	Citations
199	Interplay of Intrinsic, Environmental, and Dynamic Effects in Tuning the EPR Parameters of Nitroxides:â€‰Further Insights from an Integrated Computational Approach. Journal of Physical Chemistry B, 2007, 111, 8928-8939.	2.6	54
200	General trends in the molecular physics of azabiphenyls. Molecular Physics, 1983, 49, 599-619.	1.7	53
201	From Classical Density Functionals to Adiabatic Connection Methods. The State of the Art.. Advances in Quantum Chemistry, 2000, 36, 45-75.	0.8	53
202	The conformational behavior of polyglycine as predicted by a density functional model with periodic boundary conditions. Journal of Chemical Physics, 2001, 114, 2541-2549.	3.0	53
203	Experimental Evidence for a Variable First Coordination Shell of the Cadmium(II) Ion in Aqueous, Dimethyl Sulfoxide, andN,Nâ€˜-Dimethylpropyleneurea Solution. Journal of Physical Chemistry B, 2005, 109, 9178-9185.	2.6	53
204	Formation of cross-linked adducts between guanine and thymine mediated by hydroxyl radical and one-electron oxidation: a theoretical study. Organic and Biomolecular Chemistry, 2008, 6, 3300.	2.8	53
205	CYANOMETHANIMINE ISOMERS IN COLD INTERSTELLAR CLOUDS: INSIGHTS FROM ELECTRONIC STRUCTURE AND KINETIC CALCULATIONS. Astrophysical Journal, 2015, 810, 111.	4.5	53
206	Density Functional Modeling of Double Exchange Interactions in Transition Metal Complexes. Calculation of the Ground and Excited State Properties of [Fe2(OH)3(tmtacn)2]2+. Journal of the American Chemical Society, 1998, 120, 8357-8365.	13.7	52
207	The Gas Phase Anisole Dimer: A Combined High-Resolution Spectroscopy and Computational Study of a Stacked Molecular System. Journal of Physical Chemistry A, 2009, 113, 14343-14351.	2.5	52
208	On the Calculation of Vibrational Frequencies for Molecules in Solution Beyond the Harmonic Approximation. Journal of Chemical Theory and Computation, 2010, 6, 1660-1669.	5.3	52
209	A general time-dependent route to Resonance-Raman spectroscopy including Franck-Condon, Herzberg-Teller and Duschinsky effects. Journal of Chemical Physics, 2014, 141, 114108.	3.0	52
210	Immersive virtual reality in computational chemistry: Applications to the analysis of QM and MM data. International Journal of Quantum Chemistry, 2016, 116, 1731-1746.	2.0	52
211	Antitumor Agents. 2. Synthesis, Structureâ^'Activity Relationships, and Biological Evaluation of Substituted 5H-Pyridophenoxazin-5-ones with Potent Antiproliferative Activity. Journal of Medicinal Chemistry, 2002, 45, 5217-5223.	6.4	51
212	Environmental Effects in Computational Spectroscopy: Accuracy and Interpretation. ChemPhysChem, 2010, 11, 1812-1832.	2.1	51
213	Stability and structure of formamide and urea dimers in aqueous solution. A theoretical study. Journal of the Chemical Society Faraday Transactions I, 1989, 85, 621.	1.0	50
214	The excited states of adenine and thymine nucleoside and nucleotide in aqueous solution: a comparative study by time-dependent DFT calculations. Theoretical Chemistry Accounts, 2008, 120, 491-497.	1.4	50
215	Integrated experimental and theoretical approach for the structural characterization of Hg2+ aqueous solutions. Journal of Chemical Physics, 2008, 128, 084502.	3.0	50
216	Toward Ab Initio Anharmonic Vibrational Circular Dichroism Spectra in the Condensed Phase. Journal of Physical Chemistry Letters, 2012, 3, 1766-1773.	4.6	50

#	Article	IF	Citations
217	General Strategy for Computing Nonlinear Optical Properties of Large Neutral and Cationic Organic Chromophores in Solution. Journal of Physical Chemistry B, 2015, 119, 3155-3173.	2.6	50
218	Accurate Simulation of Resonance-Raman Spectra of Flexible Molecules: An Internal Coordinates Approach. Journal of Chemical Theory and Computation, 2015, 11, 3267-3280.	5.3	50
219	Development and Implementation of Advanced Fitting Methods for the Calculation of Accurate Molecular Structures. Journal of Chemical Theory and Computation, 2017, 13, 3060-3075.	5.3	50
220	Accuracy Meets Interpretability for Computational Spectroscopy by Means of Hybrid and Double-Hybrid Functionals. Frontiers in Chemistry, 2020, 8, 584203.	3.6	50
221	Dielsâ€“Alder reactions: An assessment of quantum chemical procedures. Journal of Chemical Physics, 1997, 106, 8727-8732.	3.0	49
222	Computational Evidence for a Variable First Shell Coordination of the Cadmium(II) Ion in Aqueous Solution. Journal of Physical Chemistry B, 2005, 109, 9186-9193.	2.6	49
223	Theory for Vibrationally Resolved Two-Photon Circular Dichroism Spectra. Application to (R)-(+)-3-Methylcyclopentanone. Journal of Physical Chemistry A, 2009, 113, 4198-4207.	2.5	49
224	Unveiling the Sulfurâ€“Sulfur Bridge: Accurate Structural and Energetic Characterization of a Homochalcogen Intermolecular Bond. Angewandte Chemie - International Edition, 2018, 57, 15822-15826.	13.8	49
225	Extending the perturbed matrix method beyond the dipolar approximation: comparison of different levels of theory. Physical Chemistry Chemical Physics, 2018, 20, 24369-24378.	2.8	49
226	Coriolis couplings in variational computations of vibrational spectra beyond the harmonic approximation: implementation and validation. Chemical Physics Letters, 2004, 392, 365-371.	2.6	48
227	Structural and Dynamical Properties of the Hg²⁺ Aqua Ion:â€‰ A Molecular Dynamics Study. Journal of Physical Chemistry B, 2008, 112, 4694-4702.	2.6	48
228	Toward spectroscopic studies of biologically relevant systems: Vibrational spectrum of adenine as a test case for performances of long-range/dispersion corrected density functionals. Chemical Physics Letters, 2009, 475, 105-110.	2.6	48
229	Towards an accurate description of anharmonic infrared spectra in solution within the polarizable continuum model: Reaction field, cavity field and nonequilibrium effects. Journal of Chemical Physics, 2011, 135, 104505.	3.0	48
230	Fully ab initio IR spectra for complex molecular systems from perturbative vibrational approaches: Glycine as a test case. Journal of Molecular Structure, 2012, 1009, 74-82.	3.6	48
231	Vertical Electronic Excitations in Solution with the EOM-CCSD Method Combined with a Polarizable Explicit/Implicit Solvent Model. Journal of Chemical Theory and Computation, 2013, 9, 3035-3042.	5.3	48
232	Reversible vapochromic response of polymer films doped with a highly emissive molecular rotor. Journal of Materials Chemistry C, 2014, 2, 9224-9232.	5.5	48
233	Toward spectroscopic accuracy for organic free radicals: Molecular structure, vibrational spectrum, and magnetic properties of F2NO. Journal of Chemical Physics, 2008, 129, 084306.	3.0	47
234	Role of Hostâ€“Guest Interactions in Tuning the Optical Properties of Coumarin Derivatives Incorporated in MCM-41: A TD-DFT Investigation. Journal of Physical Chemistry C, 2012, 116, 17807-17818.	3.1	47

#	Article	IF	Citations
235	A gauge invariant multiscale approach to magnetic spectroscopies in condensed phase: General three-layer model, computational implementation and pilot applications. Journal of Chemical Physics, 2013, 138, 234108.	3.0	47
236	ACCURATE SPECTROSCOPIC CHARACTERIZATION OF OXIRANE: A VALUABLE ROUTE TO ITS IDENTIFICATION IN TITAN'S ATMOSPHERE AND THE ASSIGNMENT OF UNIDENTIFIED INFRARED BANDS. Astrophysical Journal, 2014, 785, 107.	4.5	47
237	Reliable vibrational wavenumbers for Cî€O and Nâ€“H stretchings of isolated and hydrogen-bonded nucleic acid bases. Physical Chemistry Chemical Physics, 2016, 18, 8479-8490.	2.8	47
238	Discovering the Elusive Global Minimum in a Ternary Chiral Cluster: Rotational Spectra of Propylene Oxide Trimer. Angewandte Chemie - International Edition, 2020, 59, 22427-22430.	13.8	47
239	Solvent effects on an SN2 reaction profile. Chemical Physics Letters, 1998, 297, 1-7.	2.6	46
240	Antitumor Agents. 1. Synthesis, Biological Evaluation, and Molecular Modeling of 5H-Pyrido[3,2-a]phenoxazin-5-one, a Compound with Potent Antiproliferative Activity. Journal of Medicinal Chemistry, 2002, 45, 5205-5216.	6.4	46
241	Hyperfine coupling constants of dimethyl nitroxide in aqueous solution: Carâ€“Parrinello molecular dynamics and discrete-continuum approaches. Chemical Physics Letters, 2004, 395, 120-126.	2.6	46
242	A mean field approach for molecular simulations of fluid systems. Journal of Chemical Physics, 2005, 122, 154109.	3.0	46
243	Periodic and High-Temperature Disordered Conformations of Polytetrafluoroethylene Chains:Â An ab Initio Modeling. Journal of the American Chemical Society, 2006, 128, 1099-1108.	13.7	46
244	Implementation and validation of DFT-D for molecular vibrations and dynamics: The benzene dimer as a case study. Chemical Physics Letters, 2008, 452, 333-339.	2.6	46
245	The excited electronic states of adenine-guanine stacked dimers in aqueous solution: a PCM/TD-DFT study. Physical Chemistry Chemical Physics, 2010, 12, 4934.	2.8	46
246	Toward an Accurate Modeling of Optical Rotation for Solvated Systems: Anharmonic Vibrational Contributions Coupled to the Polarizable Continuum Model. Journal of Chemical Theory and Computation, 2012, 8, 585-597.	5.3	46
247	Anharmonicity Effects in the Vibrational CD Spectra of Propylene Oxide. Journal of Physical Chemistry Letters, 2013, 4, 3424-3428.	4.6	46
248	High-Accuracy Vibrational Computations for Transition-Metal Complexes Including Anharmonic Corrections: Ferrocene, Ruthenocene, and Osmocene as Test Cases. Journal of Chemical Theory and Computation, 2014, 10, 4565-4573.	5.3	46
249	Vibrational Density Matrix Renormalization Group. Journal of Chemical Theory and Computation, 2017, 13, 3764-3777.	5.3	46
250	Assessing the acidâ€“base and conformational properties of histidine residues in human prion protein (125â€“228) by means of pK a calculations and molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2006, 64, 167-177.	2.6	45
251	New quantum chemical computations of formamide deuteration support gas-phase formation of this prebiotic molecule. Monthly Notices of the Royal Astronomical Society: Letters, 2017, 468, L1-L5.	3.3	45
252	Accurate Biomolecular Structures by the Nano-LEGO Approach: Pick the Bricks and Build Your Geometry. Journal of Chemical Theory and Computation, 2021, 17, 7290-7311.	5.3	45

#	Article	IF	Citations
253	Comparison of convetional and hybrid density functional approaches. Cationic hydrides of first-row transition metals as a case study. Chemical Physics Letters, 1996, 249, 290-296.	2.6	44
254	Catalytic and bulk solvent effects on proton transfer: Formamide as a case study. Journal of Computational Chemistry, 1997, 18, 1993-2000.	3.3	44
255	Systematic phenomenological study of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>cos</mml:mi><mml:mo>ï»¿</mml:mo><mml:mn>2</mml:mn><mml:mi>Ï•</mml:mi></mml:math>asymmetry in unpolarized semi-inclusive DIS. Physical Review D, 2008, 78, .	4.7	44
256	Lack of Visible Chromophore Development in the Pulse Radiolysis Oxidation of 5,6-Dihydroxyindole-2-carboxylic Acid Oligomers: DFT Investigation and Implications for Eumelanin Absorption Properties. Journal of Organic Chemistry, 2009, 74, 3727-3734.	3.2	44
257	New Hints on the pH-Driven Tautomeric Equilibria of the Topotecan Anticancer Drug in Aqueous Solutions from an Integrated Spectroscopic and Quantum-Mechanical Approach. Journal of the American Chemical Society, 2005, 127, 15429-15436.	13.7	43
258	Spectroscopic Properties in the Liquid Phase: Combining High-Level Ab Initio Calculations and Classical Molecular Dynamics. ChemPhysChem, 2006, 7, 148-156.	2.1	43
259	Accurate Density Functional Calculations of Near-Edge X-Ray and Optical Absorption Spectra of Liquid Water Using Nonperiodic Boundary Conditions: The Role of Self-Interaction and Long-Range Effects. Physical Review Letters, 2008, 100, 107401.	7.8	43
260	Unraveling solvent effects on the electronic absorption spectra of TRITC fluorophore in solution: a theoretical TD-DFT/PCM study. Physical Chemistry Chemical Physics, 2010, 12, 2722.	2.8	43
261	Theoretical multilevel approach for studying the photophysical properties of organic dyes in solution. Physical Chemistry Chemical Physics, 2010, 12, 10550.	2.8	43
262	The Interplay between Ï€Ï€*/nÏ€* Excited States in Gasâ€Phase Thymine: A Quantum Dynamical Study. ChemPhysChem, 2011, 12, 1957-1968.	2.1	43
263	Computational Design, Synthesis, and Mechanochromic Properties of New Thiopheneâ€Based Ï€â€Conjugated Chromophores. Chemistry - A European Journal, 2013, 19, 1996-2004.	3.3	43
264	Computational Spectroscopy of Large Systems in Solution: The DFTB/PCM and TD-DFTB/PCM Approach. Journal of Chemical Theory and Computation, 2013, 9, 2052-2071.	5.3	43
265	Analytical gradients for <scp>MP</scp>2, double hybrid functionals, and <scp>TD</scp>â€<scp>DFT</scp> with polarizable embedding described by fluctuating charges. Journal of Computational Chemistry, 2015, 36, 2271-2290.	3.3	43
266	Precursors of the RNA World in Space: Detection of (Z)-1,2-ethenediol in the Interstellar Medium, a Key Intermediate in Sugar Formation. Astrophysical Journal Letters, 2022, 929, L11.	8.3	43
267	Conformational behavior of ?,?-dialkylated peptides: Ab initio and empirical results for cyclopropylglycine. Biopolymers, 1988, 27, 1673-1685.	2.4	42
268	Structure and ESR features of glycine radical in its zwitterionic form. Chemical Physics Letters, 1995, 242, 351-354.	2.6	42
269	Micellar aggregation of sulfonate surfactants studied by electron paramagnetic resonance of a cationic nitroxide: an experimental and computational approach. Physical Chemistry Chemical Physics, 2002, 4, 2180-2188.	2.8	42
270	UVâ^'Vis Spectra of the Anticancer Campothecin Family Drugs in Aqueous Solution: Specific Spectroscopic Signatures Unraveled by a Combined Computational and Experimental Study. Journal of Physical Chemistry B, 2009, 113, 5369-5375.	2.6	42

#	Article	IF	Citations
271	Efficient Excitedâ€State Symmetry Breaking in a Cationic Quadrupolar System Bearing Diphenylamino Donors. ChemPhysChem, 2016, 17, 136-146.	2.1	42
272	Effective yet reliable computation of hyperfine coupling constants in solution by a QM/MM approach: Interplay between electrostatics and non-electrostatic effects. Journal of Chemical Physics, 2019, 150, 124102.	3.0	42
273	Structural versatility of peptides from C?,?-disubstituted glycines: Preferred conformation of the C?,?-diphenylglycine residue. Biopolymers, 1990, 30, 1-11.	2.4	40
274	Role of Polar and Enthalpic Effects in the Addition of Methyl Radical to Substituted Alkenes:â€‰ A Density Functional Study Including Solvent Effects. Journal of the American Chemical Society, 1998, 120, 5733-5740.	13.7	40
275	Through-bond and through-space effects in the magnetic properties of nitroxide biradicals by an integrated QM/MM approach including solvent effects. Chemical Physics Letters, 1999, 302, 240-248.	2.6	40
276	Unraveling Solvent-Driven Equilibria between Î±- and 3₁₀-Helices through an Integrated Spin Labeling and Computational Approach. Journal of the American Chemical Society, 2007, 129, 11248-11258.	13.7	40
277	Unraveling the Role of Stereo-electronic, Dynamical, and Environmental Effects in Tuning the Structure and Magnetic Properties of Glycine Radical in Aqueous Solution at Different pH Values. Journal of the American Chemical Society, 2007, 129, 15380-15390.	13.7	40
278	Effect of the Ï€ Bridge and Acceptor on Intramolecular Charge Transfer in Pushâ€“Pull Cationic Chromophores: An Ultrafast Spectroscopic and TDâ€DFT Computational Study. ChemPhysChem, 2015, 16, 1440-1450.	2.1	40
279	Structural features of the carbonâ€“sulfur chemical bond: a semi-experimental perspective. Canadian Journal of Chemistry, 2016, 94, 1065-1076.	1.1	40
280	Simulation of Vibronic Spectra of Flexible Systems: Hybrid DVR-Harmonic Approaches. Journal of Chemical Theory and Computation, 2017, 13, 2804-2822.	5.3	40
281	Ab-initio mechanistic studies of radical reactions. Directive effects in the addition of methyl radical to unsymmetrical fluoroethenes. Journal of the Chemical Society Perkin Transactions II, 1986, , 1517-1524.	0.9	39
282	Quantum Mechanical Conformational Analysis of Î²-Alanine Zwitterion in Aqueous Solution. Journal of the American Chemical Society, 2000, 122, 3151-3155.	13.7	39
283	Electron Transfer in the [Pt(NH3)4]2+ [W(CN)8]3- Donorâ^'Acceptor System. The Environment Effect:â€‰ A Time-Dependent Density Functional Study. Journal of the American Chemical Society, 2001, 123, 10742-10743.	13.7	39
284	Computation of the acetone ultraviolet spectrum in gas phase and in aqueous solution by a mixed discrete/continuum model. Molecular Physics, 2003, 101, 1945-1953.	1.7	39
285	Reliable molecular simulations of solute-solvent systems with a minimum number of solvent shells. Journal of Chemical Physics, 2006, 124, 214505.	3.0	39
286	Absorption Spectrum of Aâ€“T DNA Unraveled by Quantum Mechanical Calculations in Solution on the (dA)₂â‹…(dT)₂ Tetramer. ChemPhysChem, 2008, 9, 2531-2537.	2.1	39
287	Structural Effects on the Electronic Absorption Properties of 5,6â€Dihydroxyindole Oligomers: The Potential of an Integrated Experimental and DFT Approach to Model Eumelanin Optical Properties^{â€}. Photochemistry and Photobiology, 2008, 84, 600-607.	2.5	39
288	Insight into the mechanism of action of plakortins, simple 1,2-dioxaneantimalarials. Organic and Biomolecular Chemistry, 2010, 8, 846-856.	2.8	39

#	Article	IF	Citations
289	Excited States Behavior of Nucleobases in Solution: Insights from Computational Studies. Topics in Current Chemistry, 2014, 355, 329-357.	4.0	39
290	Noncovalent Interactions and Internal Dynamics in Pyridineâ€“Ammonia: A Combined Quantumâ€Chemical and Microwave Spectroscopy Study. Chemistry - A European Journal, 2017, 23, 4876-4883.	3.3	39
291	Force Field Parametrization of Metal Ions from Statistical Learning Techniques. Journal of Chemical Theory and Computation, 2018, 14, 255-273.	5.3	39
292	Structures and properties of lanthanide and actinide complexes by a new density functional approach: Lanthanum, gadolinium, lutetium, and thorium halides as case studies. Journal of Computational Chemistry, 2000, 21, 1153-1166.	3.3	38
293	Development and Validation of an Integrated Computational Approach for the Modeling of cw-ESR Spectra of Free Radicals in Solution:Âp-(Methylthio)phenyl Nitronylnitroxide in Toluene as a Case Study. Journal of the American Chemical Society, 2006, 128, 15865-15873.	13.7	38
294	Noncovalent Interactions in the Gas Phase: The Anisoleâ€“Phenol Complex. Journal of Physical Chemistry A, 2011, 115, 9603-9611.	2.5	38
295	Identification of Serine Conformers by Matrix-Isolation IR Spectroscopy Aided by Near-Infrared Laser-Induced Conformational Change, 2D Correlation Analysis, and Quantum Mechanical Anharmonic Computations. Journal of Physical Chemistry B, 2015, 119, 10496-10510.	2.6	38
296	Simulation of Vacuum UV Absorption and Electronic Circular Dichroism Spectra of Methyl Oxirane: The Role of Vibrational Effects. Journal of Chemical Theory and Computation, 2016, 12, 2820-2833.	5.3	38
297	Electronic absorption spectra of pyridine and nicotine in aqueous solution with a combined molecular dynamics and polarizable QM/MM approach. Journal of Computational Chemistry, 2017, 38, 319-335.	3.3	38
298	Theoretical approach to the structure and hyperfine coupling constants of nonrigid radicals: the case of dihydronitrosyl radical. The Journal of Physical Chemistry, 1993, 97, 6355-6361.	2.9	37
299	Structure and Magnetic Properties of Nitroxide Molecular Crystals by Density Functional Calculations Employing Periodic Boundary Conditions. Journal of the American Chemical Society, 2002, 124, 113-120.	13.7	37
300	Toward spectroscopic accuracy for open-shell systems: Molecular structure and hyperfine coupling constants of H2CN, H2CP, NH2, and PH2 as test cases. Journal of Chemical Physics, 2010, 133, 184301.	3.0	37
301	Reliable structural, thermodynamic, and spectroscopic properties of organic molecules adsorbed on silicon surfaces from computational modeling: the case of glycine@Si(100). Physical Chemistry Chemical Physics, 2011, 13, 16713.	2.8	37
302	Molecular Structure and Spectroscopic Signatures of Acrolein: Theory Meets Experiment. Journal of Physical Chemistry A, 2014, 118, 6648-6656.	2.5	37
303	Presence of Two Emissive Minima in the Lowest Excited State of a Pushâ€“Pull Cationic Dye Unequivocally Proved by Femtosecond Up-Conversion Spectroscopy and Vibronic Quantum-Mechanical Computations. Journal of Physical Chemistry B, 2015, 119, 6035-6040.	2.6	37
304	Temperature Dependence of Radiative and Nonradiative Rates from Time-Dependent Correlation Function Methods. Journal of Chemical Theory and Computation, 2016, 12, 774-786.	5.3	37
305	Insights into structural and dynamical features of water at halloysite interfaces probed by DFT and classical molecular dynamics simulations. Physical Chemistry Chemical Physics, 2016, 18, 2164-2174.	2.8	37
306	Density functional theory: An effective theoretical tool for the study of ? radicals. International Journal of Quantum Chemistry, 1994, 52, 963-971.	2.0	36

#	Article	IF	Citations
307	Study of prototypical Diels-Alder reactions by a hybrid density functional/Hartree-Fock approach. Chemical Physics Letters, 1996, 251, 393-399.	2.6	36
308	Vibrational analyses for CHFClBr and CDFClBr based on high levelab initiocalculations. Journal of Chemical Physics, 2006, 125, 054308.	3.0	36
309	Chemical, Pulse Radiolysis and Density Functional Studies of a New, Labile 5,6-Indolequinone and Its Semiquinone. Journal of Organic Chemistry, 2007, 72, 1595-1603.	3.2	36
310	Assessment of a computational strategy approaching spectroscopic accuracy for structure, magnetic properties and vibrational frequencies of organic free radicals: the F2CN and F2BO case. Physical Chemistry Chemical Physics, 2008, 10, 6991.	2.8	36
311	Hydrodynamic modeling of diffusion tensor properties of flexible molecules. Journal of Computational Chemistry, 2009, 30, 2-13.	3.3	36
312	Methyl Phosphate Dianion Hydrolysis in Solution Characterized by Path Collective Variables Coupled with DFT-Based Enhanced Sampling Simulations. Journal of Chemical Theory and Computation, 2011, 7, 539-543.	5.3	36
313	Absorption and emission spectra of fluorescent silica nanoparticles from TD-DFT/MM/PCM calculations. Physical Chemistry Chemical Physics, 2011, 13, 16689.	2.8	36
314	Unraveling the peculiar modus operandi of a new class of solvatochromic fluorescent molecular rotors by spectroscopic and quantum mechanical methods. Chemical Science, 2013, 4, 2502.	7.4	36
315	An integrated experimental and quantum-chemical investigation on the vibrational spectra of chlorofluoromethane. Journal of Chemical Physics, 2013, 139, 164302.	3.0	36
316	Accurate prediction of bulk properties in hydrogen bonded liquids: amides as case studies. Physical Chemistry Chemical Physics, 2016, 18, 25342-25354.	2.8	36
317	The challenging playground of astrochemistry: an integrated rotational spectroscopy â€“ quantum chemistry strategy. Physical Chemistry Chemical Physics, 2020, 22, 6507-6523.	2.8	36
318	A new general form of molecular force fields. Application to intra- and interresidue interactions in peptides. Journal of the American Chemical Society, 1992, 114, 9085-9093.	13.7	35
319	Structure and ESR Features of Glycine Radical. Journal of the American Chemical Society, 1995, 117, 12618-12624.	13.7	35
320	Structure and Magnetic Properties of Oxoverdazyl Radicals and Biradicals by an Integrated Computational Approach. Journal of Physical Chemistry A, 1999, 103, 4275-4282.	2.5	35
321	Conformational and Spectroscopic Analysis of the Tyrosyl Radical Dipeptide Analogue in the Gas Phase and in Aqueous Solution by a Density Functional/Continuum Solvent Model. Journal of the American Chemical Society, 2002, 124, 11531-11540.	13.7	35
322	Evidence of Variable H-Bond Network for Nitroxide Radicals in Protic Solvents. Journal of Physical Chemistry B, 2006, 110, 16189-16192.	2.6	35
323	On the properties of microsolvated molecules in the ground (S) and excited (S1) states: The anisole-ammonia 1:1 complex. Journal of Chemical Physics, 2007, 127, 144303.	3.0	35
324	Halogen Bonds between 2,2,6,6-Tetramethylpiperidine-N-oxyl Radical and C_xH_yF_zI Species:â€‰ DFT Calculations of Physicochemical Properties and Comparison with Hydrogen Bonded Adducts. Journal of Physical Chemistry A, 2007, 111, 8482-8490.	2.5	35

#	Article	IF	Citations
325	Pulse ENDOR and density functional theory on the peridinin triplet state involved in the photo-protective mechanism in the peridininâ€“chlorophyll aâ€“protein from Amphidinium carterae. Biochimica Et Biophysica Acta - Bioenergetics, 2008, 1777, 295-307.	1.0	35
326	PCM/TD-DFT study of the two lowest excited states of uracil derivatives in solution: The effect of the functional and of the cavity model. Computational and Theoretical Chemistry, 2009, 914, 87-93.	1.5	35
327	An integrated computational protocol for the accurate prediction of EPR and PNMR parameters of aminoxyl radicals in solution. Magnetic Resonance in Chemistry, 2010, 48, S11-S22.	1.9	35
328	Vibronic Coupling Dominates the Electronic Circular Dichroism of the Benzene Chromophore ¹L_b band. Journal of Organic Chemistry, 2013, 78, 7398-7405.	3.2	35
329	Stereoelectronic, Vibrational, and Environmental Contributions to Polarizabilities of Large Molecular Systems: A Feasible Anharmonic Protocol. Journal of Chemical Theory and Computation, 2014, 10, 2456-2464.	5.3	35
330	New Developments of a Multifrequency Virtual Spectrometer: Stereoâ€Electronic, Dynamical, and Environmental Effects on Chiroptical Spectra. Chirality, 2014, 26, 588-600.	2.6	35
331	Rotational and Infrared Spectroscopy of Ethanimine: A Route toward Its Astrophysical and Planetary Detection. Astrophysical Journal, 2018, 855, 123.	4.5	35
332	Conformational behaviour of isomeric bithienyls. An ab initio study. Journal of the Chemical Society Perkin Transactions II, 1986, , 907.	0.9	34
333	Towards linear scaling in continuum solvent models.. Chemical Physics Letters, 1998, 293, 221-229.	2.6	34
334	Tuning of Structural and Magnetic Properties of Nitronyl Nitroxides by the Environment. A Combined Experimental and Computational Study. Journal of Physical Chemistry A, 1999, 103, 3481-3488.	2.5	34
335	Performance of ab initio and DFT PCM methods in calculating vibrational spectra in solution: Formaldehyde in acetonitrile as a test case. Chemical Physics Letters, 2005, 416, 206-211.	2.6	34
336	Free Radical Coupling of o-Semiquinones Uncovered. Journal of the American Chemical Society, 2013, 135, 12142-12149.	13.7	34
337	Vibronic Coupling Investigation to Compute Phosphorescence Spectra of Pt(II) Complexes. Inorganic Chemistry, 2015, 54, 5588-5595.	4.0	34
338	VMS-ROT: A New Module of the Virtual Multifrequency Spectrometer for Simulation, Interpretation, and Fitting of Rotational Spectra. Journal of Chemical Theory and Computation, 2017, 13, 4382-4396.	5.3	34
339	Development and Validation of a Parameter-Free Model Chemistry for the Computation of Reliable Reaction Rates. Journal of Chemical Theory and Computation, 2021, 17, 4913-4928.	5.3	34
340	Experimental and theoretical approach to the electronic structure and the molecular conformation of azabiphenyls. Assymetric bipyridines. Chemical Physics, 1985, 96, 435-445.	1.9	33
341	Interplay of stereo-electronic, environmental, and dynamical effects in determining the EPR parameters of aromatic spin-probes: INDCO as a test case. Physical Chemistry Chemical Physics, 2010, 12, 3741.	2.8	33
342	Validation of Hybrid Density Functional/Hartreeâ€“Fock Approaches for the Study of Homogeneous Catalysis. The Journal of Physical Chemistry, 1996, 100, 2094-2099.	2.9	32

#	Article	IF	Citations
343	Intrinsic and environmental effects in the physico-chemical properties of nitroxides. The case of 2-phenyl-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazol-1-oxyl 3-oxide. Chemical Physics Letters, 1999, 310, 159-165.	2.6	32
344	Conformational analysis of the tyrosine dipeptide analogue in the gas phase and in aqueous solution by a density functional/continuum solvent model. Journal of Computational Chemistry, 2002, 23, 650-661.	3.3	32
345	Ab initiostudy of electron affinity variation induced by organic molecule adsorption on the silicon (001) surface. Physical Review B, 2007, 76, .	3.2	32
346	Ab InitioModeling of CW-ESR Spectra of the Double Spin Labeled Peptide Fmoc-(Aib-Aib-TOAC)2-Aib-OMe in Acetonitrile. Journal of Physical Chemistry B, 2007, 111, 2668-2674.	2.6	32
347	Ab Initio Prediction of the Emission Color in Phosphorescent Iridium(III) Complexes for OLEDs. Journal of Physical Chemistry B, 2008, 112, 13181-13183.	2.6	32
348	Double Cï£¿H Activation of Ethane by Metalâ€Free SO₂^{.+} Radical Cations. Chemistry - A European Journal, 2010, 16, 6234-6242.	3.3	32
349	An Integrated Protocol for the Accurate Calculation of Magnetic Interactions in Organic Magnets. Journal of Chemical Theory and Computation, 2011, 7, 699-706.	5.3	32
350	Barrierless photoisomerisation of the â€œsimplest cyanineâ€: Joining computational and femtosecond optical spectroscopies to trace the full reaction path. Physical Chemistry Chemical Physics, 2012, 14, 13350.	2.8	32
351	Environmental and complexation effects on the structures and spectroscopic signatures of organic pigments relevant to cultural heritage: the case of alizarin and alizarinâ€“Mg(ii)/Al(iii) complexes. Physical Chemistry Chemical Physics, 2014, 16, 2897.	2.8	32
352	Accuracy and Reliability in the Simulation of Vibrational Spectra: A Comprehensive Benchmark of Energies and Intensities Issuing From Generalized Vibrational Perturbation Theory to Second Order (GVPT2). Frontiers in Astronomy and Space Sciences, 2021, 8, .	2.8	32
353	Relative ordering and spacing of n and .pi. levels in isomeric bipyrimidines. A theoretical and gas-phase UV photoelectron spectroscopic study. Journal of the American Chemical Society, 1982, 104, 4571-4578.	13.7	31
354	Chemisorption of atomic and molecular oxygen on the (100) surface of silicon; a theoretical study. Surface Science, 1985, 162, 230-238.	1.9	31
355	A theoretical investigation of potential energy surfaces governing the photochemical tautomerization of 2-pyridone. Chemical Physics Letters, 1994, 226, 399-404.	2.6	31
356	Conformational Behavior and Magnetic Properties of Organic Radicals Derived from Amino Acid Residues. The Dipeptide Analog of Glycine Radical. Journal of the American Chemical Society, 1995, 117, 1083-1089.	13.7	31
357	Understanding Electron Transfer across Negatively-Charged Aib Oligopeptides. Journal of Physical Chemistry B, 2005, 109, 1023-1033.	2.6	31
358	Understanding the photophysical properties of coumarin-based Pluronicâ€“silica (PluS) nanoparticles by means of time-resolved emission spectroscopy and accurate TDDFT/stochastic calculations. Physical Chemistry Chemical Physics, 2013, 15, 12360.	2.8	31
359	A Multifrequency Virtual Spectrometer for Complex Bioâ€Organic Systems: Vibronic and Environmental Effects on the UV/Vis Spectrum of Chlorophyll a. ChemPhysChem, 2014, 15, 3355-3364.	2.1	31
360	Laboratory measurements and astronomical search for cyanomethanimine. Astronomy and Astrophysics, 2018, 609, A121.	5.1	31

#	Article	IF	Citations
361	On the chemisorption of water on the (100) surface of silicon. Surface Science, 1987, 180, 599-604.	1.9	30
362	A theoretical study of proton transfer in [2,2â€²-bipyridyl]-3,3â€²-diol. Chemical Physics Letters, 1995, 241, 1-6.	2.6	30
363	Development and Validation of Effective Computational Strategies for the Study of Metal Nitroxide Complexes. Journal of Physical Chemistry A, 1999, 103, 7676-7685.	2.5	30
364	Conformational Behavior of Macromolecules in Solution. Homopolypeptides of Î±-Aminoisobutyric Acid as Test Cases. Macromolecules, 2001, 34, 7550-7557.	4.8	30
365	Ab initio computation of spectroscopic parameters as a tool for the structural elucidation of organic systems. Computational and Theoretical Chemistry, 2007, 811, 323-335.	1.5	30
366	Magnetic coupling in bis-nitronylnitroxide radicals: The role of aromatic bridges. Journal of Chemical Physics, 2009, 130, 094306.	3.0	30
367	Benzothiopyranoindole-Based Antiproliferative Agents: Synthesis, Cytotoxicity, Nucleic Acids Interaction, and Topoisomerases Inhibition Properties. Journal of Medicinal Chemistry, 2009, 52, 5429-5441.	6.4	30
368	An ultrafast spectroscopic and quantum mechanical investigation of multiple emissions in pushâ€“pull pyridinium derivatives bearing different electron donors. Physical Chemistry Chemical Physics, 2015, 17, 20981-20989.	2.8	30
369	Diving into chemical bonding: An immersive analysis of the electron charge rearrangement through virtual reality. Journal of Computational Chemistry, 2018, 39, 2607-2617.	3.3	30
370	Unsupervised search of low-lying conformers with spectroscopic accuracy: A two-step algorithm rooted into the island model evolutionary algorithm. Journal of Chemical Physics, 2020, 153, 124110.	3.0	30
371	junChS and junChS-F12 Models: Parameter-free Efficient yet Accurate Composite Schemes for Energies and Structures of Noncovalent Complexes. Journal of Chemical Theory and Computation, 2021, 17, 6974-6992.	5.3	30
372	Density Functional Calculations of Isotropic Hyperfine Coupling Constants in .beta.-Ketoenolyl Radicals. The Journal of Physical Chemistry, 1994, 98, 8648-8652.	2.9	29
373	Radiation-induced formation of DNA intrastrand crosslinks between thymine and adenine bases: a theoretical approach. Organic and Biomolecular Chemistry, 2006, 4, 3986.	2.8	29
374	Isotopomeric Conformational Changes in the Anisoleâ‹¯Water Complex:Â New Insights from HR-UV Spectroscopy and Theoretical Studiesâ€. Journal of Physical Chemistry A, 2007, 111, 12363-12371.	2.5	29
375	Vibrational analysis of x-ray absorption fine structure thermal factors by ab initio molecular dynamics: The Zn(II) ion in aqueous solution as a case study. Journal of Chemical Physics, 2011, 134, 074504.	3.0	29
376	Methods for Calculating Partition Functions of Molecules Involving Large Amplitude and/or Anharmonic Motions. Journal of Chemical Theory and Computation, 2016, 12, 1011-1018.	5.3	29
377	Astrochemistry and Astrobiology: Materials Sciencein Wonderland?. International Journal of Molecular Sciences, 2019, 20, 4079.	4.1	29
378	Unbiased Determination of Absolute Configurations by vis-Ã-vis Comparison of Experimental and Simulated Spectra: The Challenging Case of Diplopyrone. Journal of Physical Chemistry B, 2019, 123, 9230-9237.	2.6	29

#	Article	IF	Citations
379	Optimization of highly excited matrix product states with an application to vibrational spectroscopy. Journal of Chemical Physics, 2019, 150, 094113.	3.0	29
380	The cluster approach in the study of atomic and molecular chemisorption on silicon. Surface Science, 1987, 189-190, 106-113.	1.9	28
381	Effective modeling of intrinsic and environmental effects on the structure and electron paramagnetic resonance parameters of nitroxides by an integrated quantum mechanical/molecular mechanics/polarizable continuum model approach. Theoretical Chemistry Accounts, 2000, 104, 273-279.	1.4	28
382	Benchmark calculations for molecules in the gas phase: Stateâ€ofâ€theâ€art coupledâ€cluster computations. International Journal of Quantum Chemistry, 2010, 110, 637-655.	2.0	28
383	Accurate structure, thermodynamics, and spectroscopy of medium-sized radicals by hybrid coupled cluster/density functional theory approaches: The case of phenyl radical. Journal of Chemical Physics, 2013, 138, 234303.	3.0	28
384	Characterization and Fate of Hydrogen-Bonded Free-Radical Intermediates and Their Coupling Products from the Hydrogen Atom Transfer Agent 1,8-Naphthalenediol. ACS Omega, 2018, 3, 3918-3927.	3.5	28
385	A never-ending story in the sky: The secrets of chemical evolution. Physics of Life Reviews, 2020, 32, 59-94.	2.8	28
386	Extending the Applicability of the Semi-experimental Approach by Means of â€œTemplate Moleculeâ€•and â€œLinear Regressionâ€•Models on Top of DFT Computations. Journal of Physical Chemistry A, 2021, 125, 9904-9916.	2.5	28
387	Proton transfer in small model systems: A density functional study. International Journal of Quantum Chemistry, 1995, 56, 697-705.	2.0	27
388	Conformational Behavior and Magnetic Properties of a Nitroxide Amino Acid Derivative in Vacuo and in Aqueous Solution. Journal of Physical Chemistry A, 2003, 107, 6264-6269.	2.5	27
389	Accurate First-Principle Prediction of ²⁹Si and ¹⁷O NMR Parameters in SiO₂ Polymorphs: The Cases of Zeolites Sigma-2 and Ferrierite. Journal of Chemical Theory and Computation, 2008, 4, 2130-2140.	5.3	27
390	First principle simulation of vibrationally resolved <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si127.gif" display="inline" overflow="scroll"><mml:mrow><mml:msup><mml:mrow><mml:mi>A</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msup><mml:mrow><mml:mo>(</mml:mo><mml:mover accent="true"><mml:mrow><mml:mtext>X</mml:mtext></mml:mrow><mml:mrow><mml:mo>Ëœ</mml:mo></mml:mrow></mml:mover><mml:mo>)</mml:mo></mml:mrow></mml:mrow></mml:math> Chemical Physics Letters, 2009, 471, 143-147.	2.6	27
391	Extending the Range of Computational Spectroscopy by QM/MM Approaches: Time-Dependent and Time-Independent Routes. Advances in Quantum Chemistry, 2010, , 17-57.	0.8	27
392	The Proton Affinity and Gasâ€Phase Basicity of Sulfur Dioxide. ChemPhysChem, 2011, 12, 112-115.	2.1	27
393	Oxygen Adsorption on Î²-Quartz Model Surfaces: Some Insights from Density Functional Theory Calculations and Semiclassical Time-Dependent Dynamics. Journal of Physical Chemistry A, 2012, 116, 1975-1983.	2.5	27
394	Ultrasound-induced transformation of fluorescent organic nanoparticles from a molecular rotor into rhomboidal nanocrystals with enhanced emission. Chemical Communications, 2014, 50, 12955-12958.	4.1	27
395	Combining the Fluctuating Charge Method, Non-periodic Boundary Conditions and Meta-dynamics: Aqua Ions as Case Studies. Journal of Chemical Theory and Computation, 2014, 10, 1150-1163.	5.3	27
396	State-of-the-Art Quantum Chemistry Meets Variable Reaction Coordinate Transition State Theory to Solve the Puzzling Case of the H₂S + Cl System. Journal of Chemical Theory and Computation, 2020, 16, 5090-5104.	5.3	27

#	Article	IF	Citations
397	Model Hamiltonians in the study of chemisorption and catalysis. Surface Science, 1985, 152-153, 690-701.	1.9	26
398	Sensitivity of peptide conformation to methods and geometrical parameters. A comparative ab initio and molecular mechanics study of oligomers of .alpha.-aminoisobutyric acid. Macromolecules, 1990, 23, 2038-2044.	4.8	26
399	Role of Hartree-Fock exchange in density functional theory. Chemical Physics Letters, 1994, 230, 189-195.	2.6	26
400	Methyl addition to acetylene and ethylene from a density functional approach. Chemical Physics Letters, 1995, 246, 45-52.	2.6	26
401	Structure and hyperfine parameters of cyclopropyl and bicyclobutyl radicals from postâ€Hartreeâ€“Fock computations. Journal of Chemical Physics, 1996, 104, 2630-2637.	3.0	26
402	Solvent effects on the conformational behavior of model peptides. A comparison between different continuum models. Chemical Physics Letters, 1996, 263, 113-118.	2.6	26
403	Performance of a new hybrid Hartreeâ€“Fock/Kohnâ€“Sham model (B98) in predicting vibrational frequencies, polarisabilities and NMR chemical shifts. Chemical Physics Letters, 1999, 311, 69-76.	2.6	26
404	First-principle molecular dynamics of the Berry pseudorotation: Insights on 19F NMR in SF4. Journal of Chemical Physics, 2004, 120, 9167-9174.	3.0	26
405	Unraveling the interplay of different contributions to the stability of the quinhydrone dimer. RSC Advances, 2014, 4, 876-885.	3.6	26
406	Extracting the transversity distributions from single-hadron and dihadron production. Physical Review D, 2015, 91, .	4.7	26
407	On the competition between weak O Hâ‹¯F and C Hâ‹¯F hydrogen bonds, in cooperation with C Hâ‹¯O contacts, in the difluoromethane â€“ tert-butyl alcohol cluster. Journal of Molecular Spectroscopy, 2017, 337, 90-95.	1.2	26
408	An ab initio study of Cu-based delafossites as an alternative to nickel oxide in photocathodes: effects of Mg-doping and surface electronic features. Physical Chemistry Chemical Physics, 2018, 20, 14082-14089.	2.8	26
409	Time-Dependent Formulation of Resonance Raman Optical Activity Spectroscopy. Journal of Chemical Theory and Computation, 2018, 14, 6370-6390.	5.3	26
410	Toward Fully Unsupervised Anharmonic Computations Complementing Experiment for Robust and Reliable Assignment and Interpretation of IR and VCD Spectra from Mid-IR to NIR: The Case of 2,3-Butanediol and trans-1,2-Cyclohexanediol. Journal of Physical Chemistry A, 2020, 124, 1011-1024.	2.5	26
411	Theoretical approach to fluorine substitution in X2NO and X2CN free radicals. Comparison between ab initio UHF and RHF + perturbation treatments. Chemical Physics, 1983, 76, 385-396.	1.9	25
412	Structural and electronic origin of the conformational behavior of biphenyl-like Î±-diimine ligands. A theoretical study. Canadian Journal of Chemistry, 1988, 66, 1313-1317.	1.1	25
413	Vibro-rotational analysis of Si2C from an ab initio potential energy surface. A comparison between perturbative and variational methods. Journal of Molecular Spectroscopy, 1992, 154, 252-264.	1.2	25
414	Improving performance of polarizable continuum model for study of large molecules in solution. Journal of Computational Chemistry, 1999, 20, 1186-1198.	3.3	25

#	Article	IF	Citations
415	Effective generation of molecular cavities in polarizable continuum model by DefPol procedure. Journal of Computational Chemistry, 1999, 20, 1693-1701.	3.3	25
416	A first-principle study of the adsorption of 1-amino-3-cyclopentene on the (100) silicon surface. Journal of Chemical Physics, 2005, 122, 184714.	3.0	25
417	Magnetic Interactions in Phenyl-Bridged Nitroxide Diradicals: Conformational Effects by Multireference and Broken Symmetry DFT Approaches. Journal of Physical Chemistry A, 2009, 113, 15150-15155.	2.5	25
418	Magnetic Properties of Nitroxide Spin Probes: Reliable Account of Molecular Motions and Nonspecific Solvent Effects by Time-Dependent and Time-Independent Approaches. Journal of Physical Chemistry B, 2010, 114, 11509-11514.	2.6	25
419	Origin invariance in vibrational resonance Raman optical activity. Journal of Chemical Physics, 2015, 142, 174101.	3.0	25
420	On the relation between carbonyl stretching frequencies and the donor power of chelating diphosphines in nickel dicarbonyl complexes. Physical Chemistry Chemical Physics, 2017, 19, 9028-9038.	2.8	25
421	Transition-metal tetrahydroborate complexes as catalysts. 1. Nonempirical determination of static, dynamic, and chemical properties of the model compounds sodium tetrahydroborate and aluminum borate (AlH2BH4). Inorganic Chemistry, 1981, 20, 1687-1691.	4.0	24
422	Conformational behaviour of phenylpyrimidines. a quantum mechanical study. Tetrahedron, 1985, 41, 1915-1918.	1.9	24
423	Nonempirical cluster-model study of the chemisorption of atomic hydrogen on the (111) surface of diamondlike crystals. Physical Review B, 1986, 34, 7203-7208.	3.2	24
424	Toward a general protocol for the study of static and dynamic properties of hydrogen-bonded systems. International Journal of Quantum Chemistry, 1997, 61, 429-442.	2.0	24
425	Comparative Static and Dynamic Study of a Prototype SN2 Reaction. Journal of Chemical Theory and Computation, 2006, 2, 1220-1227.	5.3	24
426	Cyclic Structural Motifs in 5,6-Dihydroxyindole Polymerization Uncovered: Biomimetic Modular Buildup of a Unique Five-Membered Macrocycle. Organic Letters, 2010, 12, 3250-3253.	4.6	24
427	Integrated experimental and computational spectroscopy study on Ï€-stacking interaction: the anisole dimer. Physical Chemistry Chemical Physics, 2010, 12, 13547.	2.8	24
428	Structureâ€“Properties Relationships in Triplet Ground State Organic Diradicals: A Computational Study. Journal of Chemical Theory and Computation, 2013, 9, 300-307.	5.3	24
429	Correct Modeling of Cisplatin: a Paradigmatic Case. Angewandte Chemie - International Edition, 2017, 56, 13838-13841.	13.8	24
430	Exploiting coordination geometry to selectively predict the Ïƒ-donor and Ï€-acceptor abilities of ligands: a back-and-forth journey between electronic properties and spectroscopy. Chemical Communications, 2018, 54, 2397-2400.	4.1	24
431	A twist on the reaction of the CN radical with methylamine in the interstellar medium: new hints from a state-of-the-art quantum-chemical study. Monthly Notices of the Royal Astronomical Society, 2020, 496, 4298-4310.	4.4	24
432	Molecular Perception for Visualization and Computation: The Proxima Library. Journal of Chemical Information and Modeling, 2020, 60, 2668-2672.	5.4	24

#	Article	IF	Citations
433	Methanimine as a Key Precursor of Imines in the Interstellar Medium: The Case of Propargylimine. Astrophysical Journal Letters, 2020, 903, L35.	8.3	24
434	Theoretical investigation of the EPR spectrum of the cyclopropyl radical. Chemical Physics Letters, 1993, 205, 324-330.	2.6	23
435	Theoretical Characterization of the Mechanism of Hgâ^'C Bond Cleavage by Halogenic Acids. Organometallics, 1996, 15, 1465-1469.	2.3	23
436	Computation of Spectroscopic Parameters in vacuo and in Condensed Phases by Methods based on the Density Functional Theory. QSAR and Combinatorial Science, 2002, 21, 105-118.	1.2	23
437	Building cavities in a fluid of spherical or rod-like particles: A contribution to the solvation free energy in isotropic and anisotropic polarizable continuum model. Journal of Computational Chemistry, 2005, 26, 1096-1105.	3.3	23
438	The effects of ferulic acid on Î²-amyloid fibrillar structures investigated through experimental and computational techniques. Biochimica Et Biophysica Acta - General Subjects, 2013, 1830, 2924-2937.	2.4	23
439	A benchmark study of electronic excitation energies, transition moments, and excited-state energy gradients on the nicotine molecule. Journal of Chemical Physics, 2014, 141, 224114.	3.0	23
440	Acidâ€"Base Strength and Acidochromism of Some Dimethylaminoâ€"Azinium Iodides. An Integrated Experimental and Theoretical Study. Journal of Physical Chemistry A, 2015, 119, 323-333.	2.5	23
441	Colourless p -phenylene-spaced bis-azoles for luminescent concentrators. Dyes and Pigments, 2016, 134, 118-128.	3.7	23
442	Effective Inclusion of Mechanical and Electrical Anharmonicity in Excited Electronic States: VPT2-TDDFT Route. Journal of Chemical Theory and Computation, 2017, 13, 2789-2803.	5.3	23
443	Potential-Energy Surfaces for Ring-Puckering Motions of Flexible Cyclic Molecules through Cremerâ€"Pople Coordinates: Computation, Analysis, and Fitting. Journal of Chemical Theory and Computation, 2019, 15, 4280-4294.	5.3	23
444	DFT meets the segmented polarization consistent basis sets: Performances in the computation of molecular structures, rotational and vibrational spectroscopic properties. Journal of Molecular Structure, 2020, 1208, 127886.	3.6	23
445	Direct catalytic effect and fine modulation of solvent in the keto-enol isomerization of amides. Computational and Theoretical Chemistry, 1995, 330, 325-333.	1.5	22
446	Structures, hyperfine parameters, and inversion barriers of cyclopropyl and oxiranyl radicals. Journal of Chemical Physics, 1996, 105, 3168-3174.	3.0	22
447	The mechanism of spin polarization in aromatic free radicals. Theoretical Chemistry Accounts, 2000, 104, 207-209.	1.4	22
448	Interplay of Intrinsic and Environmental Effects on the Magnetic Properties of Free Radicals Issuing from H-Atom Addition to Cytosine. Journal of the American Chemical Society, 2001, 123, 7113-7117.	13.7	22
449	The cos2Ï† asymmetry of Drellâ€"Yan and J/Ïˆ production in unpolarized ppÌ„ scattering. European Physical Journal C, 2007, 49, 967-971.	3.9	22
450	Chemistry of Nitrated Lipids: Remarkable Instability of 9-Nitrolinoleic Acid in Neutral Aqueous Medium and a Novel Nitronitrate Ester Product by Concurrent Autoxidation/Nitric Oxide-Release Pathways. Journal of Organic Chemistry, 2008, 73, 7517-7525.	3.2	22

#	Article	IF	Citations
451	Development of a Virtual Spectrometer for Chiroptical Spectroscopies: The Case of Nicotine. Chirality, 2013, 25, 701-708.	2.6	22
452	Computational Chemistry Meets Experiments for Explaining the Behavior of Bibenzyl: A Thermochemical and Spectroscopic (Infrared, Raman, and NMR) Investigation. Journal of Chemical Theory and Computation, 2014, 10, 5586-5592.	5.3	22
453	The Unexplored World of Cycloalkeneâ€“Water Complexes: Primary and Assisting Interactions Unraveled by Experimental and Computational Spectroscopy. Angewandte Chemie - International Edition, 2019, 58, 13935-13941.	13.8	22
454	An ab initio reinvestigation of the geometric and electronic structure of boron trioxide. Computational and Theoretical Chemistry, 1981, 76, 29-35.	1.5	21
455	A molecular dynamics study of associations in solution. an NPT simulation of the urea dimer in water. Chemical Physics Letters, 1987, 140, 401-405.	2.6	21
456	Medium-dependent competitive pathways in the reactions of polyunsaturated fatty acids with nitric oxide in the presence of oxygen. Structural characterisation of nitration products and a theoretical insight. Tetrahedron, 1999, 55, 9297-9308.	1.9	21
457	Toward an effective yet reliable many-body computation of magnetic couplings in bisnitronyl nitroxide biradicals. Journal of Chemical Physics, 2008, 128, 174303.	3.0	21
458	The electronic structure of the lutein triplet state in plant light-harvesting complex II. Physical Chemistry Chemical Physics, 2012, 14, 12238.	2.8	21
459	Environmental and dynamical effects on the optical properties of molecular systems by time-independent and time-dependent approaches: Coumarin derivatives as test cases. Computational and Theoretical Chemistry, 2014, 1037, 35-48.	2.5	21
460	EXPLORING A CHEMICAL ROUTE FOR THE FORMATION OF STABLE ANIONS OF POLYYNES [C_nH^{â^'} (nÂ=Â2, 4)] IN MOLECULAR CLOUDS. Astrophysical Journal, 2016, 830, 2.	4.5	21
461	Models of Aged Magnesiumâ€“Silicateâ€“Hydrate Cements Based on the Lizardite and Talc Crystals: A Periodic DFT-GIPAW Investigation. Journal of Physical Chemistry C, 2017, 121, 7319-7330.	3.1	21
462	Two-level stochastic search of low-energy conformers for molecular spectroscopy: implementation and validation of MM and QM models. Physical Chemistry Chemical Physics, 2019, 21, 19921-19934.	2.8	21
463	Chemical promenades: Exploring potentialâ€energy surfaces with immersive virtual reality. Journal of Computational Chemistry, 2020, 41, 1310-1323.	3.3	21
464	Formation of Phosphorus Monoxide (PO) in the Interstellar Medium: Insights from Quantum-chemical and Kinetic Calculations. Astrophysical Journal, 2021, 922, 169.	4.5	21
465	Mapping the many-electron generalised spin-exchange Hamiltonian to accurate post-HF calculations. Chemical Physics, 2005, 309, 133-141.	1.9	20
466	A Combined Theoretical and Experimental Approach to Determining Order Parameters of Solutes in Liquid Crystals from13C NMR Data. Journal of Physical Chemistry B, 2005, 109, 2584-2590.	2.6	20
467	Microsolvation of the Zn(II) ion in aqueous solution: A hybrid QM/MM MD approach using non-periodic boundary conditions. Chemical Physics Letters, 2008, 451, 53-57.	2.6	20
468	On the interpretation of continuous wave electron spin resonance spectra of tempo-palmitate in 5-cyanobiphenyl. Journal of Chemical Physics, 2008, 128, 024501.	3.0	20

#	Article	IF	Citations
469	Accurate yet feasible post-Hartreeâ€“Fock computation of magnetic interactions in large biradicals through a combined variational/perturbative approach: Setup and validation. Journal of Chemical Physics, 2009, 131, 224103.	3.0	20
470	Simulation of electron spin resonance spectroscopy in diverse environments: An integrated approach. Computer Physics Communications, 2009, 180, 2680-2697.	7.5	20
471	Computational Investigation on the Spectroscopic Properties of Thiophene Based Europium Î²-Diketonate Complexes. Journal of Chemical Theory and Computation, 2014, 10, 767-777.	5.3	20
472	Hydration Shell of Antifreeze Proteins: Unveiling the Role of Non-Ice-Binding Surfaces. Journal of Physical Chemistry B, 2019, 123, 6474-6480.	2.6	20
473	The Role of State-of-the-Art Quantum-Chemical Calculations in Astrochemistry: Formation Route and Spectroscopy of Ethanimine as a Paradigmatic Case. Molecules, 2020, 25, 2873.	3.8	20
474	A non-empirical and HAM/3 study of the geometry, conformational behaviour and electronic structure of isomeric vinylpyridines. Computational and Theoretical Chemistry, 1984, 108, 35-43.	1.5	19
475	Conformational behavior of azabiphenyls. International Journal of Quantum Chemistry, 1986, 29, 541-551.	2.0	19
476	Structure and EPR parameters of CuC2H2 from a density functional approach. Chemical Physics Letters, 1995, 237, 189-194.	2.6	19
477	Theoretical Study of the Electronic Structure and of the Mercury-Carbon Bonding of Methylmercury(II) Compounds. The Journal of Physical Chemistry, 1995, 99, 12743-12750.	2.9	19
478	Substituent Effects in the Hetero-Dielsâ˜Alder Reaction of Thiocarbonyl Compounds with Butadiene. Journal of Organic Chemistry, 1996, 61, 5121-5129.	3.2	19
479	Ring-Opening Reaction of Cyclobutene Radical Cation: Effect of Solvent on Competing Pathways. Journal of Physical Chemistry A, 1999, 103, 217-219.	2.5	19
480	Singletâ€“triplet energy gap of a diarylnitroxide diradical by an accurate many-body perturbative approach. Physical Chemistry Chemical Physics, 2011, 13, 4709.	2.8	19
481	Reassessment of the Thermodynamic, Kinetic, and Spectroscopic Features of Cyanomethanimine Derivatives: A Full Anharmonic Perturbative Treatment. Journal of Chemical Theory and Computation, 2015, 11, 1165-1171.	5.3	19
482	Anharmonicity Effects in IR Spectra of [Re(X)(CO)₃(Î±-diimine)] (Î±-diimine = 2,2â€²-bipyridine or) Tj ETQq0 0 0 rgBT /Overl Journal of Physical Chemistry A, 2015, 119, 10137-10146.	2.5	19
483	Photoexcitation and relaxation kinetics of molecular systems in solution: towards a complete in silico model. Physical Chemistry Chemical Physics, 2016, 18, 28919-28931.	2.8	19
484	From ascorbic acid to furan derivatives: the gas phase acid catalyzed degradation of vitamin C. Physical Chemistry Chemical Physics, 2018, 20, 17132-17140.	2.8	19
485	Ferrocenes with simple chiral substituents: an in-depth theoretical and experimental VCD and ECD study. Physical Chemistry Chemical Physics, 2019, 21, 9419-9432.	2.8	19
486	Exploring the Maze of Cycloserine Conformers in the Gas Phase Guided by Microwave Spectroscopy and Quantum Chemistry. Journal of Physical Chemistry A, 2021, 125, 2121-2129.	2.5	19

#	Article	IF	Citations
487	The challenge of non-covalent interactions: theory meets experiment for reconciling accuracy and interpretation. Journal of Physics Condensed Matter, 2020, 32, 343002.	1.8	19
488	Ab initio mechanistic studies of radical reactions. Addition of methyl radical to acetylene and ethylene. Chemical Physics Letters, 1985, 118, 573-579.	2.6	18
489	Protomeric equilibria in the ground and excited states of 2-pyridone. A semiempirical study including solvent effects. Journal of the Chemical Society Perkin Transactions II, 1993, , 697.	0.9	18
490	Theoretical Study of a New Building Block for Organic Conductors:Â Tetrathiapentalene and Its Radical Cation. Journal of Physical Chemistry B, 1999, 103, 6863-6869.	2.6	18
491	A density functional study of thorium tetrahalides. Physical Chemistry Chemical Physics, 2000, 2, 3111-3114.	2.8	18
492	New computational strategies for the quantum mechanical study of biological systems in condensed phases. Theoretical and Computational Chemistry, 2001, , 467-538.	0.4	18
493	Solvent Effects on the UV (n â†' Ï€*) and NMR (17O) Spectra of Acetone in Aqueous Solution: Development and Validation of a Modified AMBER Force Field for an Integrated MD/DFT/PCM Approach. Theoretical Chemistry Accounts, 2006, 116, 456-461.	1.4	18
494	Thermodynamics of protonation of polymeric bases whose repeating units behave independently. Journal of Polymer Science, Polymer Symposia, 1981, 69, 49-66.	0.1	18
495	Three-dimensional diabatic models for the Ï€Ï€*Âσ†' nÏ€* excited-state decay of uracil derivatives in solution. Theoretical Chemistry Accounts, 2009, 123, 273-286.	1.4	18
496	Molecular Dynamics Simulations of the Self-Assembly of Tetraphenylporphyrin-Based Monolayers and Bilayers at a Silver Interface. Journal of Physical Chemistry C, 2011, 115, 18434-18444.	3.1	18
497	Computational tools for the interpretation of electron spin resonance spectra in solution. Molecular Physics, 2013, 111, 2746-2756.	1.7	18
498	Conformational Effects on the Magnetic Properties of an Organic Diradical: A Computational Study. Journal of Chemical Theory and Computation, 2013, 9, 1958-1963.	5.3	18
499	Accurate yet feasible computations of resonance Raman spectra for metal complexes in solution: [Ru(bpy)₃]²⁺ as a case study. Dalton Transactions, 2014, 43, 17610-17614.	3.3	18
500	Fine-tuning of atomic point charges: Classical simulations of pyridine in different environments. Chemical Physics Letters, 2017, 677, 120-126.	2.6	18
501	A Modular Implementation for the Simulation of 1D and 2D Solid-State NMR Spectra of Quadrupolar Nuclei in the Virtual Multifrequency Spectrometerâ€"Draw Graphical Interface. Journal of Chemical Theory and Computation, 2017, 13, 2215-2229.	5.3	18
502	Binding of Nucleic Acid Components to the Serpentinite-Hosted Hydrothermal Mineral Brucite. Astrobiology, 2018, 18, 989-1007.	3.0	18
503	Reinvestigation of the Deceptively Simple Reaction of Toluene with OH and the Fate of the Benzyl Radical: The â€œHiddenâ€•Routes to Cresols and Benzaldehyde. Journal of Physical Chemistry A, 2020, 124, 5917-5930.	2.5	18
504	Insoluble organic matter in chondrites: Archetypal melanin-like PAH-based multifunctionality at the origin of life?. Physics of Life Reviews, 2021, 37, 65-93.	2.8	18

#	Article	IF	Citations
505	Theoretical analysis of conduction in acid and base solutions. The Journal of Physical Chemistry, 1982, 86, 4436-4446.	2.9	17
506	Surface relaxation and reconstruction in diamond-like crystals. Solid State Communications, 1984, 49, 925-928.	1.9	17
507	Cluster model study of the chemisorption of atomic hydrogen on the basal plane of graphite. Surface Science, 1987, 189-190, 185-189.	1.9	17
508	Use of molecular symmetry in the computation of solvation energies and their analytical derivatives by the polarizable continuum model. Chemical Physics Letters, 1999, 301, 263-269.	2.6	17
509	Disordered Chain Conformations of Poly(tetrafluoroethylene) in the High-Temperature Crystalline Form I. Macromolecules, 2004, 37, 9473-9480.	4.8	17
510	Structural, thermodynamic, and magnetic properties of adducts between TEMPO radical and alcohols in solution: New insights from DFT and discreteâ€“continuum solvent models. Chemical Physics Letters, 2006, 419, 106-110.	2.6	17
511	A polarizable continuum approach for the study of heterogeneous dielectric environments. Journal of Chemical Physics, 2006, 124, 184103.	3.0	17
512	The role of accurate quantum mechanical computations in the assignment of vibrational spectra for unstable free radicals: H2CN and F2CN as test cases. Chemical Physics Letters, 2009, 467, 276-280.	2.6	17
513	An integrated computational tool to model the broadening of the absorption bands of flexible dyes in solution: cationic chromophores as test cases. Physical Chemistry Chemical Physics, 2014, 16, 26963-26973.	2.8	17
514	Vibrationally resolved NEXAFS at C and N K-edges of pyridine, 2-fluoropyridine and 2,6-difluoropyridine: A combined experimental and theoretical assessment. Journal of Chemical Physics, 2015, 143, 204102.	3.0	17
515	Accurate Infrared (IR) Spectra for Molecules Containing the Câ‰¡N Moiety by Anharmonic Computations with the Double Hybrid B2PLYP Density Functional. Journal of Chemical Theory and Computation, 2015, 11, 4364-4369.	5.3	17
516	Virtual Eyes Designed for Quantitative Spectroscopy of Inorganic Complexes: Vibronic Signatures in the Phosphorescence Spectra of Terpyridine Derivatives. Journal of Physical Chemistry B, 2015, 119, 7253-7257.	2.6	17
517	Correction to Semi-Experimental Equilibrium Structure Determinations by Employing B3LYP/SNSD Anharmonic Force Fields: Validation and Application to Semirigid Organic Molecules. Journal of Physical Chemistry A, 2016, 120, 3754-3754.	2.5	17
518	Noncovalent Interactions in the Catechol Dimer. Biomimetics, 2017, 2, 18.	3.3	17
519	Tyrosine absorption spectroscopy: Backbone protonation effects on the side chain electronic properties. Journal of Computational Chemistry, 2018, 39, 1747-1756.	3.3	17
520	State-of-the-art computation of the rotational and IR spectra of the methyl-cyclopropyl cation: hints on its detection in space. Physical Chemistry Chemical Physics, 2019, 21, 3431-3439.	2.8	17
521	Assessment of Multi-Scale Approaches for Computing UVâ€“Vis Spectra in Condensed Phases: Toward an Effective yet Reliable Integration of Variational and Perturbative QM/MM Approaches. Journal of Chemical Theory and Computation, 2019, 15, 3170-3184.	5.3	17
522	The ONIOM/PMM Model for Effective Yet Accurate Simulation of Optical and Chiroptical Spectra in Solution: Camphorquinone in Methanol as a Case Study. Journal of Chemical Theory and Computation, 2020, 16, 3294-3306.	5.3	17

#	Article	IF	Citations
523	Integration of theory, simulation, artificial intelligence and virtual reality: a four-pillar approach for reconciling accuracy and interpretability in computational spectroscopy. Physical Chemistry Chemical Physics, 2021, 23, 17079-17096.	2.8	17
524	Structural versatility of peptides from CÎ±,Î±-disubstituted glycines. Preferred conformation of the CÎ±,Î±-dibenzylglycine residue. Journal of the Chemical Society Perkin Transactions II, 1990, , 1481-1487.	0.9	16
525	Modulation of intramolecular proton transfer by electronic excitation and environment: 2-Pyridone as a case study. Journal of Computational Chemistry, 1994, 15, 395-404.	3.3	16
526	A theoretical study of the competition between ethylene insertion and chain transfer in cationic aluminum systems. Chemical Physics Letters, 2000, 329, 99-105.	2.6	16
527	Observed and calculated1H- and13C-NMR chemical shifts of substituted 5H-pyrido[3,2-a]- and 5H-pyrido[2,3-a]phenoxazin-5-ones and of some 3H-phenoxazin-3-one derivatives. Organic and Biomolecular Chemistry, 2004, 2, 1577-1581.	2.8	16
528	Molecular dynamics simulations in a NpT ensemble using non-periodic boundary conditions. Chemical Physics Letters, 2009, 483, 177-181.	2.6	16
529	Sensors for DNA detection: theoretical investigation of the conformational properties of immobilized single-strand DNA. Physical Chemistry Chemical Physics, 2009, 11, 10644.	2.8	16
530	Silicon Nanocrystal Functionalization: Analytic Fitting of DFTB Parameters. Journal of Chemical Theory and Computation, 2011, 7, 713-719.	5.3	16
531	Towards the SMART workflow system for computational spectroscopy. Physical Chemistry Chemical Physics, 2018, 20, 26034-26052.	2.8	16
532	Solid State Photochemistry of Hydroxylated Naphthalenes on Minerals: Probing Polycyclic Aromatic Hydrocarbon Transformation Pathways under Astrochemically-Relevant Conditions. ACS Earth and Space Chemistry, 2018, 2, 977-1000.	2.7	16
533	The Quest for a Plausible Formation Route of Formyl Cyanide in the Interstellar Medium: a State-of-the-art Quantum-chemical and Kinetic Approach. Astrophysical Journal, 2020, 900, 85.	4.5	16
534	Accurate Quantum Chemical Spectroscopic Characterization of Glycolic Acid: A Route Toward its Astrophysical Detection. Journal of Physical Chemistry A, 2022, 126, 2373-2387.	2.5	16
535	Theoretical study of oxygen chemisorption on (111) and (100) silicon surfaces. Physics Letters, Section A: General, Atomic and Solid State Physics, 1985, 113, 321-324.	2.1	15
536	Shadowing in deuterium and the small-x limit of and F2p. Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics, 1994, 321, 137-139.	4.1	15
537	Towards an effective computational tool for the study of radiation-induced lesions of DNA bases. Chemical Physics Letters, 1999, 301, 255-262.	2.6	15
538	Modeling Polymerization Reactions at Aluminum-Based Catalysts:Â Is DFT a Reliable Computational Tool?. Journal of Physical Chemistry A, 2001, 105, 9014-9023.	2.5	15
539	A Parameter-Free Quantum-Mechanical Approach for Calculating Electron-Transfer Rates for Large Systems in Solution. ChemPhysChem, 2006, 7, 1211-1214.	2.1	15
540	Calculated spectroscopic and electric properties of the alkali metal-ammonia complexes from Knâ€“NH3 to Frnâ€“NH3 (n=0,+1). Journal of Chemical Physics, 2007, 127, 104313.	3.0	15

#	Article	IF	Citations
541	Integrated Approach for Modeling the Emission Fluorescence of 4-(N,N-Dimethylamino)benzonitrile in Polar Environments. Journal of Physical Chemistry B, 2008, 112, 8106-8113.	2.6	15
542	An improved AMBER force field for Î±,Î±-dialkylated peptides: intrinsic and solvent-induced conformational preferences of model systems. Physical Chemistry Chemical Physics, 2013, 15, 17395.	2.8	15
543	Interaction of collagen with chlorosulphonated paraffin tanning agents: Fourier transform infrared spectroscopic analysis and molecular dynamics simulations. Physical Chemistry Chemical Physics, 2013, 15, 14736.	2.8	15
544	ACCURATE SPECTROSCOPIC CHARACTERIZATION OF PROTONATED OXIRANE: A POTENTIAL PREBIOTIC SPECIES IN TITAN'S ATMOSPHERE. Astrophysical Journal, 2014, 792, 118.	4.5	15
545	Flexible and Comprehensive Implementation of MD-PMM Approach in a General and Robust Code. Journal of Chemical Theory and Computation, 2017, 13, 5506-5514.	5.3	15
546	Direct extraction of the Sivers distributions from spin asymmetries in pion and kaon leptoproduction. Physical Review D, 2017, 95, .	4.7	15
547	Computational simulation of vibrationally resolved spectra for spinâ€forbidden transitions. Chirality, 2018, 30, 850-865.	2.6	15
548	Molecular synthons for accurate structural determinations: the equilibrium geometry of 1-chloro-1-fluoroethene. Physical Chemistry Chemical Physics, 2019, 21, 3615-3625.	2.8	15
549	General Perturb-Then-Diagonalize Model for the Vibrational Frequencies and Intensities of Molecules Belonging to Abelian and Non-Abelian Symmetry Groups. Journal of Chemical Theory and Computation, 2021, 17, 4332-4358.	5.3	15
550	Stacked but not Stuck: Unveiling the Role of Ï€â†'Ï€* Interactions with the Help of the Benzofuranâ€“Formaldehyde Complex. Angewandte Chemie - International Edition, 2022, 61, .	13.8	15
551	Vibrational spectra of difluorosilane from a hybrid ab initio and DFT quartic force field. Chemical Physics Letters, 2005, 415, 25-29.	2.6	14
552	Modified virtual orbitals for CI calculations of energy splitting in organic diradicals. Physical Chemistry Chemical Physics, 2009, 11, 3854.	2.8	14
553	Extension of the AMBER force field to cyclic Î±,Î± dialkylated peptides. Physical Chemistry Chemical Physics, 2012, 14, 15308.	2.8	14
554	Red-Hair-Inspired Chromogenic System Based on a Proton-Switched Dehydrogenative Free-Radical Coupling. Organic Letters, 2013, 15, 4944-4947.	4.6	14
555	The Borderline between Reactivity and Preâ€reactivity of Binary Mixtures of Gaseous Carboxylic Acids and Alcohols. Angewandte Chemie - International Edition, 2017, 56, 3872-3875.	13.8	14
556	Theory meets experiment for elucidating the structure and stability of non-covalent complexes: waterâ€“amine interaction as a proof of concept. Physical Chemistry Chemical Physics, 2020, 22, 5024-5032.	2.8	14
557	Rich Collection of n-Propylamine and Isopropylamine Conformers: Rotational Fingerprints and State-of-the-Art Quantum Chemical Investigation. Journal of Physical Chemistry A, 2020, 124, 1372-1381.	2.5	14
558	1,2-Disubstituted Planar Chiral Ferrocene Derivatives from Sulfonamide-Directed ortho-Lithiation: Synthesis, Absolute Configuration, and Chiroptical Properties. Organometallics, 2021, 40, 578-590.	2.3	14

#	Article	IF	Citations
559	Looking for the Elusive Imine Tautomer of Creatinine: Different States of Aggregation Studied by Quantum Chemistry and Molecular Spectroscopy. ChemPlusChem, 2021, 86, 1374-1386.	2.8	14
560	Gas-phase identification of (Z)-1,2-ethenediol, a key prebiotic intermediate in the formose reaction. Chemical Communications, 2022, 58, 2750-2753.	4.1	14
561	A rationalization of the enthalpy of protonation of polyamines. Journal of Solution Chemistry, 1979, 8, 427-438.	1.2	13
562	Ab initio pseudopotential study of the fluxional behavior in tetrahydroborate complexes. Many-body contributions to the energy barriers of NaBH4, AlH2BH4, and GaH2BH4. Journal of Computational Chemistry, 1988, 9, 518-521.	3.3	13
563	Comparison between post-Hartree-Fock and DFT methods for the study of strength and mechanism of cleavage of Hg(SINGLE BOND)C bond. International Journal of Quantum Chemistry, 1997, 61, 361-367.	2.0	13
564	Nitration versus Nitrosation Chemistry of Menthofuran:â€‰ Remarkable Fragmentation and Dimerization Pathways and Expeditious Entry into Dehydromenthofurolactone. Journal of Organic Chemistry, 2007, 72, 10123-10129.	3.2	13
565	Theoretical Study of the X2NO Systems (X = F, Cl, Br, I): Effects of Halogen Substitution on Structural and Spectroscopic Properties. Journal of Chemical Theory and Computation, 2009, 5, 2378-2387.	5.3	13
566	Timeâ€dependent and timeâ€independent approaches for the computation of absorption spectra of Uracil derivatives in solution. International Journal of Quantum Chemistry, 2010, 110, 624-636.	2.0	13
567	Simulating DNA Hybridization on an Amine-Functionalized Silicon Substrate. Journal of Physical Chemistry B, 2010, 114, 8341-8349.	2.6	13
568	Neutral molecular shuttle in acetonitrile dilute solution investigated by molecular dynamics and density functional theory. Computational and Theoretical Chemistry, 2012, 985, 53-61.	2.5	13
569	Synthesis and Optical Properties of Imidazoleâ€Based Fluorophores having High Quantum Yields. ChemPlusChem, 2014, 79, 366-370.	2.8	13
570	Phenomenological analysis of azimuthal asymmetries in unpolarized semi-inclusive deep inelastic scattering. Physical Review D, 2015, 91, .	4.7	13
571	Organic solvent simulations under non-periodic boundary conditions: A library of effective potentials for the GLOB model. Chemical Physics Letters, 2015, 625, 186-192.	2.6	13
572	Toward the design of alkynylimidazole fluorophores: computational and experimental characterization of spectroscopic features in solution and in poly(methyl methacrylate). Physical Chemistry Chemical Physics, 2015, 17, 26710-26723.	2.8	13
573	Tuning dispersion correction in DFT-D2 for metal-molecule interactions: A tailored reparameterization strategy for the adsorption of aromatic systems on Ag(1â€¯1â€¯1). Chemical Physics Letters, 2018, 693, 28-33.	2.6	13
574	Measurement of P-weighted Sivers asymmetries in leptoproduction of hadrons. Nuclear Physics B, 2019, 940, 34-53.	2.5	13
575	Exploring the Maze of C₂N₂H₅ Radicals and Their Fragments in the Interstellar Medium with the Help of Quantum-Chemical Computations. ACS Earth and Space Chemistry, 2020, 4, 774-782.	2.7	13
576	Unveiling Bifunctional Hydrogen Bonding with the Help of Quantum Chemistry: The Imidazole-Water Adduct as Test Case. Journal of Physical Chemistry A, 2021, 125, 2989-2998.	2.5	13

#	Article	IF	Citations
577	Structures and relative stabilities of [C2H6N]+ ions: A non-empirical and MNDO study. Computational and Theoretical Chemistry, 1985, 124, 319-324.	1.5	12
578	On the interaction of halogen atoms with (111) and (100) surfaces of silicon. Solid State Communications, 1986, 59, 433-436.	1.9	12
579	Applications of density functional theory approaching chemical accuracy to the study of typical carbon-carbon and carbon-hydrogen bonds. Computational and Theoretical Chemistry, 1996, 369, 29-37.	1.5	12
580	Toward an effective and reliable representation of solvent effects in the study of biochemical systems. International Journal of Quantum Chemistry, 1999, 73, 219-227.	2.0	12
581	Hydrogen-bonding between the hydrogen peroxide molecule and the hydroperoxy radical (H2O2â€“HO2): the global minimum. Chemical Physics Letters, 2004, 391, 134-137.	2.6	12
582	A discrete/continuum QM/MM MD study of the triplet state of acetone in aqueous solution. Chemical Physics Letters, 2008, 453, 202-206.	2.6	12
583	Ï€-Electron Manipulation of the 5,6-Dihydroxyindole/Quinone System by 3-Alkynylation: Mild Acid-Mediated Entry to (Cross)-Conjugated Scaffolds and Paradigms for Medium-Tunable Chromophores. Journal of Organic Chemistry, 2011, 76, 4457-4466.	3.2	12
584	Tuning of NMR and EPR parameters by vibrational averaging and environmental effects: an integrated computational approach. Molecular Physics, 2013, 111, 1345-1354.	1.7	12
585	Computational study of the DPAP molecular rotor in various environments: from force field development to molecular dynamics simulations and spectroscopic calculations. Physical Chemistry Chemical Physics, 2017, 19, 30590-30602.	2.8	12
586	Encapsulating Iodine and Copper into Copper(I) Clusters Stabilized by Dichalcogenolate Ligands: Stability, Structure, and Optical Properties. Inorganic Chemistry, 2017, 56, 14135-14146.	4.0	12
587	Spectroscopic Characterization of Key Aromatic and Heterocyclic Molecules: A Route toward the Origin of Life. Astronomical Journal, 2017, 154, 82.	4.7	12
588	Sextic centrifugal distortion constants: interplay of density functional and basis set for accurate yet feasible computations. Molecular Physics, 2020, 118, e1734678.	1.7	12
589	Recent Advances in Density Functional Methods. Recent Advances in Computational, 2002, , .	0.8	12
590	Unbiased disentanglement of conformational baths with the help of microwave spectroscopy, quantum chemistry, and artificial intelligence: The puzzling case of homocysteine. Journal of Chemical Physics, 2022, 157, .	3.0	12
591	Structural and energetic characteristics of electron deficient M2H6 compounds from a density functional approach. Chemical Physics Letters, 1994, 222, 597-602.	2.6	11
592	Proton transfer in excited electronic states: environmental effects on the tautomerization of 2-pyridone. Journal of Photochemistry and Photobiology A: Chemistry, 1994, 80, 211-219.	3.9	11
593	Development and validation of force-field parameters for molecular simulations of peptides and proteins containing open-shell residues. Journal of Computational Chemistry, 1997, 18, 1720-1728.	3.3	11
594	Accurate prediction of electron-paramagnetic-resonance tensors for spin probes dissolved in liquid crystals. Journal of Chemical Physics, 2005, 123, 194909.	3.0	11

#	Article	IF	Citations
595	The catecholic antioxidant piceatannol is an effective nitrosation inhibitor via an unusual double bond nitration. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 2238-2242.	2.2	11
596	Parameterization and validation of an accurate force-field for the simulation of alkylamine functionalized silicon (111) surfaces. Physical Chemistry Chemical Physics, 2010, 12, 4201.	2.8	11
597	Interactions of Nucleotide Bases with Decorated Si Surfaces from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2011, 115, 9146-9156.	3.1	11
598	Melaninâ€inspired Organic Electronics: Electroluminescence in Asymmetric Triazatruxenes. ChemPlusChem, 2015, 80, 919-927.	2.8	11
599	Tuning of dye optical properties by environmental effects: a QM/MM and experimental study. Physical Chemistry Chemical Physics, 2016, 18, 9724-9733.	2.8	11
600	New atomistic model of pyrrole with improved liquid state properties and structure. International Journal of Quantum Chemistry, 2018, 118, e25554.	2.0	11
601	Discovering the Elusive Global Minimum in a Ternary Chiral Cluster: Rotational Spectra of Propylene Oxide Trimer. Angewandte Chemie, 2020, 132, 22613-22616.	2.0	11
602	The challenging equilibrium structure of HSSH: Another success of the rotational spectroscopy / quantum chemistry synergism. Journal of Molecular Structure, 2020, 1211, 127933.	3.6	11
603	Isomerization and Fragmentation Reactions on the [C₂SH₄] Potential Energy Surface: The Metastable Thione S-Methylide Isomer. Journal of Organic Chemistry, 2021, 86, 2941-2956.	3.2	11
604	High Water Density at Non-Ice-Binding Surfaces Contributes to the Hyperactivity of Antifreeze Proteins. Journal of Physical Chemistry Letters, 2021, 12, 8777-8783.	4.6	11
605	Quantum-mechanical study of the chemisorption of atomic and molecular oxygen on graphite clusters. Computational and Theoretical Chemistry, 1986, 136, 313-322.	1.5	10
606	Quantum mechanical study of regioselectivity of radical additions to substituted olefins. Journal of Computational Chemistry, 2000, 21, 675-691.	3.3	10
607	Solvent effects on molecular interactions: new hints from an integrated density functional/polarizable continuum model. Computational and Theoretical Chemistry, 2005, 729, 1-9.	1.5	10
608	A computational protocol to probe the role of solvation effects on the reduction potential of azurin mutants. Proteins: Structure, Function and Bioinformatics, 2005, 62, 262-269.	2.6	10
609	Harmonic and anharmonic contributions to parity-violating vibrational frequency difference between enantiomers of chiral molecules. Journal of Chemical Physics, 2005, 123, 234304.	3.0	10
610	Excited state properties of sizable molecules in solution: from structure to reactivity. Theoretical Chemistry Accounts, 2007, 117, 1073-1084.	1.4	10
611	On the stability of X2NO radicals (X = F, Cl, Br, I). Physical Chemistry Chemical Physics, 2009, 11, 11463.	2.8	10
612	Absorption spectra of natural pigments as sensitizers in solar cells by TD-DFT and MRPT2: protonated cyanidin. Physical Chemistry Chemical Physics, 2012, 14, 16130.	2.8	10

#	Article	IF	Citations
613	The Î”^{2,2â€²}â€Bi(2Hâ€1,4â€benzothiazine) Structural Motif of Red Hair Pigments Revisited: Photochromism and Acidichromism in a Unique Fourâ€State System. European Journal of Organic Chemistry, 2012, 2012, 5136-5140.	2.4	10
614	Unravelling electronic and structural requisites of tripletâ€“triplet energy transfer by advanced electron paramagnetic resonance and density functional theory. Molecular Physics, 2013, 111, 2914-2932.	1.7	10
615	Structural, dynamic and photophysical properties of a fluorescent dye incorporated in an amorphous hydrophobic polymer bundle. Physical Chemistry Chemical Physics, 2014, 16, 16573-16587.	2.8	10
616	BALOO: A Fast and Versatile Code for Accurate Multireference Variational/Perturbative Calculations. Journal of Chemical Theory and Computation, 2015, 11, 2024-2035.	5.3	10
617	A â€œTwistâ€•on the Interpretation of the Multifluorescence Patterns of DASPMI. Journal of Chemical Theory and Computation, 2015, 11, 4803-4813.	5.3	10
618	Vibrational Comfort on Board the Vehicle: Influence of Speed Bumps and Comparison between Different Categories of Vehicle. Advances in Acoustics and Vibration, 2016, 2016, 1-6.	0.5	10
619	Vapochromic behavior of polycarbonate films doped with a luminescent molecular rotor. Polymers for Advanced Technologies, 2016, 27, 429-435.	3.2	10
620	Assessment of Electron Propagator Methods for the Simulation of Vibrationally Resolved Valence and Core Photoionization Spectra. Journal of Chemical Theory and Computation, 2017, 13, 3120-3135.	5.3	10
621	Tailorâ€•made computational protocols for precise characterization of small biological building blocks using QM and MM approaches. Biopolymers, 2018, 109, e23109.	2.4	10
622	Modeling amino-acid side chain infrared spectra: the case of carboxylic residues. Physical Chemistry Chemical Physics, 2020, 22, 3008-3016.	2.8	10
623	Gas-Phase Formation and Isomerization Reactions of Cyanoacetaldehyde, a Prebiotic Molecule of Astrochemical Interest. ACS Earth and Space Chemistry, 2021, 5, 1071-1082.	2.7	10
624	On the shapes of weakly adsorbed two-dimensional clusters. Surface Science, 1980, 97, 537-552.	1.9	9
625	Theoretical studies on the geometric and electronic structure of substituted SCN isomers. Computational and Theoretical Chemistry, 1982, 86, 239-253.	1.5	9
626	Theoretical investigation of the torsional potential of 2,2â€²-bipyrimidine. Chemical Physics Letters, 1993, 215, 40-44.	2.6	9
627	Regioselectivity of methyl radical addition to fluoroethenes: a quantum mechanical study. Chemical Physics Letters, 1998, 293, 295-301.	2.6	9
628	Reaction between quinone and thiazolidine. A study on the formation mechanism of new antiproliferative quinolindiones. Tetrahedron, 2004, 60, 8189-8197.	1.9	9
629	Oxidative chemistry of 2-nitro and 4-nitroestradiol: Dichotomous behavior of radical intermediates and novel potential routes for oxyfunctionalization and B-ring fission of steroidal scaffolds. Steroids, 2005, 70, 543-550.	1.8	9
630	Dissociative Electron Transfer in Donorâ^'Peptideâ^'Acceptor Systems:Â Results for Kinetic Parameters from a Density Functional/Polarizable Continuum Model. Journal of Physical Chemistry B, 2006, 110, 12632-12639.	2.6	9

#	Article	IF	Citations
631	Uracil anion radical in aqueous solution: thermodynamics versus spectroscopy. Physical Chemistry Chemical Physics, 2010, 12, 10736.	2.8	9
632	Density functional theory study of the interaction of vinyl radical, ethyne, and ethene with benzene, aimed to define an affordable computational level to investigate stability trends in large van der Waals complexes. Journal of Chemical Physics, 2013, 139, 244306.	3.0	9
633	A new Gaussian MCTDH program: Implementation and validation on the levels of the water and glycine molecules. Journal of Chemical Physics, 2014, 140, 244104.	3.0	9
634	Vibronic Effects on Rates of Excitation Energy Transfer and Their Temperature Dependence. Journal of Chemical Theory and Computation, 2016, 12, 2357-2365.	5.3	9
635	New insights into the vibrational and optical signatures of trans-stilbene via integrated experimental and quantum mechanical approaches. Physical Chemistry Chemical Physics, 2016, 18, 19378-19385.	2.8	9
636	Unraveling the role of additional OH-radicals in the Hâ€“Abstraction from Dimethyl sulfide using quantum chemical computations. Chemical Physics Letters, 2020, 739, 136963.	2.6	9
637	H-Abstraction from Dimethyl Sulfide in the Presence of an Excess of Hydroxyl Radicals. A Quantum Chemical Evaluation of Thermochemical and Kinetic Parameters Unveils an Alternative Pathway to Dimethyl Sulfoxide. ACS Earth and Space Chemistry, 2020, 4, 403-419.	2.7	9
638	Non-empirical and MNDO study of the geometry and electronic structure of H2XO radicals. Computational and Theoretical Chemistry, 1982, 90, 59-64.	1.5	8
639	A theoretical characterization of the structure formation enthalpy, and fluzional behaviour of B2H6 and AlBH6. Theoretica Chimica Acta, 1989, 76, 53-64.	0.8	8
640	Ab initio study of the nitronyl and imino nitroxides: relation between electronic structure and magnetic properties in metal-nitroxide complexes. The Journal of Physical Chemistry, 1991, 95, 9238-9242.	2.9	8
641	Theoretical energies of representative carbon-carbon bonds. International Journal of Quantum Chemistry, 1995, 55, 469-476.	2.0	8
642	Free Energy Landscapes of Ion Coordination in Aqueous Solution. Journal of Physical Chemistry B, 2011, 115, 12875-12878.	2.6	8
643	Extension of the AMBER Force Field for Nitroxide Radicals and Combined QM/MM/PCM Approach to the Accurate Determination of EPR Parameters of DMPO-H in Solution. Journal of Chemical Theory and Computation, 2013, 9, 3626-3636.	5.3	8
644	Proton and Electron Transfer Mechanisms in the Formation of Neutral and Charged Quinhydrone-Like Complexes: A Multilayered Computational Study. Journal of Chemical Theory and Computation, 2014, 10, 4883-4895.	5.3	8
645	Solar collectors based on luminescent 2,5-diarylimidazoles. Dyes and Pigments, 2018, 157, 334-341.	3.7	8
646	CPL Spectra of Camphor Derivatives in Solution by an Integrated QM/MD Approach. Frontiers in Chemistry, 2020, 8, 584.	3.6	8
647	Rotational Spectroscopy Meets Quantum Chemistry for Analyzing Substituent Effects on Non-Covalent Interactions: The Case of the Trifluoroacetophenone-Water Complex. Molecules, 2020, 25, 4899.	3.8	8
648	A General User-Friendly Tool for Kinetic Calculations of Multi-Step Reactions within the Virtual Multifrequency Spectrometer Project. Applied Sciences (Switzerland), 2020, 10, 1872.	2.5	8

#	Article	IF	Citations
649	Proton transfer in the ground and excited electronic states of [2,2â€²-bipyridyl]-3,3â€²-diol. A semiempirical study. Journal of the Chemical Society Perkin Transactions II, 1995, , 1141-1147.	0.9	7
650	Structure and magnetic properties of aza-aromatic triplet states. The case of quinoxaline. Chemical Physics Letters, 2001, 335, 427-434.	2.6	7
651	Regioselectivity and Nucleophilic Control in the Cyclopropane Ring Opening of Duocarmycin SA Derivatives under Neutral and Acid Conditions:Â A Quantum Mechanical Study in the Gas Phase and in Solution. Journal of Organic Chemistry, 2004, 69, 7414-7422.	3.2	7
652	UV-vis spectra of p-benzoquinone anion radical in solution by a TD-DFT/PCM approach. Theoretical Chemistry Accounts, 2007, 118, 143-148.	1.4	7
653	Theoretical modeling of open-shell molecules in solution: a QM/MM molecular dynamics approach. Theoretical Chemistry Accounts, 2008, 120, 499-506.	1.4	7
654	Structure and ESR features of a radiation-induced radical in Î±-glycine crystals. Chemical Physics Letters, 2008, 452, 89-93.	2.6	7
655	A critical analysis of the structure and vibrational frequencies of F2NO+ and Cl2NO+ from accurate quantum chemical computations. Chemical Physics Letters, 2008, 462, 49-52.	2.6	7
656	Microsolvation of uracil anion radical in aqueous solution: a QM/MM study. Chemical Physics Letters, 2010, 500, 104-110.	2.6	7
657	DNA hybridization mechanism on silicon nanowires: a molecular dynamics approach. Molecular BioSystems, 2010, 6, 2230.	2.9	7
658	Theoretical study of the conformational and optical properties of a fluorescent dye. A step toward modeling sensors grafted on polymer structures. Physical Chemistry Chemical Physics, 2011, 13, 21471.	2.8	7
659	In Silico Study of Molecular-Engineered Nanodevices: A Lockable Light-Driven Motor in Dichloromethane Solution. Journal of Physical Chemistry Letters, 2013, 4, 3885-3890.	4.6	7
660	Evidences of long lived cages in functionalized polymers: Effects on chromophore dynamic and spectroscopic properties. Chemical Physics Letters, 2014, 601, 134-138.	2.6	7
661	Breaking the Hydrophobicity of the MscL Pore: Insights into a Charge-Induced Gating Mechanism. PLoS ONE, 2015, 10, e0120196.	2.5	7
662	Definition of an On-Board Comfort Index (Rail) for the Railway Transport. Journal of Advanced Transportation, 2017, 2017, 1-11.	1.7	7
663	Theory Meets Experiment for Noncovalent Complexes: The Puzzling Case of Pnicogen Interactions. Angewandte Chemie, 2018, 130, 14049-14053.	2.0	7
664	Virtual reality tools for advanced modeling. AIP Conference Proceedings, 2019, , .	0.4	7
665	Mechanistic insights into metal ions transit through threefold ferritin channel. Biochimica Et Biophysica Acta - General Subjects, 2019, 1863, 472-480.	2.4	7
666	A Journey from Thermally Tunable Synthesis to Spectroscopy of Phenylmethanimine in Gas Phase and Solution. Chemistry - A European Journal, 2020, 26, 15016-15022.	3.3	7

#	Article	IF	Citations
667	Toward Accurate Formation Routes of Complex Organic Molecules in the Interstellar Medium: The Paradigmatic Cases of Acrylonitrile and Cyanomethanimine. Frontiers in Astronomy and Space Sciences, 2022, 8, .	2.8	7
668	Bond orbital models. Computational and Theoretical Chemistry, 1983, 105, 191-200.	1.5	6
669	A theoretical study of relaxation and reconstruction of the (111) surface of diamond. Surface Science, 1985, 162, 169-174.	1.9	6
670	The fragmentation of C2H6N+ ions: an alternative mechanism. Chemical Physics Letters, 1987, 133, 548-552.	2.6	6
671	Intramolecular C-H--O interaction between lactam oxygen and N-alkyl protons. Journal of Molecular Graphics and Modelling, 2001, 19, 318-324.	2.4	6
672	General computational strategy to study polymerization reactions at aluminum-based catalysts. International Journal of Quantum Chemistry, 2003, 91, 474-482.	2.0	6
673	On the role of stereo-electronic effects in tuning the selectivity and rate of DNA alkylation by duocarmycins. Organic and Biomolecular Chemistry, 2006, 4, 1242.	2.8	6
674	Organic Functionalization and Optimal Coverage of a Silicon(111) Surface in Solvent: A Computational Study. Journal of Physical Chemistry C, 2011, 115, 4145-4154.	3.1	6
675	Trichocyanines: a Red-Hair-Inspired Modular Platform for Dye-Based One-Time-Pad Molecular Cryptography. ChemistryOpen, 2015, 4, 370-377.	1.9	6
676	Theoretical evidence of metal-induced structural distortions in a series of bipyrimidine-based ligands. Dalton Transactions, 2015, 44, 506-510.	3.3	6
677	The Unexplored World of Cycloalkeneâ€“Water Complexes: Primary and Assisting Interactions Unraveled by Experimental and Computational Spectroscopy. Angewandte Chemie, 2019, 131, 14073-14079.	2.0	6
678	Transversity distributions from difference asymmetries in semi-inclusive DIS. Physical Review D, 2019, 99, .	4.7	6
679	Theory meets experiment for unravelling the C1s X-ray photoelectron spectra of pyridine, 2-fluoropyridine, and 2,6-difluoropyridine. Journal of Chemical Physics, 2019, 151, 124105.	3.0	6
680	Systematic Study on the Absorption Features of Interstellar Ices in the Presence of Impurities. ACS Earth and Space Chemistry, 2020, 4, 920-946.	2.7	6
681	Dipolar 1,3â€cycloaddition of thioformaldehyde S â€methylide (<scp> CH ₂ SCH) Tj ETQq1 1 0.784314 rgBT /Over ₃ </scp> , <scp> SO ₂ </scp> , <scp>. Journal of Computational Chemistry, 2022, 43, 1420-1433.	3.3	6
682	Transition state structure and isotope effects in unimolecular hydrogen elimination from carbocations. Chemical Physics Letters, 1983, 98, 463-466.	2.6	5
683	Hybridization and surface relaxation in diamond-like crystals. Computational and Theoretical Chemistry, 1983, 94, 173-185.	1.5	5
684	ESR features of the bicyclobutyl radical revisited. A counterintuitive ordering of short- and long-range isotropic hyperfine coupling constants. Chemical Physics Letters, 1995, 246, 53-58.	2.6	5

#	Article	IF	Citations
685	Accurate and effective calculation of amide proton magnetic shieldings in a calcium binding peptide. Physical Chemistry Chemical Physics, 2004, 6, 2557.	2.8	5
686	Order parameters of Î±,Ï‰-diphenylpolyenes in a nematic liquid crystal from an integrated computational and C13 NMR spectroscopic approach. Journal of Chemical Physics, 2006, 125, 174904.	3.0	5
687	Gas-Phase Chemistry of Diphosphate Anions as a Tool To Investigate the Intrinsic Requirements of Phosphate Ester Enzymatic Reactions: The [M1M2HP2O7]â¯ Ions. Chemistry - A European Journal, 2007, 13, 2096-2108.	3.3	5
688	Conformational preferences and selfâ€association modes of two diastereomeric statine derivatives. International Journal of Peptide and Protein Research, 1987, 30, 583-595.	0.1	5
689	Theoretical study of a molecular junction with asymmetric current/voltage characteristics. Chemical Physics Letters, 2012, 549, 1-5.	2.6	5
690	Electron Transport Properties of Diarylethene Photoswitches by a Simplified NEGF-DFT Approach. Journal of Physical Chemistry B, 2014, 118, 4976-4981.	2.6	5
691	Virtual eyes for technology and cultural heritage: towards computational strategy for new and old indigo-based dyes. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	5
692	Toward a General Yet Effective Computational Approach for Diffusive Problems: Variable Diffusion Tensor and DVR Solution of the Smoluchowski Equation along a General One-Dimensional Coordinate. Journal of Chemical Theory and Computation, 2016, 12, 3482-3490.	5.3	5
693	Neutral copper(<scp>i</scp>) complexes featuring phosphinesulfonate chelates. Dalton Transactions, 2016, 45, 6566-6573.	3.3	5
694	Magnetic gaps in organic tri-radicals: From a simple model to accurate estimates. Journal of Chemical Physics, 2017, 146, 104103.	3.0	5
695	The Sivers asymmetry in Drellâ€“Yan production at the J /Î¨ peak at COMPASS. Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics, 2017, 770, 302-306.	4.1	5
696	Unveiling the Sulfurâ€“Sulfur Bridge: Accurate Structural and Energetic Characterization of a Homochalcogen Intermolecular Bond. Angewandte Chemie, 2018, 130, 16048-16052.	2.0	5
697	Computational Spectroscopy in Solution by Integration of Variational and Perturbative Approaches on Top of Clusterized Molecular Dynamics. Journal of Chemical Theory and Computation, 2020, 16, 5747-5761.	5.3	5
698	A reinvestigation of the deceptively simple reaction of toluene with OH, and the fate of the benzyl radical: a combined thermodynamic and kinetic study on the competition between OH-addition and H-abstraction reactions. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	5
699	Length-scale dependence of protein hydration-shell density. Physical Chemistry Chemical Physics, 2020, 22, 7340-7347.	2.8	5
700	Ultraviolet resonance Raman spectroscopy of anthracene: Experiment and theory. Journal of Raman Spectroscopy, 0, , .	2.5	5
701	An improved study of HCO+ and He system: Interaction potential, collisional relaxation, and pressure broadening. Journal of Chemical Physics, 2021, 155, 234306.	3.0	5
702	Molecular Dynamics Simulations Enforcing Nonperiodic Boundary Conditions: New Developments and Application to the Solvent Shifts of Nitroxide Magnetic Parameters. Journal of Chemical Theory and Computation, 2022, , .	5.3	5

#	Article	IF	Citations
703	A Computational Journey across Nitroxide Radicals: From Structure to Spectroscopic Properties and Beyond. Molecules, 2021, 26, 7404.	3.8	5
704	Gas phase unimolecular 1,1-hydrogen elimination: Reaction mechanism and isotope effect. International Journal of Quantum Chemistry, 1984, 26, 621-636.	2.0	4
705	A theoretical study of the nitrogenâ€"graphite system. Computational and Theoretical Chemistry, 1986, 139, 277-282.	1.5	4
706	A microscopic approach to the structure and thermodynamic properties of peptides and proteins. Thermochimica Acta, 1990, 162, 141-154.	2.7	4
707	Core and valence electrons in atom-by-atom descriptions of molecules. Advances in Quantum Chemistry, 2000, 36, 27-44.	0.8	4
708	Phototransformation of the drug trazodone in aqueous solution. Journal of Photochemistry and Photobiology A: Chemistry, 2008, 199, 353-357.	3.9	4
709	Complementary and partially complementary DNA duplexes tethered to a functionalized substrate: a molecular dynamics approach to biosensing. Physical Chemistry Chemical Physics, 2011, 13, 12478.	2.8	4
710	Effective time-independent studies on resonance Raman spectroscopy of trans-stilbene including the Duschinsky effect. Molecular Physics, 2013, 111, 1511-1525.	1.7	4
711	Chain length, temperature and solvent effects on the structural properties of Î±-aminoisobutyric acid homooligopeptides. Physical Chemistry Chemical Physics, 2016, 18, 20389-20398.	2.8	4
712	Vitamin C: an experimental and theoretical study on the gasâ€phase structure and ion energetics of protonated ascorbic acid. Journal of Mass Spectrometry, 2016, 51, 1146-1151.	1.6	4
713	Low-lying electronic excitations of a water-soluble BODIPY: from the gas phase to the solvated molecule. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	4
714	Quantitative prediction and interpretation of spin energy gaps in polyradicals: the virtual magnetic balance. Physical Chemistry Chemical Physics, 2017, 19, 9039-9044.	2.8	4
715	4-Fluoro-Threonine: From Diastereoselective Synthesis to pH-Dependent Conformational Equilibrium in Aqueous Solution. ACS Omega, 2021, 6, 13170-13181.	3.5	4
716	Interplay of stereo-electronic, vibronic and environmental effects in tuning the chiroptical properties of an Ir(III) cyclometalated N-heterocyclic carbene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 254, 119631.	3.9	4
717	Moka: Designing a Simple Scene Graph Library for Cluster-Based Virtual Reality Systems. Lecture Notes in Computer Science, 2014, , 333-350.	1.3	4
718	Enhancing the Accuracy of Ab Initio Molecular Dynamics by Fine Tuning of Effective Two-Body Interactions: Acetonitrile as a Test Case. Journal of Physical Chemistry A, 2021, 125, 10475-10484.	2.5	4
719	Gliding on Ice in Search of Accurate and Cost-Effective Computational Methods for Astrochemistry on Grains: The Puzzling Case of the HCN Isomerization. Journal of Chemical Theory and Computation, 2022, 18, 3111-3121.	5.3	4
720	The mechanisms of elementary physicochemical processes: An introductory report. International Journal of Quantum Chemistry, 1984, 26, 563-591.	2.0	3

#	Article	IF	Citations
721	Properties and Spectroscopies. , 0, , 125-312.		3
722	Structural and conformational investigation of nemorosone: A combined X-ray and quantum mechanical study. Chemical Physics Letters, 2008, 462, 158-163.	2.6	3
723	Bottom-Up Approach to Innovative Memory Devices: I. Intrinsic and Environmental Effects on the Molecular Component. Journal of Physical Chemistry C, 2008, 112, 17081-17088.	3.1	3
724	Magneto-Structural Relationships for Radical Cation and Neutral Pyridinophane Structures with Intrabridgehead Nitrogen Atoms. An Integrated Experimental and Quantum Mechanical Study. Journal of Physical Chemistry B, 2009, 113, 9026-9034.	2.6	3
725	The Virtual Electron Paramagnetic Resonance Laboratory: A User Guide toab initio Modeling. , 0, , 251-284.		3
726	Nonadiabatic photodynamics of phenol on a realistic potential energy surface by a novel multilayer Gaussian MCTDH program. Chemical Physics Letters, 2015, 636, 15-21.	2.6	3
727	Anharmonic Computations Meet Experiments (IR, Raman, Neutron Diffraction) for Explaining the Behavior of 1,3,5-Tribromo-2,4,6-trimethylbenzene. Journal of Physical Chemistry A, 2016, 120, 1127-1132.	2.5	3
728	General Approach to Coupled Reactive Smoluchowski Equations: Integration and Application of Discrete Variable Representation and Generalized Coordinate Methods to Diffusive Problems. Journal of Chemical Theory and Computation, 2017, 13, 5900-5910.	5.3	3
729	On the composition of an arbitrary collection of SU(2) spins: an enumerative combinatoric approach. Journal of Physics A: Mathematical and Theoretical, 2018, 51, 105202.	2.1	3
730	Comfort Index CI(bus): A methodology to measure the comfort on board. Procedia Computer Science, 2018, 134, 439-444.	2.0	3
731	The role of the multiconfigurational character of nitronyl-nitroxide in the singletâ€“triplet energy gap of its diradicals. Physical Chemistry Chemical Physics, 2018, 20, 18547-18555.	2.8	3
732	Enthalpies of formation of the benzyloxyl, benzylperoxyl, hydroxyphenyl radicals and related species on the potential energy surface for the reaction of toluene with the hydroxyl radical. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	3
733	Chemical bonding in cuprous complexes with simple nitriles: octet rule and resonance concepts versus quantitative charge-redistribution analysis. Physical Chemistry Chemical Physics, 2020, 22, 20238-20247.	2.8	3
734	Looking for the bricks of the life in the interstellar medium: The fascinating world of astrochemistry. EPJ Web of Conferences, 2020, 246, 00021.	0.3	3
735	Nonempirical analysis of unusual chemical bonds. II. AlH2BH4 and AlH2C3H5. International Journal of Quantum Chemistry, 1981, 19, 1197-1201.	2.0	2
736	Hybridization and surface relaxation in diamond-like crystals. Journal of Molecular Structure, 1983, 94, 173-185.	3.6	2
737	Towards the Understanding of the Excited State Dynamics of Nucleic Acids: Solvent and Stacking Effect on the Photophysical Behavior of Nucleobases. AIP Conference Proceedings, 2007, , .	0.4	2
738	An integrated approach for the interpretation of emission fluorescence of DMABN-Crown derivatives in polar environments. Chemical Physics Letters, 2008, 467, 204-209.	2.6	2

#	Article	IF	Citations
739	Interplay of Stereoelectronic Vibrational and Environmental Effects in Tuning Physicochemical Properties of Carbon-Centered Radicals. , 0, , 105-139.		2
740	Bottom-Up Approach to Innovative Memory Devices: II. Molecular Adsorption on Electrodes and the Asymmetric Response. Journal of Physical Chemistry C, 2010, 114, 21439-21443.	3.1	2
741	Computational Spectroscopy. , 2013, , .		2
742	Discrete variable representation of the Smoluchowski equation using a sinc basis set. Physical Chemistry Chemical Physics, 2015, 17, 17362-17374.	2.8	2
743	Effects of music playing on biological molecules. MATEC Web of Conferences, 2018, 210, 05006.	0.2	2
744	Machine Learning of Potential-Energy Surfaces Within a Bond-Order Sampling Scheme. Lecture Notes in Computer Science, 2019, , 388-400.	1.3	2
745	Computational Evidence Suggests That 1-Chloroethanol May Be an Intermediate in the Thermal Decomposition of 2-Chloroethanol into Acetaldehyde and HCl. Journal of Physical Chemistry A, 2019, 123, 1983-1998.	2.5	2
746	Stacked but not Stuck: Unveiling the Role of Ï€ â†' Ï€* Interactions with the Help of the Benzofuranâ€Formaldehyde Complex. Angewandte Chemie, 2022, 134, e202113737.	2.0	2
747	Spectroscopic Characterization of 3-Aminoisoxazole, a Prebiotic Precursor of Ribonucleotides. Molecules, 2022, 27, 3278.	3.8	2
748	Theoretical studies on the protonation of diamines in aqueous solution. Inorganica Chimica Acta, 1980, 40, X57-X58.	2.4	1
749	Non-empirical analysis of unusual chemical bonds. Journal of Molecular Structure, 1983, 92, 103-108.	3.6	1
750	Nonempirical cluster model study of the on-top chemisorption of fluorine and chlorine on C(111) surface. Solid State Communications, 1988, 65, 945-947.	1.9	1
751	Conformational behaviour of nonâ€fused biheterocycles. Part XV. Isomeric phenylisoxazoles. Journal of Heterocyclic Chemistry, 1988, 25, 1709-1712.	2.6	1
752	Non-empirical cluster-model study of the relaxation of (111) surfaces of C, Si, Ge. Computational and Theoretical Chemistry, 1990, 204, 325-329.	1.5	1
753	Photochemical behavior of some substituted benzophenoxazinones. Journal of Heterocyclic Chemistry, 1995, 32, 743-746.	2.6	1
754	Interpretation of the emission fluorescence spectra of two fluoroionophores: DMABNâ€Crown4 and DMABNâ€Crown5. International Journal of Quantum Chemistry, 2010, 110, 368-375.	2.0	1
755	Transport properties of binuclear metal complexes of the VIII group using a simplified NEGF-DFT approach. Physical Chemistry Chemical Physics, 2013, 15, 11409.	2.8	1
756	Reprint of â€œEnvironmental and dynamical effects on the optical properties of molecular systems by time-independent and time-dependent approaches: Coumarin derivatives as test casesâ€• Computational and Theoretical Chemistry, 2014, 1040-1041, 144-157.	2.5	1

#	Article	IF	Citations
757	Computational Spectroscopy in Solution: Methods and Models for Investigating Complex Systems. Challenges and Advances in Computational Chemistry and Physics, 2015, , 447-517.	0.6	1
758	Challenges in astrochemistry: The spectroscopic point of view. Physics of Life Reviews, 2020, 34-35, 143-146.	2.8	1
759	Interplay of Stereoelectronic and Vibrational Modulation Effects in Tuning the UPS Spectra of Unsaturated Hydrocarbon Cage Compounds. Journal of Chemical Theory and Computation, 2020, 16, 5218-5226.	5.3	1
760	A computational journey in the CH2O2S land: an accurate rotational and ro-vibrational analysis of the sulfene molecule and the O,S- and O,O-monothiocarbonic acids. Molecular Physics, 2020, 118, e1766707.	1.7	1
761	Transverseâ€“Spin Quark Distributions from Asymmetry Data and Symmetry Arguments. Symmetry, 2021, 13, 116.	2.2	1
762	A computational insight into the relationship between side chain IR line shapes and local environment in fibril-like structures. Journal of Chemical Physics, 2021, 154, 084105.	3.0	1
763	Virtual Reality bridge between Chemistry and Cultural Heritage: the â€œSala degli Stemmiâ€•Case Study.. IOP Conference Series: Materials Science and Engineering, 2020, 949, 012020.	0.6	1
764	Analysis of L-DOPA and droxidopa binding to human Î²2-adrenergic receptor. Biophysical Journal, 2021, , .	0.5	1
765	Synchrotron-based far-infrared spectroscopy of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="normal">HC</mml:mi></mml:mrow><mml:mn>3</mml:mn></mml:msub><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math>: Extended ro-vibrational analysis and new line list up to 3360 Âcm<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.s	2.3	1
766	Development, Validation, and Pilot Application of a Generalized Fluctuating Charge Model for Computational Spectroscopy in Solution. ACS Omega, 2022, 7, 13382-13394.	3.5	1
767	Non-empirical analysis of unusual chemical bonds. Computational and Theoretical Chemistry, 1983, 92, 103-108.	1.5	0
768	Interaction of Atomic Hydrogen with the (111) and (100) Surfaces of Diamond-Like Crystals. Studies in Surface Science and Catalysis, 1989, , 69-73.	1.5	0
769	Interplay of Electronic, Environmental, and Vibrational Effects in Determining the Hyperfine Coupling Constants of Organic Free Radicals. ChemInform, 2004, 35, no.	0.0	0
770	Thiazolidin-4-one Formation. Mechanistic and Synthetic Aspects of the Reaction of Imines and Mercaptoacetic Acid under Microwave and Conventional Heating.. ChemInform, 2005, 36, no.	0.0	0
771	Theoretical and computational chemistry in Italy: an overview. Theoretical Chemistry Accounts, 2007, 117, 599-602.	1.4	0
772	Tribute to Jacopo Tomasi. Journal of Physical Chemistry A, 2015, 119, 5039-5040.	2.5	0
773	Theoretical and computational chemistry in Italy. International Journal of Quantum Chemistry, 2016, 116, 1499-1500.	2.0	0
774	Correct Modeling of Cisplatin: a Paradigmatic Case. Angewandte Chemie, 2017, 129, 14026-14029.	2.0	0

#	Article	IF	Citations
775	Collisional broadening and hyperfine structure of rotational transitions. Reply to the comments on â€œA never-ending story in the sky: The secrets of chemical evolutionâ€• Physics of Life Reviews, 2020, 32, 124-128.	2.8	0
776	PhysChem: A New Physical Chemistry Journal. Physchem, 2021, 1, 1-3.	1.1	0
777	Graphical Interfaces and Virtual Reality for Molecular Sciences. , 2014, , .		0
778	Status and perspectives of a virtual multifrequency spectrometer for ESR. Electron Paramagnetic Resonance, 2016, , 98-156.	0.2	0
779	A Diabatic Electronic State System to Describe the Internal Conversion of Azulene. Lecture Notes in Computer Science, 2017, 10408, 328-337.	1.3	0
780	Probing Liquid-Ordered and Disordered Phases in Lipid Model Membranes: A Combined Theoretical and Spectroscopic Study of a Fluorescent Molecular Rotor. Journal of Physical Chemistry B, 2022, , .	2.6	0
781	Welcome to Physchem: Status and Prospects. Physchem, 2022, 2, 16-17.	1.1	0
782	PROTEUS: an immersive tool for exploring the world of cultural heritage across space and time scales. Heritage Science, 2022, 10, .	2.3	0