

Toward a systematic molecular orbital theory for excite

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Citation Report

#	ARTICLE	IF	CITATIONS
7	The Response of Electrons to Structural Changes. <i>Science</i> , 1991, 252, 1266-1272.	6.0	58
8	Ground state properties and optical response of $\text{Li}_x\text{Na}_{4-x}\text{O}_4$: An ab initio study. <i>Journal of Chemical Physics</i> , 1992, 96, 4924-4933.	1.2	38
9	The use of the point charge model in the evaluation of spectral shifts within the INDO/CIS approximation. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1992, , 2197.	0.9	0
10	One-electron density matrices and energy gradients in second-order electron propagator theory. <i>Journal of Chemical Physics</i> , 1992, 96, 8379-8389.	1.2	38
11	$\tilde{\pi}^*$ negative ion resonance states of (E)- and (Z)-1,3,5-hexatriene. Prediction of electron affinities near threshold. <i>Chemical Physics Letters</i> , 1992, 200, 527-533.	1.2	4
12	Ab initio quantum-chemical study of the lower-lying electronic states of o-benzyne. <i>Chemical Physics Letters</i> , 1992, 198, 259-265.	1.2	16
13	Towards an accurate molecular orbital theory for excited states: the benzene molecule. <i>Chemical Physics Letters</i> , 1992, 192, 5-13.	1.2	213

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25	Use of calculated quantum chemical properties as surrogates for solvatochromic parameters in structure-activity relationships. <i>Accounts of Chemical Research</i> , 1993, 26, 599-605.	7.6	89
26	Franck-Condon structure of the $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions in norbornadiene. <i>Journal of Chemical Physics</i> , 1993, 98, 14-20.	1.2	22
27	Electronic and vibrational spectra of matrix isolated anthracene radical cations: Experimental and theoretical aspects. <i>Journal of Chemical Physics</i> , 1993, 98, 4494-4511.	1.2	144
28	Application of the CI-Singles Method in Predicting the Energy, Properties, and Reactivity of Molecules in Their Excited States. , 1993, , 11-26.		6
29	Towards an accurate molecular orbital theory for excited states: Ethene, butadiene, and hexatriene. <i>Journal of Chemical Physics</i> , 1993, 98, 3151-3162.	1.2	407
30	Simulation of defect processes: experiences with the self-trapped exciton. <i>Modelling and Simulation in Materials Science and Engineering</i> , 1993, 1, 673-692.	0.8	34
31	On the vibronic structure of the $S_0 \rightarrow S_1$ transitions in azulene. <i>Journal of Chemical Physics</i> , 1993, 99, 4318-4326.	1.2	56
32	The Franck-Condon structure of the $1A \rightarrow 1B$ transition of cis- and trans-hexatriene: An ab initio modeling. <i>Journal of Chemical Physics</i> , 1993, 98, 4822-4829.	1.2	30
33	Calculations on the competition between association and reaction for $C_3H + H_2$. <i>Journal of Chemical Physics</i> , 1993, 99, 2812-2820.	1.2	38
34	Methyl rotor effects on acetone Rydberg spectra. II. The $1B_2(3s \rightarrow n) \rightarrow 1A_1$ transition. <i>Journal of Chemical Physics</i> , 1993, 98, 3795-3802.	1.2	35
35	van der Waals broadening of the $X^1\Sigma^+ \rightarrow B^1\Sigma^+$ (3s Rydberg) transition of acetone by He, Ar, and CH_4 : Inversion of the spectra to the interaction pair potentials. <i>Journal of Chemical Physics</i> , 1993, 98, 8593-8600.	1.2	2
36	Photodecomposition of acetyl chloride on the excited singlet state surface. <i>Journal of Chemical Physics</i> , 1993, 99, 6531-6536.	1.2	24
37	The $S_0 \rightarrow S_1$ transition of trans- β -methyl styrene. <i>Journal of Chemical Physics</i> , 1994, 101, 11082-11083.	1.2	5
38	Theoretical study of Na-atom emission from NaCl (100) surfaces. <i>Physical Review B</i> , 1994, 49, 11364-11373.	1.1	54
39	Role of the $HNO_3 \rightarrow NOH$ Isomerization in reactions (i) $NH(3^1\Sigma^+) + O(3P)$ and (ii) $N(4S) + OH(2^1\Sigma^+)$: Ab initio calculations and quantum statistical Rice-Ramsperger-Kassel analysis of the potential energy surfaces. <i>Journal of Chemical Physics</i> , 1994, 101, 3906-3915.	1.2	22
40	Chemistry of Higher Group 14 Homologues of Thioketones $R_1R_2M[\text{dbnd}]S$ ($M[\text{dbnd}]Si, Ge, Sn, Pb$). Phosphorus, Sulfur and Silicon and the Related Elements, 1994, 95, 21-33.	0.8	6
41	Franck-Condon modeling of the structure of the $S_0 \rightarrow S_2$ transition of trans, trans-, cis, trans-, and cis-cis-octatetraene. <i>Journal of Chemical Physics</i> , 1994, 101, 1842-1851.	1.2	29
42	Second-order perturbation theory using correlated orbitals. I. Full-valence reference functions. <i>Chemical Physics</i> , 1994, 189, 1-16.	0.9	16

#	ARTICLE	IF	CITATIONS
43	EHF theory of chemical reactions Part 4. UNO CASSCF, UNO CASPT2 and R(U)HF coupled-cluster (CC) wavefunctions. <i>Journal of Molecular Structure</i> , 1994, 310, 205-218.	1.8	87
44	Electronic spectra of finite polyenes and polyacetylene obtained by electron and polarization propagator calculations. <i>Theoretica Chimica Acta</i> , 1994, 89, 335-362.	0.9	2
45	The origin of differences between coupled cluster theory and quadratic configuration interaction for excited states. <i>Chemical Physics Letters</i> , 1994, 218, 139-146.	1.2	36
46	A doubles correction to electronic excited states from configuration interaction in the space of single substitutions. <i>Chemical Physics Letters</i> , 1994, 219, 21-29.	1.2	610
47	Theoretical determination of the electronic spectrum of free base porphyrin. <i>Chemical Physics Letters</i> , 1994, 226, 27-36.	1.2	87
48	The geometric and electronic structures of C ₆ H and its ions. <i>Chemical Physics Letters</i> , 1994, 227, 371-376.	1.2	24
49	A theoretical study of the reaction of P ⁺ with water. <i>Chemical Physics Letters</i> , 1994, 230, 358-364.	1.2	5
50	Ground state free base porphyrin: C _{2v} or D _{2h} symmetry? A theoretical contribution. <i>Chemical Physics Letters</i> , 1994, 221, 136-144.	1.2	57
51	Matrix Spectroscopy of 2-Adamantylidene, a Dialkylcarbene with Singlet Ground State. <i>Angewandte Chemie International Edition in English</i> , 1994, 33, 1964-1966.	4.4	44
52	Spektroskopie von matrixisoliertem 2-Adamantyliden, einem Dialkylcarben mit Singulett-Grundzustand. <i>Angewandte Chemie</i> , 1994, 106, 2048-2051.	1.6	5
53	The vibrational structure of the S ₀ \hat{a}^1 S ₁ transition of anthracene. <i>Chemical Physics</i> , 1994, 186, 303-316.	0.9	32
54	Dissociation dynamics of acetyl chloride and cis-trans isomerisation of methoxychloro carbene and chlorohydroxymethyl carbene. <i>Chemical Physics</i> , 1994, 181, 73-84.	0.9	19
55	Solvent effects on the tautomerism of apigeninidin. <i>Tetrahedron Letters</i> , 1994, 35, 9751-9754.	0.7	1
56	Proton transfer in methyleneimine complexed with formic acid. <i>Journal of Molecular Structure</i> , 1994, 322, 9-20.	1.8	5
57	An ab initio calculation of the vertical excitation energies of naphthalene. <i>Computational and Theoretical Chemistry</i> , 1994, 309, 13-19.	1.5	3
58	On the electronic structure of the cations, radicals and anions of H ₂ SiP, H ₂ PSi and related compounds. <i>Computational and Theoretical Chemistry</i> , 1994, 313, 27-40.	1.5	16
59	Substituent effect of second row elements on silyl centers. <i>Computational and Theoretical Chemistry</i> , 1994, 313, 73-81.	1.5	43
60	Ab initio calculation of the molecular structure and conformational composition of dihalotetrasilanes. <i>Computational and Theoretical Chemistry</i> , 1994, 313, 83-89.	1.5	1

#	ARTICLE	IF	CITATIONS
61	The structure of methimazole and its consequences for current therapeutic models of graves' disease.. Bioorganic and Medicinal Chemistry Letters, 1994, 4, 1357-1360.	1.0	25
62	EHF theory of chemical reactions Part 4. UNO CASSCF, UNO CASPT2 and R(U)HF coupled-cluster (CC) wavefunctions. Computational and Theoretical Chemistry, 1994, 310, 205-218.	1.5	45
63	Theoretical study of hydrogen bonding and proton transfer in the ground and lowest excited singlet states of tropolone. Journal of Chemical Physics, 1994, 101, 9755-9765.	1.2	91
64	Nonoptical excited state spectroscopy of CHF ₂ Cl: Characterization of nondipole $\pi \rightarrow \pi^*$ valence transitions by angle-resolved electron energy loss spectroscopy. Journal of Chemical Physics, 1994, 100, 1011-1020.	1.2	17
65	Ab initio study of the molecular structure, polarizability and first hyperpolarizability of 6-hydroxy-1-formylfulvene. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 2873.	1.7	18
66	The $S_0(1A_g) \rightarrow S_1(1B_{2u})$ vibronic transition in benzene: Anabinitio study. Journal of Chemical Physics, 1994, 100, 2458-2464.	1.2	60
67	One-electron density matrices and energy gradients in the random phase approximation. Journal of Chemical Physics, 1994, 101, 6743-6749.	1.2	24
68	Configuration interaction studies on the S_2 surface of H ₂ CO: $2^1A'' \rightarrow (1^1f, 1^1e^*/1^1e, 1^1e^*)$ as perturber of $1^1B_2(n, 3s)$. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 683-688.	1.7	19
69	The vibronic structure of the $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions in simple oligomers of thiophene. Journal of Chemical Physics, 1994, 100, 2571-2587.	1.2	93
70	Considerations in constructing a multireference second-order perturbation theory. Journal of Chemical Physics, 1994, 100, 3672-3682.	1.2	181
71	Analysis of the absorption spectrum ($1^1A_g \rightarrow 1^1B_u$) and resonance Raman excitation profiles of trans-1,3,5-hexatriene based on ab initio molecular orbital calculations. Journal of Chemical Physics, 1994, 101, 4496-4504.	1.2	31
72	Quantum chemistry and density functional calculations of formyl chloride. Molecular Physics, 1994, 82, 825-829.	0.8	7
73	UV photoelectron and ab initio quantum mechanical characterization of valence electrons in Na(+)-water-2'-deoxyguanosine 5'-phosphate clusters: electronic influences on DNA alkylation by methylating and ethylating carcinogens.. Proceedings of the National Academy of Sciences of the United States of America, 1994, 91, 3725-3729.	3.3	26
74	<title>Vibronic spectroscopy of simple peptides: resonance Raman studies of solvation effects</title> , 1995, , .		0
75	A theoretical study of the reaction of Si ⁺ with ammonia. Chemical Physics Letters, 1995, 240, 193-198.	1.2	9
76	An application of the equation-of-motion coupled cluster method to the excited states of formaldehyde, acetaldehyde, and acetone. Chemical Physics Letters, 1995, 241, 26-32.	1.2	76
77	A REMPI study of indene and its clusters with argon and krypton. Chemical Physics Letters, 1995, 242, 139-146.	1.2	16
78	Ab initio MO study of the geometries and energetics of the C ₃ H ⁻ anion. Chemical Physics Letters, 1995, 242, 527-534.	1.2	18

#	ARTICLE	IF	CITATIONS
79	Ab initio calculations of vibronic spectra for indole. Chemical Physics Letters, 1995, 244, 53-58.	1.2	82
80	A perturbative correction to restricted open shell configuration interaction with single substitutions for excited states of radicals. Chemical Physics Letters, 1995, 246, 114-121.	1.2	158
81	The molecular structures and the absorption maxima of the H-chromophores of the indigoid dyes. Journal of Computational Chemistry, 1995, 16, 945-950.	1.5	3
82	Potential energy curves of HgCd and spectroscopic constants of group IIB metal dimers. Chemical Physics, 1995, 197, 129-137.	0.9	15
83	Ground-state and some excited states of Li ₂ by the half-projected Hartree-Fock method. International Journal of Quantum Chemistry, 1995, 54, 305-311.	1.0	9
84	Configuration interaction with single substitutions for excited states of open-shell molecules. International Journal of Quantum Chemistry, 1995, 56, 361-370.	1.0	54
85	Excited-state gradients via CPHF equations. International Journal of Quantum Chemistry, 1995, 56, 395-410.	1.0	7
86	Analytical gradient of the CIS(D) perturbative correction to single-excitation configuration interaction excited states. International Journal of Quantum Chemistry, 1995, 56, 421-427.	1.0	6
87	The electronic spectrum of phthalazine. Theory and experiment. Chemical Physics, 1995, 198, 183-206.	0.9	14
88	Ab initio quantum mechanical vibrational analysis of planar AX ₃ molecules (A is Al, Ga, In; X is F, Cl, Br.) <small>Tj ETQq1 1 0.784314 rgBT / Over 2.0 16</small>	2.0	16
89	Ab initio quantum chemical calculations of geometry and vibrational frequencies of chlorine heptoxide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1995, 51, 2453-2458.	2.0	4
90	Hydrogen bond patterns in solid state carboxylic acids. Vibrational study of the hydrogen bond patterns in oxamic, malonamic and succinamic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1995, 51, 1601-1615.	2.0	22
91	Ab initio study on the As-stabilized surface structure in AlAs molecular beam epitaxy. Journal of Crystal Growth, 1995, 150, 163-167.	0.7	4
92	UV spectroscopic study and conformational analysis of domperidone. Journal of Molecular Structure, 1995, 350, 43-47.	1.8	17
93	Theoretical synthesis of vibrational spectra of polycyclic aromatic hydrocarbons. Infrared spectra of coronene. Journal of Molecular Structure, 1995, 352-353, 475-479.	1.8	15
94	Structure and enantiomerization of helically twisted lactone-bridged biaryls: A theoretical study. Tetrahedron, 1995, 51, 3149-3158.	1.0	30
95	Ab initio and PM3 analysis of 1,3-dipolar cycloaddition reaction between pyridine N-oxides and isocyanates. Theoretical evidence of concerted and nonsynchronous mechanism with zwitterionic character. Tetrahedron, 1995, 51, 6451-6458.	1.0	22
96	Electronic spectrum of porphyrins. CS INDO CI study. Computational and Theoretical Chemistry, 1995, 333, 121-133.	1.5	25

#	ARTICLE	IF	CITATIONS
97	Theoretical vibrational spectra of spiropentane and deuterated isotopomers. Computational and Theoretical Chemistry, 1995, 341, 271-278.	1.5	4
98	Should the standard basis sets be augmented with diffuse functions on hydrogens to provide a reasonable description of the lowest Rydberg state of hydrogen-containing molecules?. Computational and Theoretical Chemistry, 1995, 357, 237-242.	1.5	3
99	Ground and excited state isomeric forms of the anthracene-diethylaniline molecular exciplex. Computational and Theoretical Chemistry, 1995, 343, 11-23.	1.5	12
100	Bidimensional tunneling splitting in the A_1^2 and X_1^1 states of tropolone. Journal of Chemical Physics, 1995, 103, 353-359.	1.2	58
101	Excited state reaction pathways for cis buta-1,3-diene. Journal of Chemical Physics, 1995, 102, 5733-5742.	1.2	92
102	Laser-induced fluorescence studies of jet-cooled S ₂ O: Axis-switching and predissociation effects. Journal of Chemical Physics, 1995, 103, 67-79.	1.2	21
103	Electron correlation in the self-trapped hole and exciton in the NaCl crystal. Physical Review B, 1995, 52, 6254-6264.	1.1	23
104	Ab initio study of styrene and p-methyl styrene in the ground and in the two lowest excited singlet states. Journal of Chemical Physics, 1995, 103, 20-36.	1.2	68
105	S ₀ →S ₁ transition of trans-p-methyl styrene: Vibronic structure and dynamics. Journal of Chemical Physics, 1995, 103, 37-47.	1.2	24
106	Optical transitions of the H centers in alkali halides. Physical Review B, 1995, 52, 4017-4028.	1.1	26
107	Properties of small clusters at ionic surfaces: (NaCl) _n clusters (n=1-48) at the (100) MgO surface. Physical Review B, 1995, 51, 13631-13644.	1.1	22
108	Molecular dynamics with electronic frictions. Journal of Chemical Physics, 1995, 103, 10137-10145.	1.2	286
109	A theoretical determination of the electronic spectrum of formaldehyde. Theoretica Chimica Acta, 1995, 92, 227-239.	0.9	75
110	A comparison of single reference methods for characterizing stationary points of excited state potential energy surfaces. Journal of Chemical Physics, 1995, 103, 4160-4174.	1.2	164
111	A theoretical study of the electronic spectra of pyridine and phosphabenzene. Theoretica Chimica Acta, 1995, 92, 67-81.	0.9	40
112	Calculated properties of P ₂ , P ₄ , and of closed-shell clusters up to P ₁₈ . Journal of Chemical Physics, 1995, 102, 3703-3711.	1.2	93
113	Theoretical approach and first examples of N-acyl-thioformamides as dienophiles in the Diels-Alder reaction. Journal of the Chemical Society Chemical Communications, 1995, , 1897-1898.	2.0	11
114	The resonance Raman spectrum of cyclobutene. Journal of Chemical Physics, 1995, 103, 5911-5918.	1.2	21

#	ARTICLE	IF	CITATIONS
115	Analysis of Electronic Transitions as the Difference of Electron Attachment and Detachment Densities. <i>The Journal of Physical Chemistry</i> , 1995, 99, 14261-14270.	2.9	288
116	H-Atom Transfer and Rotational Processes in the Ground and First Singlet Excited Electronic States of 2-(2-Hydroxyphenyl)oxazole Derivatives: An Experimental and Theoretical Study. <i>The Journal of Physical Chemistry</i> , 1996, 100, 19789-19794.	2.9	86
117	Theoretical Calculations on Excited Electronic States of Benzaldehyde and Observation of the S ₂ †S ₀ Jet-Cooled Spectrum. <i>The Journal of Physical Chemistry</i> , 1996, 100, 17111-17123.	2.9	43
118	A Theoretical Study of Chlorine Atom and Methyl Radical Addition to Nitrogen Bases: Why Do Cl Atoms Form Two-Center Three-Electron Bonds Whereas CH ₃ Radicals Form Two-Center Two-Electron Bonds?. <i>Journal of the American Chemical Society</i> , 1996, 118, 10571-10576.	6.6	46
119	Coupled cluster calculations of the excitation energies of ethylene, butadiene, and cyclopentadiene. <i>Journal of Chemical Physics</i> , 1996, 105, 6979-6988.	1.2	141
120	Requirements for activation of surface oxygen atoms in MgO using the Laplacian of the electron density. <i>Surface Science</i> , 1996, 351, 233-249.	0.8	41
121	Observation of the Hammick Intermediate: Reduction of the Pyridine-2-ylid Ion in the Gas Phase. <i>Journal of the American Chemical Society</i> , 1996, 118, 11898-11904.	6.6	84
122	Vibronic structure of the emission spectra from single vibronic levels of the S ₁ manifold in naphthalene: Theoretical simulation. <i>Journal of Chemical Physics</i> , 1996, 104, 3486-3500.	1.2	48
123	On the Nature of Electronic Transitions in Radicals: An Extended Single Excitation Configuration Interaction Method. <i>The Journal of Physical Chemistry</i> , 1996, 100, 6131-6137.	2.9	71
124	On the theoretical investigation of vibronic spectra of ethylene by ab initio calculations of the Franck-Condon factors. <i>Journal of Chemical Physics</i> , 1996, 105, 9007-9020.	1.2	68
125	One-center trapping of the holes in alkali halide crystals. <i>Physical Review B</i> , 1996, 54, 962-969.	1.1	35
126	Response theory for static and dynamic polarizabilities of excited states. <i>Journal of Chemical Physics</i> , 1996, 105, 581-587.	1.2	46
127	UV Photoelectron and ab Initio Quantum Mechanical Evaluation of Nucleotide Ionization Potentials in Water Counterion Environments: Polarization Effects on DNA Alkylation by Carcinogenic Methylating Agents. <i>Journal of the American Chemical Society</i> , 1996, 118, 3694-3707.	6.6	53
128	Electronically Excited States of 1,4:5,8-Bismethano-1,4,4a,5,8,8a-hexahydronaphthalene, a Nonconjugated Diene: Comparison of Theory and Experiment. <i>Journal of the American Chemical Society</i> , 1996, 118, 1235-1240.	6.6	7
129	[31] Predicting physical properties of peroxytrinitrite by quantum mechanics. <i>Methods in Enzymology</i> , 1996, 269, 329-346.	0.4	2
130	Î±-Bond cleavage upon electronic excitation of acetyl chloride study of Cl single surfaces by full geometry optimization. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1996, 92, 373-375.	1.7	9
131	Time-Dependent Density Functional Response Theory of Molecular Systems: Theory, Computational Methods, and Functionals. <i>Theoretical and Computational Chemistry</i> , 1996, , 391-439.	0.2	255
132	Investigating the C-Cl Antibonding Character in the Î±* Excited State of Vinyl, Allyl, and Propargyl Chloride: Emission Spectra and ab Initio Calculations. <i>The Journal of Physical Chemistry</i> , 1996, 100, 7765-7771.	2.9	34

#	ARTICLE	IF	CITATIONS
133	Density functional study of isomerization of fluoro- and chloroformaldehyde radical cations. <i>Journal of Computational Chemistry</i> , 1996, 17, 1309-1317.	1.5	10
134	The Electronic Spectra of Ethylene. <i>Bulletin of the Chemical Society of Japan</i> , 1996, 69, 1901-1906.	2.0	9
135	Theoretical Study of the Electronic Structure of 2,2-Bisilole in Comparison with 1,1-Bi-1,3-cyclopentadiene: π -Conjugation and a Low-Lying LUMO as the Origin of the Unusual Optical Properties of 3,3,4,4-Tetraphenyl-2,2-bisilole. <i>Bulletin of the Chemical Society of Japan</i> , 1996, 69, 2327-2334.	2.0	236
136	Dissociation and isomerization reactions of formalimine on the ground and excited state surface. <i>Computational and Theoretical Chemistry</i> , 1996, 364, 97-106.	1.5	15
137	The photochemical isomerization of DAMN to ACI: stability of potential intermediates. <i>Computational and Theoretical Chemistry</i> , 1996, 364, 121-130.	1.5	4
138	Estimating molecular collision diameters using computational methods. <i>Computational and Theoretical Chemistry</i> , 1996, 365, 9-12.	1.5	19
139	An ab initio study of excited states of the phthalocyanine magnesium complex and its cation radical. <i>Chemical Physics Letters</i> , 1996, 260, 178-185.	1.2	19
140	Conformational potential energy surface of the FSO radical and its isomer FOS in the ground $2A_1$ state. <i>Computational and Theoretical Chemistry</i> , 1996, 388, 1-6.	1.5	5
141	Hartree-Fock symmetry-breaking in magnesium and nickel porphyrins. <i>Computational and Theoretical Chemistry</i> , 1996, 388, 293-297.	1.5	3
142	Theoretical study of the reaction of P^+ with methane. <i>Journal of Physical Organic Chemistry</i> , 1996, 9, 419-426.	0.9	4
143	Absorption maxima study of chromophores of indigoid dyes. <i>International Journal of Quantum Chemistry</i> , 1996, 60, 681-687.	1.0	6
144	Energetic and conformational study of four benzylimidazole compounds with μ_2 agonist profile: The mivazerol and three methylated derivatives. <i>International Journal of Quantum Chemistry</i> , 1996, 60, 911-930.	1.0	5
145	UV photoelectron and ab initio quantum mechanical characterization of nucleotides: The valence electronic structure of anionic 2'-deoxyadenosine-5'-phosphate. <i>International Journal of Quantum Chemistry</i> , 1996, 60, 1735-1743.	1.0	5
146	Simplified methods for equation-of-motion coupled-cluster excited state calculations. <i>Chemical Physics Letters</i> , 1996, 248, 189-198.	1.2	112
147	Study of prototypical Diels-Alder reactions by a hybrid density functional/Hartree-Fock approach. <i>Chemical Physics Letters</i> , 1996, 251, 393-399.	1.2	36
148	Treatment of electronic excitations within the adiabatic approximation of time dependent density functional theory. <i>Chemical Physics Letters</i> , 1996, 256, 454-464.	1.2	5,263
149	Theoretical study of molecular dynamics in model base pairs. <i>Chemical Physics Letters</i> , 1996, 256, 370-376.	1.2	90
150	$\tilde{\nu}$ -vibronic spectrum of ethylene from ab initio calculations of the Franck-Condon factors. <i>Chemical Physics Letters</i> , 1996, 258, 53-62.	1.2	57

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151	Density functional calculations with configuration interaction for the excited states of molecules. <i>Chemical Physics Letters</i> , 1996, 259, 128-137.	1.2	204
152	Ab initio MO investigations of molecular structures in the ground and first excited states of heterocyclic pyridinium betaine. <i>Chemical Physics Letters</i> , 1996, 261, 18-22.	1.2	22
153	The Spectroscopy of Formaldehyde. <i>Journal of Molecular Spectroscopy</i> , 1996, 176, 375-384.	0.4	23
154	Matrix-isolation FT-IR and ab initio $6\hat{a}^{\leftarrow}31 + + G\hat{a}^{\leftarrow}\hat{a}^{\leftarrow}$ study of 1-CH ₃ -adenine tautomerism. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1996, 52, 383-396.	2.0	16
155	Second-order perturbation theory using correlated orbitals. II. A coupled MCSCF perturbation strategy for electronic spectra and its applications to ethylene, formaldehyde and vinylidene. <i>Chemical Physics</i> , 1996, 205, 323-349.	0.9	24
156	Proton transfer between phenol and ammonia in ground and excited electronic states. <i>Chemical Physics Letters</i> , 1996, 262, 567-572.	1.2	59
157	Stereochemical aspects of the asymmetric synthesis of chiral $\hat{1}\pm, \hat{1}^2$ -dihydroxy phosphonates. Synthesis of $\hat{1}\pm, \hat{1}^2$ -dihydroxy phosphonic acids. <i>Tetrahedron: Asymmetry</i> , 1996, 7, 3485-3504.	1.8	14
158	Infrared and Raman spectra, ab initio calculations and vibrational assignment for 3-fluoro-1-butyne. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1996, 52, 1861-1873.	2.0	8
159	Infrared and Raman spectra, conformational stability, ab initio calculations and vibrational assignment for 1,2-pentadiene (ethyl allene). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1996, 52, 1843-1859.	2.0	13
160	S ₁ \hat{a}^{\leftarrow} S ₀ transition of phenylacetylene: ab initio and resonant two-photon ionization studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1996, 52, 1703-1716.	2.0	26
161	Calculations on ground and excited state potential energy surfaces of floppy free radicals: HC ₄ H ₂ , HC ₃ NH, and HC ₃ O. <i>Chemical Physics</i> , 1996, 213, 139-151.	0.9	15
162	Theoretical studies of (d-p) π bonding, electronic spectra, and reactivities in homo- and heterometallic clusters: [Mo ₃ -n W _n X ₄ (H ₂ O) ₉] ₄₊ (X = O, S, Se, Te; n = 0-3). <i>Journal of Cluster Science</i> , 1996, 7, 469-500.	1.7	11
163	The spasiba force field of model compounds related to lipids of biomembranes. <i>Journal of Molecular Structure</i> , 1996, 384, 55-71.	1.8	11
164	Conformational properties of o-alkoxy-benzamides in different solvents. <i>Journal of Molecular Structure</i> , 1996, 384, 9-16.	1.8	3
165	Far infrared spectra, conformational equilibria, vibrational assignments and ab initio calculations of 2-chloroethanol. <i>Journal of Molecular Structure</i> , 1996, 385, 7-21.	1.8	23
166	Ab initio study of singlet excited states of bicyclo[2.2.0]hexasilane and tricyclo[4.2.0.0 _{2,5}]octasilane. <i>Molecular Engineering</i> , 1996, 6, 363-371.	0.2	1
167	Experimental and theoretical characterization of the S ₁ \hat{a}^{\leftarrow} S ₀ transition of benzo[a]pyrene. <i>Journal of Chemical Physics</i> , 1996, 105, 7323-7335.	1.2	30
168	Excited and ionized states of free base porphin studied by the symmetry adapted cluster \hat{a} configuration interaction (SAC \hat{a} CI) method. <i>Journal of Chemical Physics</i> , 1996, 104, 2321-2329.	1.2	164

#	ARTICLE	IF	CITATIONS
169	Electronic excitation energies in copper selenide clusters. <i>Journal of Chemical Physics</i> , 1996, 104, 7113-7121.	1.2	17
170	Exploring chromium (VI) dioxodihalides chemistry: Is density functional theory the most suitable tool?. <i>Journal of Chemical Physics</i> , 1996, 104, 9499-9510.	1.2	28
171	Proton transfer in the ground and lowest excited states of malonaldehyde: A comparative density functional and post-Hartree-Fock study. <i>Journal of Chemical Physics</i> , 1996, 105, 11007-11019.	1.2	215
172	Characterization of ground and excited electronic state deprotonation energies of systems containing double bonds using natural bond orbital analysis. <i>Journal of Chemical Physics</i> , 1996, 105, 4675-4691.	1.2	5
173	Electronic states of ketene. <i>Journal of Chemical Physics</i> , 1996, 105, 1034-1045.	1.2	35
174	Charge Transfer Processes in Surface-Enhanced Raman Scattering. Franck-Condon Active Vibrations of Pyridine. <i>The Journal of Physical Chemistry</i> , 1996, 100, 9254-9261.	2.9	120
175	Ab Initio Study of the Electronic Spectrum of HOBr. <i>The Journal of Physical Chemistry</i> , 1996, 100, 9250-9253.	2.9	45
176	Structures, Relative Stabilities, and Vibrational Spectra of Isomers of HClO ₃ . <i>The Journal of Physical Chemistry</i> , 1996, 100, 573-579.	2.9	30
177	Conformational Control during the Photolysis of Matrix-Isolated Chloroformylketene: A Kinetic and Theoretical Studies of C ₃ O ₂ Formation. <i>The Journal of Physical Chemistry</i> , 1996, 100, 7034-7041.	2.9	28
178	Ab Initio Analysis of the Effects of Aqueous Solvation on the Resonance Raman Intensities of N-Methylacetamide. <i>The Journal of Physical Chemistry</i> , 1996, 100, 2731-2737.	2.9	73
179	The Spatial Extent of the V State of Ethylene and Its Relation to Dynamic Correlation in the Cope Rearrangement. <i>The Journal of Physical Chemistry</i> , 1996, 100, 6161-6166.	2.9	60
180	Ab Initio Study of the Low-Lying Electronic States of Indene. <i>The Journal of Physical Chemistry</i> , 1996, 100, 10869-10874.	2.9	18
181	Low-Lying Electronically Excited States of CH ₃ Cl: A Comparison of Theory and Experiment. <i>The Journal of Physical Chemistry</i> , 1996, 100, 5642-5648.	2.9	11
182	Ab Initio Calculations of the Excited States of Formamide. <i>The Journal of Physical Chemistry</i> , 1996, 100, 13487-13491.	2.9	40
183	Picosecond Time-Resolved Fourier-Transform Raman Spectroscopy and Normal-Mode Analysis of the Ground State and Singlet Excited State of Anthracene. <i>The Journal of Physical Chemistry</i> , 1996, 100, 11857-11862.	2.9	15
184	CH Stretching Overtone Investigation of Relative CH Bond Lengths in Pyridine. <i>The Journal of Physical Chemistry</i> , 1996, 100, 19273-19279.	2.9	26
185	Quantum ab Initio Study of Acetylene Adsorption on NaCl(100). II. Excited States and Photochemistry. <i>The Journal of Physical Chemistry</i> , 1996, 100, 17915-17922.	2.9	22
186	Cluster models for the photoabsorption of divalent defects in silicate glasses: Basis set and cluster size dependence. <i>Applied Physics Letters</i> , 1997, 71, 770-772.	1.5	15

#	ARTICLE	IF	CITATIONS
187	Nonadiabatic coupling of the 3p Rydberg and π^* valence states of acetone. Journal of Chemical Physics, 1997, 107, 675-679.	1.2	13
188	High resolution optothermal spectroscopy of pyridine in the S1 state. Journal of Chemical Physics, 1997, 107, 10399-10405.	1.2	21
189	Photoabsorption of the neutral oxygen vacancy in silicate and germanosilicate glasses: First-principles calculations. Physical Review B, 1997, 56, 5035-5038.	1.1	38
190	Solvation and the excited states of formamide. Journal of Chemical Physics, 1997, 107, 5771-5775.	1.2	53
191	Excited State Intramolecular Proton Transfer in Anionic Analogues of Malonaldehyde. Journal of Physical Chemistry A, 1997, 101, 5901-5909.	1.1	34
192	Boron dichloride and its cation Geometries, vibrational frequencies, ionization energy and excitation energies. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 53-61.	1.7	9
193	Structures and vibrations of ortho-, meta-, and para-fluoroanilines in the S0 and S1 states by ab initio calculations and resonant two-photon ionization spectroscopy. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 2981-2987.	1.7	42
194	On the photoisomerization of 5-hydroxytropolone: An ab initio and nuclear wave function study. Journal of Chemical Physics, 1997, 107, 6275-6282.	1.2	18
195	Lowest Triplet State of Indole: An ab Initio Study. Journal of Physical Chemistry A, 1997, 101, 2686-2691.	1.1	42
196	Inter-ring Torsional Modulation in Molecular Lasers. Ultraviolet Lasing via Amplified Spontaneous Emission Spectroscopy of Phenylimidazoles. Journal of Physical Chemistry A, 1997, 101, 5284-5291.	1.1	33
197	Manipulation of Dipole Moment and Hyperpolarizability Based on Heterocyclic Pyridinium Betaine Structures: Ab Initio and INDO/S MO Calculations. Journal of Physical Chemistry B, 1997, 101, 1910-1915.	1.2	35
198	Charge Fluxes and Changes in Electronic Structures as the Origin of Infrared Intensities in the Ground and Excited Electronic States. Journal of Physical Chemistry B, 1997, 101, 466-471.	1.2	25
199	Theoretical Study of the Structure, Energetics, and the π^* Electronic Transition of the Acetone +nH ₂ O (n= 1-3) Complexes. Journal of Physical Chemistry A, 1997, 101, 9925-9934.	1.1	36
200	Metastable States of Dimethylammonium, (CH ₃) ₂ NH ⁺ . Journal of Physical Chemistry A, 1997, 101, 3789-3799.	1.1	48
201	Heterocyclic Pyridinium Betaines, A New Class of Second-Order Nonlinear Optical Materials: A Combined Theoretical and Experimental Investigation of First-Order Hyperpolarizability through ab Initio, INDO/S, and Hyper-Rayleigh Scattering. Journal of Physical Chemistry B, 1997, 101, 576-582.	1.2	46
202	Interstellar Silicon-Nitrogen Chemistry. 4. Which Reaction Paths to HSiN and HNSi? An Extensive ab Initio Investigation with Crucial Consequences for Molecular Astrophysics. Journal of Physical Chemistry A, 1997, 101, 299-309.	1.1	13
203	Fluorescence Lifetime Measurements and Spectral Analysis of Adamantylidiazirine. Journal of the American Chemical Society, 1997, 119, 3580-3591.	6.6	51
204	Theoretical Study of Hyperpolarizabilities of Spirolinked Push-Pull Polyenes. Journal of Physical Chemistry A, 1997, 101, 1-4.	1.1	32

#	ARTICLE	IF	CITATIONS
205	Intramolecular Proton or Hydrogen-Atom Transfer in the Ground and Excited States of 2-Hydroxybenzoyl Compounds. Journal of Physical Chemistry A, 1997, 101, 7914-7921.	1.1	110
206	New and Unusual Bonding in Open Shell van der Waals Molecules Revealed by the Heavy Atom Effect: The Case of BAR. Journal of Physical Chemistry A, 1997, 101, 3166-3173.	1.1	14
207	On Calculating the Electronic Spectroscopy of Very Large Molecules. , 1997, , 249-289.		13
208	Using ab Initio MO Calculations To Understand the Photodissociation Dynamics of CH ₂ CCH ₂ and CH ₂ C ₂ . Journal of Physical Chemistry A, 1997, 101, 6638-6646.	1.1	29
209	Properties of Some Condensed Aromatic Systems. Journal of Organic Chemistry, 1997, 62, 5720-5727.	1.7	144
210	On Solvent Basicity: Analysis of the SB Scale. Journal of Physical Chemistry A, 1997, 101, 5183-5189.	1.1	59
211	Theoretical investigation of the adsorption of alkali metals on a Cu(111) surface. Surface Science, 1997, 385, 24-36.	0.8	32
212	Preparation and characterization of pyridinium-n-carboxylate trioxochromate (VI) (n=3, 4) and pyridinium-4-carboxylic pyridine-4 carboxylate trioxochromate (VI) hemihydrate. Inorganica Chimica Acta, 1997, 258, 53-63.	1.2	10
213	An Experimental and Computational Investigation of the Electrocyclic Ring Opening of $\dot{\text{I}}\pm$ -Fluorocyclopropyl Radicals. Tetrahedron, 1997, 53, 10071-10082.	1.0	5
214	A photoabsorption, photodissociation and photoelectron spectroscopy study of C ₂ H ₄ and C ₂ D ₄ . Chemical Physics, 1997, 219, 91-116.	0.9	96
215	Localization of $\dot{\text{I}}f$ molecular orbitals: towards a better description of the electronic excited states of large conjugated molecules. Chemical Physics, 1997, 219, 265-278.	0.9	11
216	The relationship between the molecular structure of semiquinone radicals and their g-values. Chemical Physics, 1997, 219, 291-304.	0.9	46
217	Single determinant calculations of excited state polarizabilities. Chemical Physics, 1997, 224, 201-214.	0.9	30
218	Theoretical study of the Ni-H tautomerism in free base porphyrin. Computational and Theoretical Chemistry, 1997, 390, 149-156.	1.5	20
219	Force field parameterization of copper(I)-olefin systems from density functional calculations. Computational and Theoretical Chemistry, 1997, 397, 39-50.	1.5	19
220	An ab initio study on excited and ground state properties of the organic fluorescence probe PRODAN. Computational and Theoretical Chemistry, 1997, 398-399, 341-346.	1.5	38
221	Full configuration interaction benchmarks for the states of methylene. Computational and Theoretical Chemistry, 1997, 400, 139-156.	1.5	21
222	Ab initio study of the ground and first excited singlet states of aniline. Computational and Theoretical Chemistry, 1997, 392, 181-191.	1.5	20

#	ARTICLE	IF	CITATIONS
223	A semiempirical study of the fluorescence properties of large charge transfer compounds: N,N'-dimethylanilino-bis-pyrazolopyridine. <i>Zeitschrift Fur Elektrotechnik Und Elektrochemie</i> , 1997, 101, 1836-1843.	0.9	7
224	Spectroscopy of Amplified Spontaneous Emission Laser Spikes in Phenyloxazoles. Prototype Classes. <i>Journal of Physical Chemistry A</i> , 1997, 101, 3260-3272.	1.1	45
225	Study of surfaces properties of fumed alumina/silica materials. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 1997, 127, 11-18.	2.3	21
226	Theoretical study of electronically excited cis- and trans-glyoxal. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1997, 53, 1153-1162.	2.0	12
227	A study of the excited state structure and vibrations of hydroquinone by ab initio calculations and resonant two-photon ionization spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1997, 53, 2595-2604.	2.0	23
229	Ab initio calculations of S1 excited state vibrational spectra of benzene, naphthalene and anthracene. <i>Chemical Physics</i> , 1997, 214, 229-241.	0.9	53
230	Vibrational analyses of the tetrathiosquarate ion based on ab initio molecular orbital and density functional calculations: Effect of the Jahn-Teller distortion in the excited electronic state on Raman intensities. <i>Chemical Physics</i> , 1997, 216, 67-79.	0.9	16
231	The electronic spectroscopy of 1,2,3-triazine. <i>Chemical Physics</i> , 1997, 221, 11-21.	0.9	14
232	Ab initio prediction of the spectra of carbon cumulenes. <i>Chemical Physics</i> , 1997, 223, 149-158.	0.9	18
233	Reaction mechanisms of phosphorus fluorides: An ab initio study. <i>Journal of Fluorine Chemistry</i> , 1997, 83, 27-30.	0.9	7
234	Spectra and structure of silicon containing compounds: XXIII. Raman and infrared spectra, conformational stability, vibrational assignment and ab initio calculations of dimethyl vinyl chlorosilane. <i>Journal of Molecular Structure</i> , 1997, 403, 57-71.	1.8	15
235	¹ H and ¹³ C NMR study and AM1 calculations of some azobenzenes and N-benzylideneanilines: effect of substituents on the molecular planarity. <i>Journal of Molecular Structure</i> , 1997, 412, 153-159.	1.8	22
236	The effect of halogen substitution on the torsion of the central bond of glyoxal (COH-COH). <i>Journal of Molecular Structure</i> , 1997, 406, 51-59.	1.8	13
237	Conformational studies of cyclopropylcarbonyl chloride from temperature-dependent FT-IR spectra of xenon solutions. <i>Journal of Molecular Structure</i> , 1997, 407, 11-26.	1.8	6
238	Photochemistry of formic acid in rare gas matrices: Double-doping experiments on the 193 nm induced photodecomposition. <i>Journal of Molecular Structure</i> , 1997, 436-437, 349-358.	1.8	28
239	DFT- and post-HF-study on structure and electronic excitation of acyclic and cyclic sulfur diimides. <i>Journal of Physical Organic Chemistry</i> , 1997, 10, 33-41.	0.9	17
240	Valence ionization potentials of anionic phosphate esters: An ab initio quantum mechanical study. <i>International Journal of Quantum Chemistry</i> , 1997, 65, 1095-1106.	1.0	5
241	Low-lying excited states of 4-dimethylaminobenzonitrile: equilibrium geometries, vibrational frequencies and charge transfer character. <i>Chemical Physics Letters</i> , 1997, 266, 521-526.	1.2	41

#	ARTICLE	IF	CITATIONS
242	Ab initio molecular orbital study of excited electronic states of the vinyl radical. <i>Chemical Physics Letters</i> , 1997, 275, 19-27.	1.2	47
243	A picosecond time-resolved resonance Raman study of S1 cis-stilbene. <i>Chemical Physics Letters</i> , 1997, 278, 56-62.	1.2	30
244	A diagnostic for the applicability of the CIS and CIS(D) excitation energy methods. <i>Chemical Physics Letters</i> , 1997, 279, 151-157.	1.2	32
245	The imide ion: potential energy surface and geometries. <i>Electrochimica Acta</i> , 1998, 43, 1375-1379.	2.6	164
246	Photoabsorption and fluorescence excitation of malononitrile in the vacuum UV region. <i>Chemical Physics Letters</i> , 1998, 282, 375-380.	1.2	4
247	Towards an understanding of the molecular mechanism of the unimolecular decomposition of the N-chloro- α -amino acids on the ground and excited states surfaces in aqueous medium. <i>Chemical Physics Letters</i> , 1998, 283, 294-300.	1.2	8
248	The gas-phase $RnX\hat{=}NO^+$ ($X=O, N, S$) cations: nitroso onium cations versus ion- $\hat{=}$ molecule complexes. <i>Chemical Physics Letters</i> , 1998, 283, 357-362.	1.2	9
249	A theoretical study of the decomposition of gold(I) complexes. <i>Chemical Physics Letters</i> , 1998, 286, 73-78.	1.2	7
250	Photodissociation of chlorobenzene at 266 nm. <i>Chemical Physics Letters</i> , 1998, 288, 429-432.	1.2	49
251	Electronic factor for photoinduced electron transfer in porphyrin- $\hat{=}$ bridge- $\hat{=}$ quinone systems. <i>Chemical Physics Letters</i> , 1998, 290, 136-142.	1.2	16
252	Interpretation of the electronic absorption spectrum of free base porphyrin by using multiconfigurational second-order perturbation theory. <i>Chemical Physics Letters</i> , 1998, 295, 195-203.	1.2	105
253	Role of the intramolecular hydrogen bond and ligand rigidity in the complexation of trifluoroacetylcycloalkanones with lanthanides: novel strategy for the design of organic ligands of high selectivity. <i>Inorganica Chimica Acta</i> , 1998, 267, 201-207.	1.2	11
254	Renormalization group approach for electronic excitations in atoms. <i>Chemical Physics Letters</i> , 1998, 290, 199-204.	1.2	7
255	Epitaxial growth of squaric acid. <i>Chemical Physics Letters</i> , 1998, 291, 419-424.	1.2	2
256	A time-dependent density functional theory study of the electronically excited states of formaldehyde, acetaldehyde and acetone. <i>Chemical Physics Letters</i> , 1998, 297, 60-64.	1.2	237
257	On the localization of the electronic excitation in supramolecules built up by equivalent units linked by hydrogen bonds. <i>Chemical Physics</i> , 1998, 228, 1-7.	0.9	4
258	Hybrid procedure of the ab initio molecular orbital (MO) method and the Monte Carlo samplings; application to cluster $B^+(H_2O)$. <i>Chemical Physics</i> , 1998, 237, 81-90.	0.9	1
259	Cation vibrational spectra of pyrimidine and its van der Waals complexes with Ar and N_2 by ZEKE photoelectron spectroscopy. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 1998, 97, 121-129.	0.8	23

#	ARTICLE	IF	CITATIONS
260	On the electronic structure of dihalogenophosphenium cations. <i>Computational and Theoretical Chemistry</i> , 1998, 422, 285-291.	1.5	8
261	MO ab initio study of the structural and electronic properties of the 5-lipoxygenase inhibitor zileuton. <i>Computational and Theoretical Chemistry</i> , 1998, 427, 237-242.	1.5	2
262	A study of the structures and vibrations of C ₆ H ₅ NH ₂ , C ₆ H ₅ NHD, C ₆ H ₅ ND ₂ , C ₆ D ₅ NH ₂ , C ₆ D ₅ NHD, and C ₆ D ₅ ND ₂ in the S ₁ state by ab initio calculations. <i>Computational and Theoretical Chemistry</i> , 1998, 428, 231-240.	1.5	64
263	A CIS study of the solvent effects on the electronic absorption spectra of push-pull ethylenes. <i>Computational and Theoretical Chemistry</i> , 1998, 429, 131-141.	1.5	7
264	A comparative analysis of the QCISD(T) and the CCSD(T) potential energy surfaces for the torsional mode of glyoxal (COHâ€“COH). <i>Computational and Theoretical Chemistry</i> , 1998, 433, 161-168.	1.5	8
265	Ab Initio study of the structure, cooperativity and vibrational properties of the H ₂ O:(HCl) ₂ hydrogen bonded complex. <i>Computational and Theoretical Chemistry</i> , 1998, 452, 55-66.	1.5	5
266	Effect of nonproximate atomic substitution on excited state intramolecular proton transfer. <i>Journal of Computational Chemistry</i> , 1998, 19, 129-138.	1.5	16
267	Method of calculating band shape for molecular electronic spectra. <i>Journal of Computational Chemistry</i> , 1998, 19, 781-796.	1.5	28
268	Structure of the T ₁ -state wave function of linear polyenes. <i>International Journal of Quantum Chemistry</i> , 1998, 67, 101-106.	1.0	6
269	Application of reaction path concept in intramolecular proton transfer. <i>Computers & Chemistry</i> , 1998, 22, 13-20.	1.2	1
270	Structures and vibrations of p-methylaniline in the S ₀ and S ₁ states studied by ab initio calculations and resonant two-photon ionization spectroscopy. <i>Journal of Molecular Structure</i> , 1998, 446, 93-102.	1.8	48
271	Structures and vibrations of p-dimethoxybenzene conformers in the S ₀ and S ₁ states studied by ab initio calculations and resonant two-photon ionization spectroscopy. <i>Journal of Molecular Structure</i> , 1998, 448, 91-100.	1.8	13
272	Conformational stability and structural parameters of CH ₃ CH ₂ CClO and other (CH ₃) _n CH ₃ â€“nCClO molecules. <i>Journal of Molecular Structure</i> , 1998, 449, 131-157.	1.8	4
273	Dielectric and conformational studies of hydrogen bonded acetone and acetonitrile system. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1998, 54, 299-304.	2.0	5
274	FT-IR spectroscopy in liquid xenon solution, ab initio calculations, normal coordinate analysis, and vibrational assignments of meso-2,4-dichloropentane and racemic-2,4-dichloropentane. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1998, 54, 419-437.	2.0	7
275	Vibrational spectroscopy of hydroxy-heterobiaryls. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1998, 54, 1291-1305.	2.0	9
276	Reassignment of the vibrational spectra of CHF ₂ CH ₃ (HFC-152a), CF ₃ CH ₃ (HFC-143a), CF ₃ CHF ₂ (HFC-125), and CHCl ₂ CF ₃ (HCFC-123). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1998, 55, 9-24.	2.0	14
277	Structures and vibrations of o-methylaniline in the S ₀ and S ₁ states studied by ab initio calculations and resonant two-photon ionization spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1998, 55, 153-162.	2.0	50

#	ARTICLE	IF	CITATIONS
278	Generation of neutral and cationic hydrogen shift isomers of pyridine: a combined experimental and computational investigation. <i>International Journal of Mass Spectrometry</i> , 1998, 179-180, 7-14.	0.7	54
279	In situ analysis of ash deposits from black liquor combustion. <i>Vibrational Spectroscopy</i> , 1998, 16, 95-103.	1.2	12
280	Stereospecific synthesis and crystal structure of the racemate of 1-thia-2-tellura-1(1-allyl-4-chloro)cyclopentane 2,2,2-trichloride. <i>Polyhedron</i> , 1998, 17, 2153-2159.	1.0	9
281	Ionization spectra of XONO ₂ (X=F, Cl, Br, I) studied by the SAC-CI method. <i>Chemical Physics</i> , 1998, 226, 113-123.	0.9	21
282	The importance of electron correlation for the ground state structure of porphycene and tetraoxaporphyrin-dication. <i>Chemical Physics</i> , 1998, 227, 331-348.	0.9	36
283	A theoretical study of the unimolecular decomposition of N-chloro- α -amino acids in aqueous solution. <i>Chemical Physics</i> , 1998, 229, 125-136.	0.9	9
284	Ab initio study of excited-state intramolecular proton dislocation in salicylic acid. <i>Chemical Physics</i> , 1998, 232, 257-265.	0.9	115
285	Time-resolved resonance Raman and molecular orbital studies of charge separation and intramolecular reorganisation. <i>Chemical Physics</i> , 1998, 234, 21-34.	0.9	21
286	Intramolecular proton transfer in the ground and the two lowest-lying singlet excited states of 1-amino-3-propenal and related species. <i>Chemical Physics</i> , 1998, 234, 1-19.	0.9	24
287	Ab initio calculations and supersonic jet studies on the geometry of 4-dimethylaminobenzonitrile (DMABN) and related compounds in the ground and excited state. <i>Chemical Physics</i> , 1998, 234, 35-57.	0.9	50
288	Many-body exchange effects in clusters of rare gases with a chromophore: He ₂ CO ₂ . <i>Chemical Physics</i> , 1998, 239, 573-591.	0.9	6
289	Temperature-programmed desorption of water from fumed silica, silica/titania, and silica/alumina. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1998, 172, 161-179.	1.9	98
290	ZEKE photoelectron spectroscopy and ab initio force-field calculation of 1,2,4,5-tetrafluorobenzene. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 1998, 88-91, 137-142.	0.8	4
291	Evidence for carbocation formation during the coadsorption of methanol and hydrogen on Pt(110). <i>Surface Science</i> , 1998, 418, 329-341.	0.8	9
292	Tuning the Excited-State Properties of Luminescent Rhenium(V) Benzylidyne Complexes Containing Phosphorus and Nitrogen Donor Ligands. <i>Organometallics</i> , 1998, 17, 1946-1955.	1.1	29
293	Raman Intensities Induced by Electrostatic Intermolecular Interaction and Related Nonlinear Optical Properties of a Conjugated π -Electron System: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 1998, 102, 8422-8425.	1.1	18
294	Ab Initio Study of the Triple-Proton-Transfer Reactions of Ground and Excited States of 7-Hydroxyquinoline in Methanol Solution. <i>Journal of the American Chemical Society</i> , 1998, 120, 7568-7576.	6.6	66
295	Ti ⁴⁺ and Zr ⁴⁺ inside Aluminosilicate and Borosilicate Cages: A Computational Study. <i>Journal of Physical Chemistry A</i> , 1998, 102, 3368-3371.	1.1	6

#	ARTICLE	IF	CITATIONS
314	Ab Initio Study of the Hydrogen Bond and Proton Transfer in 2-(2-Hydroxyphenyl)benzothiazole and 2-(2-Hydroxyphenyl)benzimidazole. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1560-1567.	1.1	98
315	Density-Functional Study of the Equilibrium Structures, Vibrational Spectra, and Energetics of CH ₃ OBr and CH ₃ BrO. <i>Journal of Physical Chemistry A</i> , 1998, 102, 9970-9974.	1.1	12
316	Matrix Isolation Fourier Transform Infrared and Ab Initio Studies of the 193-nm-Induced Photodecomposition of Formamide. <i>Journal of Physical Chemistry A</i> , 1998, 102, 6643-6650.	1.1	91
317	Linear and sublinear scaling formation of Hartree-Fock-type exchange matrices. <i>Journal of Chemical Physics</i> , 1998, 109, 1663-1669.	1.2	302
318	An efficient implementation of time-dependent density-functional theory for the calculation of excitation energies of large molecules. <i>Journal of Chemical Physics</i> , 1998, 109, 8218-8224.	1.2	4,690
319	Molecular excitation energies to high-lying bound states from time-dependent density-functional response theory: Characterization and correction of the time-dependent local density approximation ionization threshold. <i>Journal of Chemical Physics</i> , 1998, 108, 4439-4449.	1.2	4,596
320	Potential role of silanones in the photoluminescence-excitation, visible-photoluminescence-emission, and infrared spectra of porous silicon. <i>Physical Review B</i> , 1998, 57, 12002-12016.	1.1	48
321	Ab initio calculation of molecular energies including parity violating interactions. <i>Journal of Chemical Physics</i> , 1998, 109, 7263-7285.	1.2	160
322	Electron Transition Current Density in Molecules. 2. Ab Initio Calculations for Electronic Transitions in Ethylene and Formaldehyde. <i>Journal of Physical Chemistry A</i> , 1998, 102, 3352-3357.	1.1	34
323	A New Class of Carborane Compounds for Second-Order Nonlinear Optics: Ab Initio Molecular Orbital Study of Hyperpolarizabilities for 1-(1-X-Dicarba-closo-dodecaborane-1-yl)-closo-dodecaborate Dianion (X = 2, 7, 12). <i>Inorganic Chemistry</i> , 1998, 37, 172-173.	1.9	44
324	Relationship between static vibrational and electronic hyperpolarizabilities of π -conjugated push-pull molecules within the two-state valence-bond charge-transfer model. <i>Journal of Chemical Physics</i> , 1998, 109, 9987-9994.	1.2	100
325	Competition between Rotamerization and Proton Transfer in o-Hydroxybenzaldehyde. <i>Journal of the American Chemical Society</i> , 1998, 120, 10497-10503.	6.6	48
326	Emission spectroscopy of jet-cooled CS ₂ upon excitation of the $1\hat{1}\hat{g}+\hat{a}\hat{1}'1B2(1\hat{1}\hat{u}+)$ transition in the 4800-51000 cm ⁻¹ region. <i>Journal of Chemical Physics</i> , 1998, 109, 7835-7843.	1.2	19
327	Coupled-cluster calculations of the electronic excitation spectrum of free base porphyrin in a polarized basis. <i>Journal of Chemical Physics</i> , 1998, 108, 6790-6798.	1.2	98
328	A theoretical study of the isotope effects on the fluorescence excitation spectrum of 5-aminotropolone. <i>Journal of Chemical Physics</i> , 1998, 108, 8114-8122.	1.2	12
329	Photochemistry of (OCS) _n ⁺ cluster ions. <i>Journal of Chemical Physics</i> , 1998, 109, 1264-1270.	1.2	35
330	Ultrafast multiphoton ionization dynamics and control of NaK molecules. <i>Journal of Chemical Physics</i> , 1998, 109, 10740-10753.	1.2	12
331	Evidence for oxide formation from the single and multiphoton excitation of a porous silicon surface or silicon nanonparticles. <i>Journal of Applied Physics</i> , 1998, 83, 5985-5991.	1.1	10

#	ARTICLE	IF	CITATIONS
332	Excited state polarizabilities in solution obtained by cubic response theory: Calculations on para-, ortho-, and meta-nitroaniline. <i>Journal of Chemical Physics</i> , 1998, 109, 6351-6357.	1.2	33
333	The Thiosulfine-Dithiirane-Dithioester Manifold $R^{1,2}$ (CS_2). <i>Sulfur Reports</i> , 1998, 21, 1-42.	0.7	31
334	Photoluminescence studies of the light-emitting species in new materials for polymer devices. , 1999, , .		0
335	Quadratic response of molecules in a nonequilibrium and equilibrium solvation model: Generalizations to include both singlet and triplet perturbations. <i>Journal of Chemical Physics</i> , 1999, 111, 2678-2685.	1.2	10
336	A surprising asymmetric structure for the short-lived excited S1 state of 4,4'-bipyridine. <i>Journal of Chemical Physics</i> , 1999, 110, 6353-6364.	1.2	7
337	Ionization potentials of Li_nO ($2 \leq n \leq 70$) clusters: Experiment and theory. <i>Journal of Chemical Physics</i> , 1999, 110, 10316-10329.	1.2	88
338	Emission spectroscopy of photodissociating N_2O_4 excited near 200 nm to the $\tilde{e}^{\prime} \text{NO}_2^*/\tilde{n}^{\prime} \text{N}^*$ avoided crossing. <i>Journal of Chemical Physics</i> , 1999, 111, 8486-8495.	1.2	13
339	Frequency-dependent polarizabilities, hyperpolarizabilities, and excitation energies from time-dependent density-functional theory based on the quasienergy derivative method. <i>Journal of Chemical Physics</i> , 1999, 111, 2878-2888.	1.2	23
340	Theoretical study of the mechanism of electron transfer at photosynthetic reaction centers. I. Singlet excited states of free base porphyrin. <i>Journal of Chemical Physics</i> , 1999, 110, 2936-2946.	1.2	19
341	Electronic spectra of carbon chain anions: $C_{2n}H^{2-}$ ($n=5-12$). <i>Journal of Chemical Physics</i> , 1999, 111, 9280-9286.	1.2	21
342	Solvation and intramolecular reorganization in 9,9'-bianthryl: Analysis of resonance Raman excitation profiles and ab initio molecular orbital calculations. <i>Journal of Chemical Physics</i> , 1999, 111, 5999-6010.	1.2	17
343	Comparison of methods for calculating the properties of intramolecular hydrogen bonds. Excited state proton transfer. <i>Journal of Chemical Physics</i> , 1999, 111, 849-858.	1.2	23
344	Photodissociation of bromobenzene at 266 nm. <i>Journal of Chemical Physics</i> , 1999, 110, 2922-2927.	1.2	82
345	Effects of halogenation on the ionized and excited states of free-base and zinc porphyrins. <i>Journal of Chemical Physics</i> , 1999, 110, 9135-9144.	1.2	68
346	Ab Initio Molecular Orbital Calculations of Electronic Couplings in the LH2 Bacterial Light-Harvesting Complex of <i>Rps. Acidophila</i> . <i>Journal of Physical Chemistry B</i> , 1999, 103, 2543-2553.	1.2	188
347	Concerning the transannular bond in silatranes and germatranes: a quantum chemical study. <i>Journal of Organometallic Chemistry</i> , 1999, 577, 205-210.	0.8	49
348	An ab initio approach to bulk and surface properties of many-body energies and adsorptivity in MgO crystal. <i>Journal of Physics and Chemistry of Solids</i> , 1999, 60, 305-315.	1.9	36
349	Matrix-isolation infrared spectra and ab initio calculations of naphthalene in the T1 state. <i>Journal of Molecular Structure</i> , 1999, 475, 253-260.	1.8	23

#	ARTICLE	IF	CITATIONS
350	He I and He II spectra of 4-haloanilines. <i>Journal of Molecular Structure</i> , 1999, 475, 241-252.	1.8	6
351	Correlations between ab initio and experimental data for isolated 1:1 hydrogen-bonded complexes of pyridine and imidazole derivatives with water. <i>Journal of Molecular Structure</i> , 1999, 476, 27-43.	1.8	64
352	Intramolecular flexibility of DNA bases in adenine-thymine and guanine-cytosine Watson-Crick base pairs. <i>Journal of Molecular Structure</i> , 1999, 477, 15-21.	1.8	65
353	Structure and dynamics of conformationally non-rigid molecules in excited electronic states: Ab initio calculations of the R2CO (R=H, F, Cl). <i>Journal of Molecular Structure</i> , 1999, 480-481, 263-267.	1.8	7
354	Abnormally long Si-Si bonds in cyclotrisilane derivatives: nonbonded interactions?. <i>Journal of Molecular Structure</i> , 1999, 485-486, 27-31.	1.8	1
355	Conformational dependence of vibrational and molecular nonlinear optical properties in substituted benzenes: the role of π -electron conjugation and back-donation. <i>Journal of Molecular Structure</i> , 1999, 509, 11-28.	1.8	62
356	Ground and excited state polarizabilities and dipole transition properties of benzene from coupled cluster response theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1999, 55, 509-524.	2.0	37
357	Ab initio calculations of the absorption spectrum of chalcone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1999, 55, 525-537.	2.0	20
358	Similarity transformed equation of motion coupled-cluster study of excited states of selected azabenzene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1999, 55, 539-559.	2.0	52
359	Metastable states of dimethylsulfonium radical, (CH ₃) ₂ SH [•] . <i>International Journal of Mass Spectrometry</i> , 1999, 185-187, 639-649.	0.7	6
360	Competitive elimination of methane and ethylene from trimethylsilyl-substituted silylenium ions. <i>International Journal of Mass Spectrometry</i> , 1999, 185-187, 449-462.	0.7	1
361	Photoisomerization of N ₂ O ₃ in an Ar matrix. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 1999, 122, 1-5.	2.0	14
362	Chemical shifts in P-1s photoabsorption spectra of gaseous phosphorus compounds. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 1999, 101-103, 125-129.	0.8	10
363	Effect of deuteration on the fluorescence excitation spectrum of tropolone: a theoretical study. <i>Chemical Physics</i> , 1999, 246, 103-113.	0.9	2
364	Effects of chemical substitution upon excited state proton transfer. Fluoroderivatives of salicylaldehyde. <i>Chemical Physics</i> , 1999, 246, 65-74.	0.9	36
365	The electronic spectrum of 1, 4, 5, 8-tetraazaphthalene. <i>Chemical Physics</i> , 1999, 246, 229-246.	0.9	8
366	The ab-initio calculation of the gas phase ion mobility of Na ⁺ in N ₂ . <i>Chemical Physics</i> , 1999, 248, 127-135.	0.9	3
367	Ab initio study of the amino group twisting and wagging reaction paths in the intramolecular charge transfer of 4-(N,N-dimethylamino)benzonitrile. <i>Chemical Physics</i> , 1999, 240, 9-18.	0.9	54

#	ARTICLE	IF	CITATIONS
368	Energy gradient method for the ground, excited, ionized, and electron-attached states calculated by the SAC (symmetry-adapted cluster)/SAC+CI (configuration interaction) method. Chemical Physics, 1999, 242, 177-193.	0.9	57
369	Photodissociation of o-dichlorobenzene at 266 nm. Chemical Physics, 1999, 248, 285-292.	0.9	22
370	Valence and inner shell non-dipole excitation spectroscopy of polyatomic molecules by angle-resolved inelastic electron scattering at high energy. Journal of Electron Spectroscopy and Related Phenomena, 1999, 100, 237-257.	0.8	33
371	Time-dependent density functional theory for radicals. Chemical Physics Letters, 1999, 302, 375-382.	1.2	431
372	Geometric derivatives of excitation energies using SCF and DFT. Chemical Physics Letters, 1999, 308, 249-255.	1.2	357
373	Theoretical calculations of methylquinolinium tricyanoquinodimethanide (CH ₃ Q ⁺ 3CNQ) using a solvation model. Chemical Physics Letters, 1999, 313, 321-331.	1.2	22
374	Infrared spectra of Dewar 2-picoline in low-temperature argon matrices. Chemical Physics Letters, 1999, 308, 403-407.	1.2	7
375	Time-dependent density functional theory within the Tamm-Dancoff approximation. Chemical Physics Letters, 1999, 314, 291-299.	1.2	1,724
376	Ab initio investigations on the photophysics of indole. Chemical Physics Letters, 1999, 315, 293-298.	1.2	213
377	Ionization potentials of hypervalent LinC (2 ≤ n ≤ 10). European Physical Journal D, 1999, 9, 289-295.	0.6	19
378	DNA Mutations Induced by Proton and Charge Transfer in the Low-Lying Excited Singlet Electronic States of the DNA Base Pairs: A Theoretical Insight. Journal of Physical Chemistry A, 1999, 103, 6251-6256.	1.1	104
379	Toward reliable density functional methods without adjustable parameters: The PBE0 model. Journal of Chemical Physics, 1999, 110, 6158-6170.	1.2	14,178
380	Potential functions of inversion of R ₂ CO (R=H, F, Cl) molecules in the lowest excited electronic states. Russian Chemical Bulletin, 1999, 48, 640-646.	0.4	7
381	The structure of CX ₂ YNO (X, Y=F, Cl) molecules in the ground and lowest excited singlet electronic states. Russian Chemical Bulletin, 1999, 48, 1436-1441.	0.4	1
382	Ab initio study on reaction path and rate constant of the hydrogen atom abstraction reaction HNCO+N ⁺ NCO+NH. Computational and Theoretical Chemistry, 1999, 459, 37-46.	1.5	12
383	Ab initio investigations of nonadiabatic electron-transfer reactivity of monohydrated transition-metal-ion redox couples M ₂ +OH ₂ /M ₃ +OH ₂ (M=V, Cr, Mn and Fe). Computational and Theoretical Chemistry, 1999, 459, 145-154.	1.5	1
384	Golden-rule treatment of the O ₂ +O ² electron-transfer reaction. Computational and Theoretical Chemistry, 1999, 459, 177-186.	1.5	7
385	An ab initio study on the vibrational and electronic spectra of the molybdenum-sulfur clusters with Mo ₂ O _n S ₄ ⁿ⁻ (n=0-4) core. Computational and Theoretical Chemistry, 1999, 460, 27-35.	1.5	6

#	ARTICLE	IF	CITATIONS
386	Effect of adjoining aromatic ring upon excited state proton transfer, o-hydroxybenzaldehyde. Computational and Theoretical Chemistry, 1999, 467, 37-49.	1.5	76
387	Single configuration interaction study on conjugated betainic chromophores based on DFT optimized geometries. Computational and Theoretical Chemistry, 1999, 469, 163-176.	1.5	32
388	Molecular and electronic structures of trithiapentalene. Computational and Theoretical Chemistry, 1999, 488, 1-10.	1.5	7
389	Cr ²⁺ /OH ₂ /Cr ³⁺ /OH ₂ electron transfer reactivity: an ab initio study at UMP2/6-311+G* level including all electron correlation. Computational and Theoretical Chemistry, 1999, 489, 141-149.	1.5	4
390	Structures and thermochemistry of BHLFm(OH) _n and several XYBO compounds at the G-2 level of theory. Computational and Theoretical Chemistry, 1999, 465, 231-242.	1.5	18
391	Intramolecular proton transfer in 2-(2-hydroxyphenyl)benzoxazole: the reliability of ab initio calculations on simplified structures. Computational and Theoretical Chemistry, 1999, 489, 255-262.	1.5	31
392	Ab initio investigation of internal rotation in conjugated molecules and the orientation of NO ₂ in nitroaromatics: nitrobenzene, o-monofluoro- and o,o-difluoro-nitrobenzenes. Computational and Theoretical Chemistry, 1999, 467, 181-186.	1.5	24
393	Quantum molecular simulation of the H abstraction at C4 of DNA sugar moiety by the free radical OH. Computational and Theoretical Chemistry, 1999, 491, 237-247.	1.5	11
394	Intermolecular Bonds Bridging Two Anthracene Molecules in a β -Cyclodextrin. Journal of Solid State Chemistry, 1999, 144, 263-271.	1.4	4
395	Ab initio molecular orbital and density functional study of the C ₆ H ₆ ...I ₂ complex in the ground and excited electronic states. International Journal of Quantum Chemistry, 1999, 72, 307-318.	1.0	18
396	Solvatochromism of fluorophores with an intramolecular hydrogen bond and their use as probes in biomolecular cavity sites. International Journal of Quantum Chemistry, 1999, 72, 421-438.	1.0	51
397	Exact size consistency of multireference Møller-Plesset perturbation theory. International Journal of Quantum Chemistry, 1999, 72, 549-558.	1.0	25
398	Anomalous failure of configuration interaction Singles (CIS) method in the computation of the electronic states of N,N-bis(4-aminophenyl)-1,4-quinonediimine. International Journal of Quantum Chemistry, 1999, 75, 623-629.	1.0	7
399	Theoretical study for the Pt ₂ Au- and PtAu ₂ - ethylene interaction. International Journal of Quantum Chemistry, 1999, 75, 699-707.	1.0	4
400	Density Functional Derived Structures and Molecular Properties of Nickel Dithiolenes and Related Complexes. European Journal of Inorganic Chemistry, 1999, 1999, 1995-2004.	1.0	84
403	Supramolecular Structure of Precipitated Nanosize β -Carotene Particles. Angewandte Chemie - International Edition, 1999, 38, 2188-2191.	7.2	224
404	Density- and density-matrix-based coupled Kohn-Sham methods for dynamic polarizabilities and excitation energies of molecules. Journal of Chemical Physics, 1999, 110, 2785-2799.	1.2	120
405	Ab initio potential-energy functions for excited state intramolecular proton transfer: a comparative study of o-hydroxybenzaldehyde, salicylic acid and 7-hydroxy-1-indanone. Physical Chemistry Chemical Physics, 1999, 1, 3065-3072.	1.3	246

#	ARTICLE	IF	CITATIONS
406	Femtosecond Dynamics of Double Proton Transfer in a Model DNA Base Pair: 7-Azaindole Dimers in the Condensed Phase. <i>Journal of Physical Chemistry A</i> , 1999, 103, 7419-7431.	1.1	182
407	Ab Initio Calculations of Vibronic Spectra and Dynamics for Small Polyatomic Molecules: A Role of Duschinsky Effect. <i>Journal of Physical Chemistry A</i> , 1999, 103, 10674-10690.	1.1	139
408	The Six-Membered Intramolecular Hydrogen Bond Position as a Switch for Inducing an Excited State Intramolecular Proton Transfer (ESIPT) in Esters of o-Hydroxynaphthoic Acids. <i>Journal of Physical Chemistry A</i> , 1999, 103, 10921-10934.	1.1	68
409	Methylsulfonyl and Methoxysulfinyl Radicals and Cations in the Gas Phase. A Variable-Time and Photoexcitation Neutralization-Reionization Mass Spectrometric and ab Initio/RRKM Study. <i>Journal of Physical Chemistry A</i> , 1999, 103, 5348-5361.	1.1	44
410	Photoabsorption of the peroxide linkage defect in silicate glasses. <i>Journal of Chemical Physics</i> , 1999, 111, 8039-8042.	1.2	15
411	On electronic structure and electronically excited states of sulfines (thione S-oxides). <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 5547-5554.	1.3	13
412	Spectroscopy of low-coordinated surface sites: Theoretical study of MgO. <i>Physical Review B</i> , 1999, 59, 2417-2430.	1.1	164
413	Quasidegenerate second-order perturbation corrections to single-excitation configuration interaction. <i>Molecular Physics</i> , 1999, 96, 593-602.	0.8	42
414	Analytical second derivatives for excited electronic states using the single excitation configuration interaction method: theory and application to benzo[a]pyrene and chalcone. <i>Molecular Physics</i> , 1999, 96, 1533-1541.	0.8	49
415	Configuration interaction singles, time-dependent Hartree-Fock, and time-dependent density functional theory for the electronic excited states of extended systems. <i>Journal of Chemical Physics</i> , 1999, 111, 10774-10786.	1.2	181
416	Evolution of the electronic states of polyaniline: an ab initio analysis of the orbital states of PANi synthons. <i>Synthetic Metals</i> , 1999, 105, 107-113.	2.1	42
417	THE PHOTOPHYSICS OF SILVER HALIDE IMAGING MATERIALS. <i>Annual Review of Physical Chemistry</i> , 1999, 50, 117-144.	4.8	102
418	Formation of hydronium and water-hydronium complexes during coadsorption of hydrogen and water on (2 $\bar{1}$ -1)Pt(110). <i>Surface Science</i> , 1999, 419, 150-157.	0.8	59
419	Electronic structure of excited states at low-coordinated surface sites of MgO. <i>Surface Science</i> , 1999, 421, L157-L165.	0.8	37
420	Theoretical Evaluation of Solvent Effects on the Conformational and Tautomeric Equilibria of 2-(2-Hydroxyphenyl)benzimidazole and on Its Absorption and Fluorescence Spectra. <i>Journal of Physical Chemistry A</i> , 1999, 103, 4525-4532.	1.1	79
421	The Configuration Interaction Method: Advances in Highly Correlated Approaches. <i>Advances in Quantum Chemistry</i> , 1999, , 143-269.	0.4	294
422	Ions and Excited Electronic States. , 1999, , 319-337.		0
423	Ground and Triplet Excited Structures and Spectroscopic Properties of Halogenated Zinc-meso-Tetraphenylporphyrin. <i>Journal of Physical Chemistry A</i> , 1999, 103, 9378-9382.	1.1	37

#	ARTICLE	IF	CITATIONS
424	Electronic Spectra of the Carbon Chain Anions C _{2n-1} H ⁻ (n= 5~8) in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 1999, 103, 9712-9716.	1.1	18
425	Molecular dynamics of pyrazine after excitation to the S ₂ electronic state using a realistic 24-mode model Hamiltonian. <i>Journal of Chemical Physics</i> , 1999, 110, 936-946.	1.2	412
426	The Fragmentation of Melamine: A Study via Electron-Impact Ionization, Laser-Desorption Ionization, Collision-Induced Dissociation, and Density Functional Calculations of Potential Energy Surface. <i>Journal of Physical Chemistry B</i> , 1999, 103, 582-596.	1.2	25
427	Theoretical Study of the Q and B Bands of Free-Base, Magnesium, and Zinc Porphyrins, and Their Derivatives. <i>Journal of Physical Chemistry A</i> , 1999, 103, 1894-1904.	1.1	157
428	Excited-State Intramolecular Proton Transfer and Rotamerism of 2-(2-hydroxyvinyl)benzimidazole and 2-(2-hydroxyphenyl)imidazole. <i>Journal of Physical Chemistry A</i> , 1999, 103, 4413-4420.	1.1	78
429	Proton-Transfer Reaction in Isolated and Water-Complexed 8-Hydroxyimidazo[1,2-a]Pyridine in the S ₀ and S ₁ Electronic States. A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 1999, 103, 5301-5306.	1.1	11
430	Modeling Nucleobase Radicals in the Gas Phase. Experimental and Computational Study of 2-Hydroxypyridinium and 2-(1H)Pyridone Radicals. <i>Journal of Physical Chemistry A</i> , 1999, 103, 6268-6281.	1.1	53
431	Theoretical Studies of Electronically Excited States of Molecular Systems Using Multiconfigurational Perturbation Theory. <i>Accounts of Chemical Research</i> , 1999, 32, 137-144.	7.6	184
432	Use of Norbornadiene in Solar Energy Storage: A Theoretical Study of a Copper(I) Photosensitizer for the Norbornadiene-Quadracyclane Transformation. <i>Inorganic Chemistry</i> , 1999, 38, 1520-1522.	1.9	32
433	Conformations of ¹² F-Fluorophenetole and Their Reactivities Studied by Supersonic Jet/REMPI Spectroscopy. <i>Journal of Physical Chemistry A</i> , 1999, 103, 2302-2309.	1.1	7
434	Extension of the Neglect of Diatomic Differential Overlap Method to Spectroscopy. NDDO-G Parametrization and Results for Organic Molecules. <i>Journal of Physical Chemistry A</i> , 1999, 103, 4553-4559.	1.1	37
435	Ab Initio and Density Functional Calculations of the Energies of the Singlet and Triplet Valence Excited States of Pyrazine. <i>Journal of Physical Chemistry A</i> , 1999, 103, 9821-9829.	1.1	52
436	Dissociative Recombination of H ₃ O ⁺ . <i>Journal of Physical Chemistry A</i> , 1999, 103, 6552-6563.	1.1	27
437	Infrared Intensity-Carrying Modes and Electron-Vibration Interactions in the Radical Cations of Polycyclic Aromatic Hydrocarbons. <i>Journal of Physical Chemistry A</i> , 1999, 103, 5557-5566.	1.1	37
438	Competition between Dipolar Relaxation and Double Proton Transfer in the Electronic Spectroscopy of Pyrroloquinolines. <i>Journal of Physical Chemistry A</i> , 1999, 103, 2467-2475.	1.1	33
439	Ab Initio and Density-Functional Calculations of the Vibrational Structure of the Singlet and Triplet Excited States of Pyrazine. <i>Journal of Physical Chemistry A</i> , 1999, 103, 9830-9841.	1.1	65
440	Heterocyclic Radicals in the Gas Phase. An Experimental and Computational Study of 3-Hydroxypyridinium Radicals and Cations. <i>Journal of the American Chemical Society</i> , 1999, 121, 6010-6018.	6.6	49
441	Accurate excitation energies from time-dependent density functional theory: Assessing the PBE0 model. <i>Journal of Chemical Physics</i> , 1999, 111, 2889-2899.	1.2	661

#	ARTICLE	IF	CITATIONS
442	Calculation of the potential energy curves of the HgZn dimer. <i>Molecular Physics</i> , 2000, 98, 1051-1055.	0.8	5
443	Molecular Modeling of a Polar Rod-Like Aromatic Polyester Forming Nematic Liquid Crystal. Part 1. Ab Initio Study of Origin of Strong SHG-Activity. <i>Molecular Crystals and Liquid Crystals</i> , 2000, 346, 107-115.	0.3	2
444	Stimulated Blue Emission and Second Harmonic Generation From Films of Ultrasmall Si Nanoparticles. <i>Materials Research Society Symposia Proceedings</i> , 2000, 638, 1.	0.1	5
445	Excited singlet state time-resolved Raman spectra of 4,4'-bipyridine and quantum chemical analysis of resonance Raman intensities. <i>Journal of Raman Spectroscopy</i> , 2000, 31, 275-281.	1.2	7
446	Theoretical characterization of intramolecular proton transfer in the ground and the lowest-lying triplet excited states of 1-amino-3-propenal: a methodological comparison. <i>Journal of Computational Chemistry</i> , 2000, 21, 257-269.	1.5	11
447	Hartree-Fock instabilities and electronic properties. <i>Journal of Computational Chemistry</i> , 2000, 21, 483-504.	1.5	36
448	Ab initio study of organic mixed valency. <i>International Journal of Quantum Chemistry</i> , 2000, 76, 552-573.	1.0	21
449	The singular coincidence of fluorescence spectra of the anionic and cationic species formed by the respective deprotonated and protonated pyrido-pyrrolo bases. <i>International Journal of Quantum Chemistry</i> , 2000, 77, 118-127.	1.0	41
450	Q-Chem 2.0: a high-performance ab initio electronic structure program package. <i>Journal of Computational Chemistry</i> , 2000, 21, 1532-1548.	1.5	617
451	A theoretical study for the Pt ₃ -ethylene molecule interaction. <i>International Journal of Quantum Chemistry</i> , 2000, 80, 298-306.	1.0	0
452	Optical properties of trans-stilbene using semiempirical and time-dependent density functional theory: A comparative study. <i>International Journal of Quantum Chemistry</i> , 2000, 80, 672-680.	1.0	51
453	Preparation of Boron and Boron Phosphide Films by Photo- and Thermal Chemical Vapor Deposition Processes. <i>Journal of Solid State Chemistry</i> , 2000, 154, 39-44.	1.4	18
454	Novel substituted 1-amino-4,5,8-naphthalenetetracarboxylic acid-1,8-lactam-4,5-imides: experimental and theoretical study. <i>Journal of Physical Organic Chemistry</i> , 2000, 13, 705-712.	0.9	5
455	The ionization energy of the diazomethyl radical (HCNN). <i>Chemical Physics Letters</i> , 2000, 321, 129-134.	1.2	7
456	Conformational landscapes in amino acids: infrared and ultraviolet ion-dip spectroscopy of phenylalanine in the gas phase. <i>Chemical Physics Letters</i> , 2000, 321, 49-56.	1.2	241
457	On the theoretical reports on 7-azaindole base-pair phototautomerization. <i>Chemical Physics Letters</i> , 2000, 324, 75-80.	1.2	27
458	Torsional potential function of phenyl acetate in the S ₁ state as studied by fluorescence excitation spectroscopy in a supersonic free jet. <i>Chemical Physics Letters</i> , 2000, 324, 260-264.	1.2	9
459	Polyhedral azadiborane chemistry. The σ -converse TM synthesis of a small family of 6,9-(NHR)-bridged-arachno-5,10-dicarbododecaboranes. <i>Inorganica Chimica Acta</i> , 2000, 304, 268-273.	1.2	26

#	ARTICLE	IF	CITATIONS
460	Oxidative fluorination of S, Se and Te compounds. <i>Journal of Fluorine Chemistry</i> , 2000, 101, 279-283.	0.9	47
461	Conformational stability, structural parameters, and vibrational frequency assignments of ethylcyclobutane using infrared and Raman spectroscopy and ab initio calculations. <i>Journal of Molecular Structure</i> , 2000, 550-551, 1-20.	1.8	1
462	Ab initio analysis of the vibrational spectra of conformers of some branched alkanes. <i>Journal of Molecular Structure</i> , 2000, 550-551, 67-91.	1.8	20
463	Vibrational transition current density in (2S,3S)-oxirane-d 2 : visualizing electronic and nuclear contributions to IR absorption and vibrational circular dichroism intensities. <i>Journal of Molecular Structure</i> , 2000, 550-551, 123-134.	1.8	7
464	Intramolecular OH... interaction: the molecular structure and conformations of 3-hexyn-1,6-diol. <i>Journal of Molecular Structure</i> , 2000, 554, 191-202.	1.8	5
465	Quantum mechanical computations of collision-induced absorption in the second overtone band of hydrogen. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2000, 67, 303-321.	1.1	13
466	Molecular structures and vibrations of m-methylaniline in the S ₀ and S ₁ states studied by laser induced fluorescence spectroscopy and ab initio calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2000, 56, 1905-1915.	2.0	33
467	Modeling of SiGe deposition using quantum chemistry techniques for detailed kinetic analysis. <i>Materials Science in Semiconductor Processing</i> , 2000, 3, 31-39.	1.9	12
468	Ab initio quantum chemistry on a ccNUMA architecture using openMP. III. <i>Parallel Computing</i> , 2000, 26, 843-856.	1.3	10
469	Photoelectron spectroscopy of vinylbromide and intramolecular dynamics of the ionic B̃ ₁ ⁺ state. <i>Chemical Physics</i> , 2000, 256, 239-249.	0.9	22
470	Vibronic analyses of the lowest singlet-singlet and singlet-triplet band systems of pyridazine. <i>Chemical Physics</i> , 2000, 257, 1-20.	0.9	15
471	The photoabsorption and constant ionic state spectroscopy of vinylbromide. <i>Chemical Physics</i> , 2000, 260, 237-247.	0.9	31
472	Substituent effects on the intramolecular proton transfer in the ground and lowest-lying singlet excited states of salicylaldehyde. <i>Chemical Physics</i> , 2000, 260, 53-64.	0.9	22
473	Electronic spectra, excited-state geometries and molecular electrostatic potentials of aromatic amino acids. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2000, 137, 79-86.	2.0	17
474	An ab initio CI study of electronic spectra of substituted free-base porphyrins. <i>Chemical Physics Letters</i> , 2000, 318, 590-596.	1.2	11
475	Light-induced electron transfer in Tl[Ag(CN) ₂]: Photochemical reaction of luminescent metal-metal exciplexes in the solid state. <i>Inorganica Chimica Acta</i> , 2000, 300-302, 314-318.	1.2	8
476	Ab initio study of anomeric effect in 2,2-difluoroglycine. <i>Computational and Theoretical Chemistry</i> , 2000, 507, 281-287.	1.5	4
477	Low-lying electronic excitations of the green fluorescent protein chromophore. <i>Computational and Theoretical Chemistry</i> , 2000, 506, 179-189.	1.5	73

#	ARTICLE	IF	CITATIONS
478	Lowest singlet excited state geometries, rotational constants and molecular electrostatic potentials of some substituted benzenes: an ab initio study. Computational and Theoretical Chemistry, 2000, 531, 249-266.	1.5	22
479	The theoretical determination of heats of formation, proton affinities and gas basicities of N and C-substituted pyrazoles: analysis of the substituent effects on the gas-phase basicity. Computational and Theoretical Chemistry, 2000, 497, 241-266.	1.5	25
480	Dimers, trimers and oligomers of sulfur oxides: an ab initio and density functional study. Computational and Theoretical Chemistry, 2000, 530, 265-279.	1.5	13
481	Quantum molecular modeling of glutathione episulfonium. Computational and Theoretical Chemistry, 2000, 501-502, 449-458.	1.5	1
482	Synthesis and Photophysics of a 1-Pyrenyl Substituted 2'-Deoxyuridine-5-Carboxamide Nucleoside: Electron Transfer Products as CIS INDO/S Excited States. Journal of Physical Chemistry B, 2000, 104, 1637-1650.	1.2	31
483	From Classical Density Functionals to Adiabatic Connection Methods. The State of the Art.. Advances in Quantum Chemistry, 2000, 36, 45-75.	0.4	53
484	Quantum chemical investigation of the Disperse Orange 3 molecule cis-trans isomerization through linear transition state and design of molecular machines. , 2000, , .		2
485	Properties of atoms in molecules: Transition probabilities. Journal of Chemical Physics, 2000, 112, 10095-10105.	1.2	38
486	Theoretical approach to photochromism of aromatic Schiff bases: A minimal chromophore salicylidene methylamine. Journal of Chemical Physics, 2000, 113, 7845-7852.	1.2	86
487	Application of time-dependent density-functional theory to the 3 rd first excited state of H ₂ . Journal of Chemical Physics, 2000, 112, 527-530.	1.2	52
488	Naphthalene dimer: Electronic states, excimers, and triplet decay. Journal of Chemical Physics, 2000, 113, 8981-8994.	1.2	84
489	Including dispersion in configuration interaction-singles calculations for the spectroscopy of chromophores in solution. Journal of Chemical Physics, 2000, 112, 7293-7299.	1.2	49
490	Direct-dynamics approach to catalytic effects: The tautomerization of 3-hydroxyisoquinoline as a test case. Journal of Chemical Physics, 2000, 113, 2662-2670.	1.2	16
491	Quantum Chemical Design of Multivariable Anisotropic Random-Walk Molecular Devices Based on Stilbene and Azo-Dyes. Molecular Crystals and Liquid Crystals, 2000, 354, 475-484.	0.3	4
492	An efficient method for calculating molecular excitation energies by time-dependent density-functional theory. Journal of Chemical Physics, 2000, 113, 2088-2099.	1.2	129
493	Electronic excitation energies of small ZnSi clusters. Physical Review A, 2000, 63, .	1.0	26
494	Magnetic circular dichroism of symmetry and spin forbidden transitions of high-spin metal ions. Journal of Chemical Physics, 2000, 113, 5003.	1.2	28
495	Ultraviolet laser spectroscopy of jet-cooled CaNC and SrNC free radicals: Observation of bent excited electronic states. Journal of Chemical Physics, 2000, 113, 8945-8952.	1.2	10

#	ARTICLE	IF	CITATIONS
496	Semiclassical molecular dynamics simulations of intramolecular proton transfer in photoexcited 2-(2-hydroxyphenyl)oxazole. <i>Journal of Chemical Physics</i> , 2000, 113, 9510-9522.	1.2	59
497	Molecular calculations of excitation energies and (hyper)polarizabilities with a statistical average of orbital model exchange-correlation potentials. <i>Journal of Chemical Physics</i> , 2000, 112, 1344-1352.	1.2	699
498	A theoretical and experimental study of cyano- and alkoxy-substituted phenylenevinylene model compounds. <i>Synthetic Metals</i> , 2000, 111-112, 539-543.	2.1	36
499	Photodissociation of Nitrosobenzene (C ₆ H ₅ NO) at 266 nm. <i>Journal of Physical Chemistry A</i> , 2000, 104, 10079-10084.	1.1	9
500	Excited-State Double Proton Transfer in 3-Formyl-7-azaindole: A Role of the π^* State in Proton-Transfer Dynamics. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8863-8871.	1.1	26
501	Ab Initio Multiple Spawning: A Photochemistry from First Principles Quantum Molecular Dynamics. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5161-5175.	1.1	717
502	Interpretation of the electronic absorption spectrum of free-base porphyrin using time-dependent density-functional theory. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 2275-2281.	1.3	109
503	Photochromism of salicylideneaniline (SA). How the photochromic transient is created: A theoretical approach. <i>Journal of Chemical Physics</i> , 2000, 112, 6329-6337.	1.2	115
504	Gas-Phase Photoelectron Spectroscopic and Theoretical Studies of 1,2-Dichalcogenins: Ionization Energies, Orbital Assignments, and an Explanation of Their Color. <i>Journal of the American Chemical Society</i> , 2000, 122, 5065-5074.	6.6	27
505	Continuum solvent effects on various isomers of bilirubin. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 4884-4890.	1.3	12
506	Theoretical Studies of Excited State Proton Transfer in Small Model Systems. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5898-5909.	1.1	171
507	Effects of Alkyl Substituents on the Excited States of Naphthalene: A Semiempirical Study. <i>Journal of Physical Chemistry A</i> , 2000, 104, 1020-1029.	1.1	10
508	Extended similarity transformed equation-of-motion coupled cluster theory (extended-STEOM-CC): Applications to doubly excited states and transition metal compounds. <i>Journal of Chemical Physics</i> , 2000, 113, 494-507.	1.2	113
509	Theoretical study of the ground and excited states of silicon clusters: Si ₈ H _x . <i>Journal of Applied Physics</i> , 2000, 88, 4340.	1.1	3
510	An approximate ab initio method based on the DIM model. <i>Canadian Journal of Chemistry</i> , 2000, 78, 1575-1586.	0.6	4
511	Molecular-dynamics simulations of solvent effects in the intramolecular charge transfer of 4-(N,N-dimethylamino)benzonitrile. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 4341-4353.	1.3	39
512	Calculation of the Vibrational Spectra of Linear Tetrapyrroles. 2. Resonance Raman Spectra of Hexamethylpyromethene Monomers. <i>Journal of Physical Chemistry B</i> , 2000, 104, 10885-10899.	1.2	27
513	Dynamics of Excited Rare-Gas Atoms with Halide Molecules: The Ar(3P) + ClF → ArCl* + F, ArF* + Cl Reaction. <i>Journal of Physical Chemistry A</i> , 2000, 104, 10529-10537.	1.1	0

#	ARTICLE	IF	CITATIONS
514	An Experimental and ab Initio Study of Hypervalent LiOZn. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2980-2984.	1.1	6
515	The Low-Lying Excited States of Pyridine. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8389-8408.	1.1	125
516	Synthesis and Photophysics of a 1-Pyrenylmethyl-Substituted 2'-Deoxyuridine-5-Carboxamide Nucleoside: An Electron-Transfer Product Lifetimes and Energies. <i>Journal of Physical Chemistry B</i> , 2000, 104, 2166-2175.	1.2	22
517	Electrostatically Driven Geometry Changes Accompanying Charge Separation in Supposedly Rigid Bichromophoric Systems. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11628-11635.	1.1	19
518	Theoretical Study of the Excited State Properties and Transitions of 2-Aminopurine in the Gas Phase and in Solution. <i>Journal of Physical Chemistry A</i> , 2000, 104, 1930-1937.	1.1	35
519	Vibrational Spectra and Structures of Long-Chain Streptocyanine Dyes: An Effects of Electron-Vibration Interactions and Vibrational Polarizabilities. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11203-11211.	1.1	11
520	Lowest Excited Triplet State of Naphthalene by Transient Polarized Resonance Raman, Matrix-Isolation Infrared, and Density-Functional-Theory Methods. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11304-11309.	1.1	28
521	Stabilities, Excitation Energies, and Dissociation Reactions of CF ₂ Cl ₂ and CF ₂ Br ₂ : A Quantum Chemical Computations of Heats of Formation of Fluorinated Methanes, Methyls, and Carbenes. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11212-11219.	1.1	25
522	Franck-Condon Simulation of the S ₁ Spectrum of Phenol. <i>Journal of Physical Chemistry A</i> , 2000, 104, 10648-10655.	1.1	70
523	Photophysical Characteristics of Directly Linked Pyrene-Dimethylaniline Derivatives. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5700-5710.	1.1	46
524	Two-Photon Absorption and Second Hyperpolarizability of the Linear Quadrupolar Molecule. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11033-11040.	1.1	60
525	Theoretical Studies on Excited States of a Phenolate Anion in the Environment of Photoactive Yellow Protein. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2939-2952.	1.1	29
526	Folding Dendrons: The Development of Solvent-, Temperature-, and Generation-Dependent Chiral Conformational Order in Intramolecularly Hydrogen-Bonded Dendrons. <i>Journal of the American Chemical Society</i> , 2000, 122, 10298-10307.	6.6	85
527	Role of SiO in the Photoluminescence of Porous Silicon. <i>Journal of Physical Chemistry B</i> , 2000, 104, 9981-9986.	1.2	62
528	Conformational Geometries and Conformation-Dependent Photophysics of Jet-Cooled 1,3-Diphenylpropane. <i>Journal of Physical Chemistry A</i> , 2000, 104, 1456-1460.	1.1	15
529	Salting Benzenes. <i>Journal of Physical Chemistry B</i> , 2000, 104, 878-892.	1.2	42
530	Resonance Raman Spectroscopy as a Probe of the Bis(1/4-oxo)copper Core. <i>Journal of the American Chemical Society</i> , 2000, 122, 792-802.	6.6	91
531	Geometry, Vibrational Frequencies, and Ionization Energies of BeX ₂ (X = F, Cl, Br, and I). <i>Journal of Physical Chemistry A</i> , 2000, 104, 974-981.	1.1	8

#	ARTICLE	IF	CITATIONS
532	Remarkably Simple Relationship Connecting the Calculated Geometries of Isomolecular States of Three Different Multiplicities. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2195-2203.	1.1	20
533	Testing the Condon Approximation for Electron Transfer via the Mulliken-Hush Model. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8566-8569.	1.1	53
534	CIS INDO/S SCRF Study of Electron Transfer Excited States in a 1-Pyrenyl Substituted 1-Methyluracil-5-Carboxamide Nucleoside Model: Dielectric Continuum Solvation Effects on Electron Transfer States. <i>Journal of Physical Chemistry B</i> , 2000, 104, 125-136.	1.2	17
535	Photoinduced Proton Transfer and Rotational Motion of 1-Hydroxy-2-acetonaphthone in the S ₁ State: A Theoretical Insight into Its Photophysics. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8424-8431.	1.1	56
536	Theoretical Study of Ultraviolet Absorption Spectra of Tetra- and Pentacoordinate Silicon Compounds. <i>Journal of Physical Chemistry A</i> , 2000, 104, 4928-4935.	1.1	24
537	A DFT/MRCI study on the excited state charge transfer states of N-pyrrolobenzene, N-pyrrolobenzonitrile and 4-N,N-dimethylaminobenzonitrile. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 5545-5552.	1.3	77
538	Excited states theory for optimized orbitals and valence optimized orbitals coupled-cluster doubles models. <i>Journal of Chemical Physics</i> , 2000, 113, 6509-6527.	1.2	125
539	Fast Evaluation of Geometries and Properties of Excited Molecules in Solution: A Tamm-Dancoff Model with Application to 4-Dimethylaminobenzonitrile. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5631-5637.	1.1	541
540	Hydrogen Atom Adducts to Nitrobenzene: Formation of the Phenylnitronic Radical in the Gas Phase and Energetics of Wheland Intermediates. <i>Journal of the American Chemical Society</i> , 2000, 122, 9511-9524.	6.6	62
541	Theoretical Calculations of Band Gaps in the Aromatic Structures of Polythieno[3,4-b]benzene and Polythieno[3,4-b]pyrazine. <i>Journal of Physical Chemistry A</i> , 2000, 104, 7106-7112.	1.1	70
542	Molecular Orbital Study of the First Excited State of the OLED Material Tris(8-hydroxyquinoline)aluminum(III). <i>Chemistry of Materials</i> , 2001, 13, 2632-2640.	3.2	221
543	Two-Photon Absorption and Nonlinear Optical Properties of Octupolar Molecules. <i>Journal of the American Chemical Society</i> , 2001, 123, 10658-10667.	6.6	200
544	Perturbative corrections to coupled-cluster and equation-of-motion coupled-cluster energies: A determinantal analysis. <i>Journal of Chemical Physics</i> , 2001, 114, 3919-3928.	1.2	168
545	Ab Initio Based Exploration of the Potential Energy Surface for the Double Proton Transfer in the First Excited Singlet Electronic State of the 7-Azaindole Dimer. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3887-3893.	1.1	70
546	Reply to "Comment on "Photoinduced Proton Transfer and Rotational Motion of 1-Hydroxy-2-acetonaphthone in the S ₁ State: A Theoretical Insight into Its Photophysics" (J.Phys.Chem.A2000,104, 8424). <i>Journal of Physical Chemistry A</i> , 2001, 105, 7317-7320.	1.1	12
547	Shape corrections to exchange-correlation potentials by gradient-regulated seamless connection of model potentials for inner and outer region. <i>Journal of Chemical Physics</i> , 2001, 114, 652.	1.2	343
548	Assessment of the quality of orbital energies in resolution-of-the-identity Hartree-Fock calculations using deMon auxiliary basis sets. <i>Journal of Chemical Physics</i> , 2001, 114, 7342-7350.	1.2	38
549	Configuration interaction study of singlet excited state of thiophene and its cyano derivative oligomers. <i>Journal of Chemical Physics</i> , 2001, 115, 184-194.	1.2	22

#	ARTICLE	IF	CITATIONS
550	Intermolecular hydrogen bonding between carotenoid and bacteriochlorophyll in LH2. <i>FEBS Letters</i> , 2001, 496, 36-39.	1.3	17
551	LIF excitation spectra of o- and m-cyanoanilines. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 4874-4888.	1.3	16
552	The improved virtual orbital-complete active space configuration interaction method, a "packageable" efficient many-body method for describing electronically excited states. <i>Journal of Chemical Physics</i> , 2001, 114, 2592-2600.	1.2	95
553	Ab initio investigation of water complexes of some atmospherically important acids: HONO, HNO ₃ and HO ₂ NO ₂ . <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 1999-2006.	1.3	54
554	The electronic spectra of symmetric cyanine dyes: A CASPT2 study. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 3906-3912.	1.3	80
555	Theoretical prediction and direct observation of the hot molecules of pyrazolotriazole azomethine dyes by steady state fluorescence. <i>Perkin Transactions II RSC</i> , 2001, , 953-960.	1.1	1
556	Calculation of the Structures, Stabilities, and Properties of Mercury Sulfide Species in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2001, 105, 935-941.	1.1	36
557	Arene-mercury Complexes Stabilized Aluminum and Gallium Chloride: Synthesis and Structural Characterization. <i>Journal of the American Chemical Society</i> , 2001, 123, 11219-11228.	6.6	34
558	Dissociation Dynamics and Stability of Cyclic Alkoxy Radicals and Alkoxide Anions. <i>Journal of the American Chemical Society</i> , 2001, 123, 3125-3132.	6.6	17
559	Photodissociation of Ethylene Sulfide at 193 nm: A Photofragment Translational Spectroscopy Study with VUV Synchrotron Radiation and ab Initio Calculations. <i>Journal of the American Chemical Society</i> , 2001, 123, 148-161.	6.6	39
560	Time-Dependent Density Functional Theory Calculations of Photoabsorption Spectra in the Vacuum Ultraviolet Region. <i>Journal of Physical Chemistry A</i> , 2001, 105, 4953-4962.	1.1	226
561	Direct Observation of a Hydrogen Atom Adduct to C-5 in Uracil. A Neutralization-Reionization Mass Spectrometric and ab Initio Study. <i>Journal of Physical Chemistry A</i> , 2001, 105, 8339-8351.	1.1	26
562	Evidence of a Double Surface Crossing between Open- and Closed-Shell Surfaces in the Photodissociation of Cyclopropyl Iodide. <i>Journal of Physical Chemistry A</i> , 2001, 105, 1693-1701.	1.1	26
563	Direct Observation of a Hydrogen Atom Adduct to O-4 in Uracil. Energetics and Kinetics of Uracil Radicals. <i>Journal of Physical Chemistry A</i> , 2001, 105, 8352-8360.	1.1	35
564	S ₀ and S ₁ States of Monochlorophenols: Ab Initio CASSCF MO Study. <i>Journal of Physical Chemistry A</i> , 2001, 105, 9252-9257.	1.1	10
565	A Laser Flash Photolysis and Quantum Chemical Study of the Fluorinated Derivatives of Singlet Phenylnitrene. <i>Journal of the American Chemical Society</i> , 2001, 123, 1951-1962.	6.6	79
566	Computing the Properties of the Copper Thioarsenite Complex, CuAs(SH)(OH). <i>Inorganic Chemistry</i> , 2001, 40, 6487-6492.	1.9	8
567	Consecutive Photolyses of Naphthalenedicarboxylic Anhydrides in Low Temperature Matrixes: Experimental and Computational Studies on Naphthynes and Benzocyclopentadienyleneketenes. <i>Journal of Physical Chemistry A</i> , 2001, 105, 7790-7798.	1.1	26

#	ARTICLE	IF	CITATIONS
568	Chiral Molecules with Achiral Excited States: A Computational Study of 1,3-Dimethylallene. <i>Journal of Physical Chemistry A</i> , 2001, 105, 9509-9517.	1.1	16
569	The Ground- and Excited-State ($1n\pi^*$ and $1\pi\pi^*$) Carboxylic Acid-Catalyzed Proton (Hydrogen) Transfer. <i>Journal of Physical Chemistry A</i> , 2001, 105, 10475-10482.	1.1	15
570	Hydrogen Atom Adducts to the Amide Bond. Generation and Energetics of the Amino(hydroxy)methyl Radical in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2001, 105, 11144-11155.	1.1	47
571	Raman and Fluorescence Spectra of Size-Selected, Matrix-Isolated C_{14} and C_{18} Neutral Carbon Clusters. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3029-3033.	1.1	26
572	Hydroxyl Radical Adducts to Pyridine. The Generation and Properties of the Elusive N-Hydroxypyridyl Radical. <i>Journal of Physical Chemistry A</i> , 2001, 105, 9130-9141.	1.1	14
573	Enhanced Nonlinear Optical Response in Zwitterionic Molecules: A Computational Study on the Role of Orbital Interactions through π Bonds. <i>Journal of Physical Chemistry A</i> , 2001, 105, 8727-8733.	1.1	45
574	Theoretical Study of 5-phenyltropone in the S_0 and S_1 States. <i>Journal of Physical Chemistry A</i> , 2001, 105, 7273-7280.	1.1	8
575	The photodissociation dynamics of cyclic sulfides probed with tunable undulator radiation. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2001, 119, 127-145.	0.8	9
576	Electronic absorption spectra of closed and open-shell tetrathiafulvalenes: the first time-dependent density-functional study. <i>Tetrahedron</i> , 2001, 57, 7883-7892.	1.0	66
577	How different can the bond angles be in two conformers?. <i>Journal of Molecular Structure</i> , 2001, 567-568, 101-106.	1.8	1
578	Inter- and intramolecular O-H \cdots H hydrogen bonding in the methanol \cdots ethene complex and syn-7-norbornenol, probed by IR, 1H NMR and quantum chemistry. <i>Journal of Molecular Structure</i> , 2001, 567-568, 319-338.	1.8	10
579	Conformations of phthalan and 1,3-benzodioxole in their S_0 and S_1 (π,π^*) electronic states: theoretical study. <i>Journal of Molecular Structure</i> , 2001, 597, 235-240.	1.8	4
580	Quadruplevoids in amorphous Si:H. <i>Physica B: Condensed Matter</i> , 2001, 308-310, 155-158.	1.3	3
581	Temperature effects on the UV-Vis electronic spectrum of trans-stilbene. <i>International Journal of Quantum Chemistry</i> , 2001, 85, 557-568.	1.0	18
582	An ab initio study of the structures and energetics of the planar ground and 90° -twisted excited states of substituted ethylenes. <i>International Journal of Quantum Chemistry</i> , 2001, 82, 242-254.	1.0	18
583	A computational study on heterodimerization of charged porphyrins. <i>Journal of Porphyrins and Phthalocyanines</i> , 2001, 05, 512-522.	0.4	1
584	Ab initio computation of the UV resonance Raman intensity pattern of aqueous imidazole. <i>Journal of Raman Spectroscopy</i> , 2001, 32, 599-605.	1.2	21
585	Theoretical prediction of vertical transition energies of diaminosilylenes and aminosubstituted disilylenes. <i>Journal of Computational Chemistry</i> , 2001, 22, 1536-1541.	1.5	23

#	ARTICLE	IF	CITATIONS
588	Theoretical Characterization of Photoisomerization Channels of Dimethylpyridines on the Singlet and Triplet Potential Energy Surfaces. <i>Chemistry - A European Journal</i> , 2001, 7, 1927-1935.	1.7	7
589	Aurophilic Attraction and Luminescence of Binuclear Gold(I) Complexes with Bridging Phosphine Ligands: ab initio Study. <i>Chemistry - A European Journal</i> , 2001, 7, 4887-4893.	1.7	94
590	Exceptionally Long ($\approx 2.9 \text{ \AA}$) C-C Bonds between [TCNE] ⁺ Ions: Two-Electron, Four-Center $\sigma^*-\sigma^*$ C-C Bonding in $[\text{TCNE}]_2^{2+}$. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 2540-2545.	7.2	164
591	Organic Nanoparticles in the Aqueous Phase—Theory, Experiment, and Use. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 4330.	7.2	905
592	Excited states of carotenoid in LH2: an ab initio study. <i>Chemical Physics Letters</i> , 2001, 334, 159-167.	1.2	30
593	The nature of the exalted Kekulé vibration of styrene and other benzene derivatives in the S1 state. <i>Chemical Physics Letters</i> , 2001, 333, 297-303.	1.2	10
594	Size-consistent wave functions for bond-breaking: the equation-of-motion spin-flip model. <i>Chemical Physics Letters</i> , 2001, 338, 375-384.	1.2	430
595	Ring-Expansion Reaction of Cyano-Substituted Singlet Phenyl Nitrenes: A Theoretical Predictions and Kinetic Results from Laser Flash Photolysis and Chemical Trapping Experiments. <i>Journal of the American Chemical Society</i> , 2001, 123, 1425-1433.	6.6	51
596	Title is missing!. <i>Aquatic Geochemistry</i> , 2001, 7, 239-254.	1.5	4
597	Photoabsorption of dioxasilyrane and silanone groups at the surface of silica. <i>Journal of Chemical Physics</i> , 2001, 114, 4657.	1.2	46
598	Finite-field Møller-Plesset perturbation theory and coupled cluster calculations of the electric multipole moments and the dipole polarizability of As ₂ . <i>Chemical Physics</i> , 2001, 269, 137-146.	0.9	14
599	Understanding the solvatochromism of 10-hydroxybenzo[h]quinoline. An appraisal of a polarity calibrator. <i>Chemical Physics</i> , 2001, 270, 1-12.	0.9	14
600	Central atom 1s photoabsorption spectra of nitrogen and phosphorus AX ₃ (A=N, P and X=F, H) molecules. <i>Chemical Physics</i> , 2001, 273, 77-89.	0.9	8
601	Quantum chemical study of the electrochemical reduction of the [Co(H ₂ O) ₆] ²⁺ and [Co(NH ₃) ₅ (H ₂ O)] ²⁺ ions. <i>Electrochimica Acta</i> , 2001, 46, 2749-2755.	2.6	6
602	The thiocarbonyl chromophore. A time-dependent density-functional study. <i>Computational and Theoretical Chemistry</i> , 2001, 538, 253-260.	1.5	32
603	Comparative theoretical study of the electronic structures and electronic spectra of Fe ²⁺ , Fe ³⁺ -porphyrin and free base porphyrin. <i>Computational and Theoretical Chemistry</i> , 2001, 539, 107-117.	1.5	17
604	Push-pull dyes containing malononitrile dimer as acceptor: synthesis, spectroscopy and quantum chemical calculations. <i>Computational and Theoretical Chemistry</i> , 2001, 543, 129-146.	1.5	18
605	Dependence of state-universal coupled-cluster energies on the model-space-defining orbitals for states of varying quasidegeneracy. <i>Computational and Theoretical Chemistry</i> , 2001, 547, 55-68.	1.5	2

#	ARTICLE	IF	CITATIONS
606	A critical comparison of theoretical and experimental electronic spectrum and potential energy curves of HF molecule and its positive and negative ions. Computational and Theoretical Chemistry, 2001, 547, 83-96.	1.5	16
607	Structural studies on conformationally defined 6-s-trans UAB retinoids. Computational and Theoretical Chemistry, 2001, 549, 39-45.	1.5	1
608	A CIS study of solvent effects on the electronic absorption spectrum of Reichardt's dye. Computational and Theoretical Chemistry, 2001, 572, 203-212.	1.5	22
609	Keeping Mars warm with new super greenhouse gases. Proceedings of the National Academy of Sciences of the United States of America, 2001, 98, 2154-2157.	3.3	43
610	Electronic excited-state wave functions for quantum Monte Carlo: Application to silane and methane. Journal of Chemical Physics, 2001, 114, 7795-7804.	1.2	28
611	Geometry optimization of excited valence states of formaldehyde using analytical multireference configuration interaction singles and doubles and multireference averaged quadratic coupled-cluster gradients, and the conical intersection formed by the $1\hat{A}'$ and $2\hat{A}'$ states. Journal of Chemical Physics, 2001, 114, 746.	1.2	38
612	Excitons in small hydrogenated Si clusters. Physical Review B, 2001, 64, .	1.1	46
613	Microstructure of local defects in amorphous Si:H: a quantum chemical study. Physical Review B, 2001, 64, .	1.1	3
614	Electronic structure studies of six-atom gold clusters. Journal of Chemical Physics, 2001, 114, 10695-10701.	1.2	38
615	Theoretical study of photochromism of N-salicylidene- \pm -methylbenzylamine. Journal of Chemical Physics, 2001, 115, 8351-8358.	1.2	20
616	Electronic structure of halogen-substituted methyl radicals: Excited states of CH ₂ Cl and CH ₂ F. Journal of Chemical Physics, 2001, 115, 7485-7494.	1.2	17
617	A crystalline orbital study of polydiacetylenes. Journal of Chemical Physics, 2001, 114, 9130-9141.	1.2	24
618	Photodissociation of the dibromomethane cation at 355 nm by means of ion velocity imaging. Journal of Chemical Physics, 2001, 115, 6012-6017.	1.2	21
619	Effect of surface reconstruction on the structural prototypes of ultrasmall ultrabright Si ₂₉ nanoparticles. Applied Physics Letters, 2001, 78, 1918-1920.	1.5	107
620	The role of charge-transfer states of the metal-adsorbate complex in surface-enhanced Raman scattering. Journal of Chemical Physics, 2002, 116, 7207-7216.	1.2	122
621	Quantitative prediction of optical excitations in conjugated organic oligomers: A density functional theory study. Journal of Chemical Physics, 2002, 117, 5921-5928.	1.2	76
622	Optical gaps of alkali borate and alkali fluoroborate glasses. Journal of Applied Physics, 2002, 91, 4149-4153.	1.1	42
623	Anisole-(H ₂ O) _n (n=1-3) complexes: An experimental and theoretical investigation of the modulation of optimal structures, binding energies, and vibrational spectra in both the ground and first excited states. Journal of Chemical Physics, 2002, 117, 8805-8822.	1.2	70

#	ARTICLE	IF	CITATIONS
624	Theoretical study of excited state proton transfer in 3,6-bis(benzoxazolyl)pyrocatechol (BBPC). <i>Journal of Chemical Physics</i> , 2002, 116, 7486-7494.	1.2	8
625	A computational study of photoisomerization in Al ₃ O ₃ ⁺ clusters. <i>Journal of Chemical Physics</i> , 2002, 117, 1077-1084.	1.2	22
626	Vibronic coupling in excited states of acetone. <i>Journal of Chemical Physics</i> , 2002, 116, 547-560.	1.2	25
627	Dissociation dynamics of gauche and anti conformations of 1-iodopropane ions prepared selectively by vacuum-ultraviolet mass-analyzed threshold ionization spectrometry: Photodissociation at 426 and 355 nm. <i>Journal of Chemical Physics</i> , 2002, 117, 124-131.	1.2	12
628	A combined nuclear dynamics and electronic study of the coupling between the internal rotation of the methyl group and the intramolecular proton transfer in 5-methyltropolone. <i>Journal of Chemical Physics</i> , 2002, 117, 7525-7533.	1.2	21
629	An experimental and ab initio investigation of the low-frequency vibrations of coumaran. <i>Journal of Chemical Physics</i> , 2002, 116, 7855-7867.	1.2	9
630	Ab Initio Quantum Molecular Dynamics. <i>Advances in Chemical Physics</i> , 2002, , 439-512.	0.3	279
631	AB Initio Reaction Paths and Potential-Energy Functions for Excited-State Intra- and Intermolecular Hydrogen-Transfer Processes. , 2002, , 93-118.		4
632	Controlled Alcohol-Ketone Interconversion by Dihydrogen Transfer: An ab Initio Study of the Methanol-Formaldehyde Complex. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9512-9519.	1.1	11
633	Vibrational Transition Current Density: Visualizing the Origin of Vibrational Circular Dichroism and Infrared Intensities. <i>ACS Symposium Series</i> , 2002, , 65-78.	0.5	1
634	FEMTO- AND PICOSECOND FLUORESCENCE DYNAMICS OF MEROCYANINE 540: EXPERIMENTS AND MODELING. , 2002, , .		1
635	Substituent Effects upon Protonation-Induced Red Shift of Phenyl-Pyridine Copolymers. <i>Journal of Physical Chemistry B</i> , 2002, 106, 534-539.	1.2	12
636	Protonated Carbonic Acid and the Trihydroxymethyl Radical in the Gas Phase. A Neutralization-Reionization Mass Spectrometric and ab Initio/RRKM Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5938-5950.	1.1	20
637	Excited States of 4-Aminobenzonitrile (ABN) and 4-Dimethylaminobenzonitrile (DMABN): Time-resolved Resonance Raman, Transient Absorption, Fluorescence, and ab Initio Calculations. <i>Journal of Physical Chemistry A</i> , 2002, 106, 3294-3305.	1.1	75
638	Switchable Electronic Coupling in Model Oligoporphyrin Molecular Wires Examined through the Measurement and Assignment of Electronic Absorption Spectra. <i>Journal of the American Chemical Society</i> , 2002, 124, 9299-9309.	6.6	106
639	Phototautomerism in Uracil: A Quantum Chemical Investigation. <i>Journal of Physical Chemistry A</i> , 2002, 106, 8642-8650.	1.1	49
640	High-Resolution Excited-State Photoelectron Spectroscopy of the Lower Rydberg States of Jet-Cooled C ₂ H ₄ and C ₂ D ₄ . <i>Journal of Physical Chemistry A</i> , 2002, 106, 3727-3737.	1.1	15
641	Vibrational Analysis of trans-Stilbene in the Ground and Excited Singlet Electronic States Revisited. <i>Journal of Physical Chemistry A</i> , 2002, 106, 3318-3324.	1.1	60

#	ARTICLE	IF	CITATIONS
642	Resonance Raman Spectra Simulation of the 4,4'-Bipyridine Anion Radical and N-Protonated Radical. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4168-4175.	1.1	18
643	Isolated Building Blocks of Photonic Materials: A High-Resolution Excited-State Photoelectron Spectroscopy of Jet-Cooled Tetramethylethylene and 1,1'-Bicyclohexylidene. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5249-5262.	1.1	13
644	Multistate Effects in Calculations of the Electronic Coupling Element for Electron Transfer Using the Generalized Mulliken-Hush Method. <i>Journal of Physical Chemistry A</i> , 2002, 106, 3930-3940.	1.1	93
645	Density Functional Theory Investigation of Cobalt Siting in Ferrierite. <i>Journal of Physical Chemistry B</i> , 2002, 106, 10864-10872.	1.2	17
646	First Gas-Phase Detection of Dimethylstannylene and Time-Resolved Study of Some of Its Reactions. <i>Journal of the American Chemical Society</i> , 2002, 124, 7555-7562.	6.6	24
647	Photodissociation Dynamics of Various Conformers of Iodobutane Isomer Ions Prepared Selectively by Vacuum Ultraviolet Mass-Analyzed Threshold Ionization. <i>Journal of the American Chemical Society</i> , 2002, 124, 7614-7621.	6.6	17
648	Interaction of Water Molecules with Cytosine Tautomers: An Excited-State Quantum Chemical Investigation. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11338-11346.	1.1	78
649	Vibrational and Electronic Spectroscopy of the Fluorene Cation. <i>Journal of Physical Chemistry A</i> , 2002, 106, 63-73.	1.1	41
650	The Nature of the Intramolecular Charge Transfer Excited State in p-Pyrrolocyanobenzene (PBN) and Other Derivatives of Benzene Substituted by Electron Donor and Acceptor Groups. <i>Journal of Physical Chemistry A</i> , 2002, 106, 1-11.	1.1	97
651	Vibrational Polarization and Opsin Shift of Retinal Schiff Bases: A Theoretical Study. <i>Journal of the American Chemical Society</i> , 2002, 124, 9272-9277.	6.6	9
652	A Time-Dependent DFT Study on Band Gaps and Effective Conjugation Lengths of Polyacetylene, Polyphenylene, Polypentafulvene, Polycyclopentadiene, Polypyrrole, Polyfuran, Polysilole, Polyphosphole, and Polythiophene. <i>Macromolecules</i> , 2002, 35, 1109-1115.	2.2	205
653	Large and Fast Relaxations inside a Protein: A Calculation and Measurement of Reorganization Energies in Alcohol Dehydrogenase. <i>Journal of Physical Chemistry B</i> , 2002, 106, 11658-11665.	1.2	86
654	The First Singlet (n, π^*) and (π, π^*) Excited States of the Hydrogen-Bonded Complex between Water and Pyridine. <i>Journal of Physical Chemistry A</i> , 2002, 106, 8769-8778.	1.1	63
655	Structure and Photophysics of an Old, New Molecule: 1,3,6,8-Tetraazatricyclo[4.4.1.1 ^{3,8}]dodecane. <i>Journal of the American Chemical Society</i> , 2002, 124, 149-158.	6.6	10
656	A Comparative Theoretical Study on DMABN: Significance of Excited State Optimized Geometries and Direct Comparison of Methodologies. <i>Journal of Physical Chemistry A</i> , 2002, 106, 804-815.	1.1	65
657	Asymmetry and long-range character of lattice deformation by neutral oxygen vacancy in $\hat{\pm}$ -quartz. <i>Physical Review B</i> , 2002, 66, .	1.1	131
658	Excited-State Intramolecular Proton Transfer in 2-(2'-Tosylaminophenyl)benzimidazole. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7655-7663.	1.1	70
659	Perturbative corrections to the equation-of-motion spin-flip self-consistent field model: Application to bond-breaking and equilibrium properties of diradicals. <i>Journal of Chemical Physics</i> , 2002, 116, 3194-3203.	1.2	192

#	ARTICLE	IF	CITATIONS
660	Photophysics of trioxatriangulenium ion. Electrophilic reactivity in the ground state and excited singlet state. <i>Photochemical and Photobiological Sciences</i> , 2002, 1, 763-773.	1.6	27
661	Effects of surface termination on the band gap of ultrabrightSi29nanoparticles: Experiments and computational models. <i>Physical Review B</i> , 2002, 65, .	1.1	43
662	Color Changes Caused by Conformational Polymorphism:Â Optical-Crystallography, Single-Crystal Spectroscopy, and Computational Chemistry. <i>Journal of Physical Chemistry A</i> , 2002, 106, 544-550.	1.1	88
663	Electron Localization in Solid Acetonitrile. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9132-9144.	1.1	28
664	A Theoretical Investigation of Excited-State Properties of the Adenineâ”Uracil Base Pair. <i>Journal of Physical Chemistry A</i> , 2002, 106, 1011-1018.	1.1	30
665	Theoretical Determination of Chromophores in the Chromogenic Effects of Aromatic Neurotoxicants. <i>Journal of the American Chemical Society</i> , 2002, 124, 2744-2752.	6.6	38
666	Thermoreversible photocyclization of a pyrazolotriazole to a triazasemibullvalene: a novel electrocyclic reaction Electronic supplementary information (ESI) available: structures and energies of all stationary points located in the course of the study, in the form of Gaussian input files, followed by energies and, where available, thermal corrections from frequency calculations. See http://www.rsc.org/suppdata/pp/b1/b106231j/ . <i>Photochemical and Photobiological Sciences</i> , 2002, 1, 38-44.	1.6	8
667	Intramolecular charge transfer and first-order hyperpolarizability of planar and twisted sesquifulvalenes. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5566-5571.	1.3	28
668	Singlet-triplet gaps in diradicals by the spin-flip approach: A benchmark study. <i>Journal of Chemical Physics</i> , 2002, 117, 4694-4708.	1.2	321
669	Functionalizing the GaN(0001)-(1Å–1) surface II. Chemisorption of 3-pyrroline. <i>Surface Science</i> , 2002, 499, 124-134.	0.8	20
671	Ground and excited states of 2-hydroxyaniline trimers: comparison of Î”SCF and CIS. <i>Computational and Theoretical Chemistry</i> , 2002, 577, 35-42.	1.5	10
672	Chalcogen-Bridged Copper Clusters. <i>European Journal of Inorganic Chemistry</i> , 2002, 2002, 279-317.	1.0	164
673	Electronic Excitations in Pyrrole: A Test Case for Determination of Chromophores in the Chromogenic Effects of Neurotoxic Hydrocarbons by Time-Dependent Density Functional Theory and Single-Excitation Configuration Interaction Methods. <i>Journal of Molecular Spectroscopy</i> , 2002, 216, 81-89.	0.4	12
674	The R2PI Spectroscopy of Tyrosine: A Vibronic Analysis. <i>Journal of Molecular Spectroscopy</i> , 2002, 215, 204-219.	0.4	105
675	Theoretical investigation of electron transfer transition in tetracyanoethylene-contained organic complexes. <i>Journal of Computational Chemistry</i> , 2002, 23, 874-886.	1.5	9
676	FA(I):Au+ andFA(II):Cu+ laser activity and photographic sensitization at the low coordinated surfaces of AgBrab initio calculations. <i>Journal of Computational Chemistry</i> , 2002, 23, 1104-1120.	1.5	13
677	F + tunable laser activity and interaction of atomic halogens (F, Cl and Br) at the low coordinated surface sites of SrO. <i>Journal of Molecular Modeling</i> , 2002, 8, 314-326.	0.8	11
678	A reinvestigation of the molecular structures, vibrations and rotation of methyl group in o-methylaniline in S0 and S1 states studied by laser induced fluorescence spectroscopy and ab initio calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2002, 58, 1069-1081.	2.0	34

#	ARTICLE	IF	CITATIONS
679	Towards the characterization of the mechanism of the sequential activation of four methane molecules by Ta+. <i>International Journal of Mass Spectrometry</i> , 2002, 219, 457-473.	0.7	20
680	Generation and characterization of ionic and neutral P(OH) ₂ ⁺ in the gas phase by tandem mass spectrometry and computational chemistry. <i>Journal of the American Society for Mass Spectrometry</i> , 2002, 13, 250-264.	1.2	11
681	Spectroscopic and structural study of complexes of quercetin with Al(III). <i>Journal of Inorganic Biochemistry</i> , 2002, 92, 19-27.	1.5	241
682	Quantum chemical studies of the spectroscopic properties of the E-64 protease inhibitor. <i>Computational and Theoretical Chemistry</i> , 2002, 585, 129-141.	1.5	1
683	Computational study of chemo- and stereoselectivity of \hat{I}^{\pm} -cis, \hat{I}^{\pm} -trans and \hat{I}^{\pm} -trans-himachalene epoxidation by MCPBA. <i>Computational and Theoretical Chemistry</i> , 2002, 588, 201-210.	1.5	6
684	An ab initio study of intermolecular potential for the He-HCl complex. <i>Computational and Theoretical Chemistry</i> , 2002, 589-590, 89-93.	1.5	14
685	A theoretical analysis of substituted formamide conformers. <i>Computational and Theoretical Chemistry</i> , 2002, 589-590, 423-429.	1.5	27
686	Non-dipole electron impact spectroscopy of a common local anesthetic: Generalized oscillator strengths of valence, Cl 2p and C 1s pre-edge transitions of chloroethane. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2002, 123, 287-302.	0.8	3
687	Sulfur-containing mesoionic compounds: Theoretical study on structure and properties. <i>International Journal of Quantum Chemistry</i> , 2002, 90, 1055-1063.	1.0	12
688	Quantum Monte Carlo calculations for ground and excited states. <i>International Journal of Quantum Chemistry</i> , 2002, 86, 218-225.	1.0	11
689	Adsorption and photodissociation of 4-haloanilines on GaN(). <i>Surface Science</i> , 2002, 519, 173-184.	0.8	16
690	The phototoxicity of polycyclic aromatic hydrocarbons: a theoretical study of excited states and correlation to experiment. <i>Computers & Chemistry</i> , 2002, 26, 371-377.	1.2	19
691	LIF excitation spectra of 2,6-dicyanoaniline. <i>Chemical Physics</i> , 2002, 285, 55-72.	0.9	13
692	Theoretical study on the ground and excited state intramolecular proton transfer in perylenequinone. <i>Chemical Physics Letters</i> , 2002, 353, 119-126.	1.2	22
693	Theoretical investigation of charge transfer to solvent in photoexcited iodide-acetonitrile clusters. <i>Chemical Physics Letters</i> , 2002, 354, 31-37.	1.2	23
694	The photoinduced intramolecular proton transfer in 2-(2-hydroxyphenyl)-4-methyloxazole embedded in β -cyclodextrin. <i>Chemical Physics Letters</i> , 2002, 356, 423-430.	1.2	15
695	Dissociative electron attachment to formic acid (HCOOH). <i>Chemical Physics Letters</i> , 2002, 361, 277-284.	1.2	91
696	Efficient use of the resolution of the identity approximation in time-dependent density functional calculations with hybrid density functionals. <i>Chemical Physics Letters</i> , 2002, 362, 170-178.	1.2	189

#	ARTICLE	IF	CITATIONS
697	On the consequences of the violation of the Hellmann-Feynman theorem in calculations of electric properties of molecules. <i>Chemical Physics Letters</i> , 2002, 363, 313-318.	1.2	10
698	Dipole moments in excited state DFT calculations. <i>Chemical Physics Letters</i> , 2002, 364, 612-615.	1.2	27
699	Molecular orbital study on the ground and excited states of methyl substituted tris(8-hydroxyquinoline) aluminum(III). <i>Chemical Physics Letters</i> , 2002, 366, 9-16.	1.2	44
700	Locally correlated equation-of-motion coupled cluster theory for the excited states of large molecules. <i>Chemical Physics Letters</i> , 2002, 366, 611-622.	1.2	98
701	Properties of Adsorbed Oxygen Forms on a Defective Ag(111) Surface. DFT Analysis. <i>Journal of Structural Chemistry</i> , 2002, 43, 26-32.	0.3	5
702	Adiabatic time-dependent density functional methods for excited state properties. <i>Journal of Chemical Physics</i> , 2002, 117, 7433-7447.	1.2	1,992
703	A Theoretical Study of Excited State Properties of Adenine-Thymine and Guanine-Cytosine Base Pairs. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4709-4717.	1.1	61
704	Bridging Nonliving and Living Matter. <i>Artificial Life</i> , 2003, 9, 269-316.	1.0	215
705	Photogeneration of o-Quinone Methides from o-Cycloalkenylphenols. <i>Journal of Organic Chemistry</i> , 2003, 68, 9643-9647.	1.7	12
706	Transition state analysis on regioselectivity in [2+2] photocycloaddition reactions of substituted 2-cyclohexenone with cycloalkenecarboxylates. <i>Tetrahedron</i> , 2003, 59, 8099-8105.	1.0	14
707	Structure and spectra of tetrasulfur S ₄ – an ab initio MO study. <i>Chemical Physics Letters</i> , 2003, 379, 162-169.	1.2	43
708	Photodissociation spectroscopy of MgCH ₃ ⁺ : dissociation processes via charge transfer and/or chemical bond rupture. <i>Chemical Physics Letters</i> , 2003, 382, 283-290.	1.2	9
709	Electronic structure of zwitterionic diamino-meta-quinonoid molecules: identity of UV absorption bands. <i>Chemical Physics Letters</i> , 2003, 382, 349-354.	1.2	20
710	Circular dichroism spectra of β -peptides: sensitivity to molecular structure and effects of motional averaging. <i>European Biophysics Journal</i> , 2003, 32, 661-670.	1.2	53
711	Direct INDO/SCI method for excited state calculations. <i>Journal of Computational Chemistry</i> , 2003, 24, 1782-1788.	1.5	19
712	Ab initio Study on Luminescence and Auophilicity of a Dinuclear [(AuPH ₃) ₂ (i-mnt)] Complex (i-mnt = Tj ETQq1 1 0.784314 ggBT /Over	1.0	37
713	Time-resolved resonance Raman study of S1 cis-stilbene and its deuterated isotopomers. <i>Journal of Raman Spectroscopy</i> , 2003, 34, 886-891.	1.2	21
714	The Quest for PdII-PdII Interactions: Structural and Spectroscopic Studies and Ab Initio Calculations on Dinuclear [Pd ₂ (CN) ₄ (-diphosphane) ₂] Complexes. <i>Chemistry - A European Journal</i> , 2003, 9, 3055-3064.	1.7	45

#	ARTICLE	IF	CITATIONS
715	Large Enhancement of the Nonlinear Optical Response of Reduced Fullerene Derivatives. Chemistry - A European Journal, 2003, 9, 1529-1534.	1.7	39
716	Excited state geometry calculations and the resonance Raman spectrum of hexamethylpyrromethene. Journal of Molecular Structure, 2003, 661-662, 611-624.	1.8	8
717	Excited states of ethylene interpreted in terms of perturbed Rydberg series. Chemical Physics, 2003, 295, 47-62.	0.9	16
718	Influence of an aromatic substituent in position 2 on photophysical properties of benzoxazol-5-yl-alanine derivatives. Chemical Physics, 2003, 295, 119-130.	0.9	17
719	Theoretical studies on photophysical properties of fullerene and its two derivatives (C60, C70). Journal of Molecular Structure, 2003, 661-662, 101-111.	1.2	50
720	Ab initio study of absorption and emission spectra of PM567. Chemical Physics Letters, 2003, 374, 206-214.	1.2	16
721	On the bathochromic shift of the absorption by astaxanthin in crustacyanin: a quantum chemical study. Chemical Physics Letters, 2003, 375, 30-38.	1.2	42
722	Double perturbation theory: a powerful tool in computational coordination chemistry. Coordination Chemistry Reviews, 2003, 238-239, 83-126.	9.5	101
723	Ab initio study of excited state protonation of monosubstituted benzenes. Computational and Theoretical Chemistry, 2003, 664-665, 309-317.	1.5	12
724	The Fourier transform infrared spectrum of the boron trifluoride-sulphur dioxide van der Waals complex. Journal of Molecular Structure, 2003, 661-662, 153-159.	1.8	7
725	Locking dendrimer conformation through metal coordination. Tetrahedron, 2003, 59, 3917-3923.	1.0	19
726	Time-dependent density functional theory calculations of the photoabsorption of fluorinated alkanes. Journal of Fluorine Chemistry, 2003, 122, 27-35.	0.9	20
727	Theoretical prediction of spectroscopic constants of 1-alkoxy radicals. Journal of Molecular Spectroscopy, 2003, 220, 276-290.	0.4	34
728	Resonance Raman spectra simulation of the biphenyl anion and cation radicals. Journal of Molecular Structure, 2003, 651-653, 747-757.	1.8	7
729	Gas-phase electron diffraction study of cyclic dimer of dimethylphosphinic acid (Me2P(O)OH)2 using quantum chemical data and a priori force field. Journal of Molecular Structure, 2003, 658, 153-170.	1.8	17
730	Does Mg4 exist? A combined Gaussian, complete basis set and density functional theory study. Computational and Theoretical Chemistry, 2003, 629, 7-10.	1.5	3
731	Ab initio MO study on the S1→S0 transitions of polychlorinated dibenzo-p-dioxins. Computational and Theoretical Chemistry, 2003, 622, 229-237.	1.5	12
732	Study of excited state properties of oligofluorenes by the singles configuration interaction (CIS) theoretical approach. Computational and Theoretical Chemistry, 2003, 625, 141-148.	1.5	33

#	ARTICLE	IF	CITATIONS
733	Theoretical study on the trihydroxy-anthraquinone tautomerism in the ground and excited states. Computational and Theoretical Chemistry, 2003, 637, 129-136.	1.5	6
734	A theoretical study of the ground and first excited singlet state proton transfer reaction in isolated 7-azaindole-water complexes. Chemical Physics, 2003, 290, 319-336.	0.9	51
735	Valence shell photoionization energies and cross-sections of NF ₃ and PF ₃ . Journal of Electron Spectroscopy and Related Phenomena, 2003, 128, 245-260.	0.8	8
736	The role of FA(I):Tl ⁺ and FA(II):Ga ⁺ defects in laser light generation and photographic sensitization at the low-coordination surface sites of AgBr first principles calculations. Physica B: Condensed Matter, 2003, 337, 17-35.	1.3	1
737	Electronic absorption spectra of amino substituted anthraquinones and their interpretation using the ZINDO/S and AM1 methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 1409-1426.	2.0	26
738	Metastable states of dimethyloxonium, (CH ₃) ₂ OH. International Journal of Mass Spectrometry, 2003, 222, 49-61.	0.7	20
739	Anisotropic photodissociation of vinyl chloride molecular cation in the ground and first excited electronic states. International Journal of Mass Spectrometry, 2003, 227, 21-32.	0.7	8
740	Calculation of the visible-UV absorption spectra of hydrogen sulfide, bisulfide, polysulfides, and As and Sb sulfides, in aqueous solution. Geochemical Transactions, 2003, 4, 1.	1.8	24
741	Theory of excitation energy transfer regarded as nonadiabatic transition 2: Computational evidence of nonadiabatic interaction causing intermolecular excitation energy transfer. International Journal of Quantum Chemistry, 2003, 94, 36-43.	1.0	5
742	Theoretical investigation of charge transfer excitation and charge recombination in acenaphthylene-tetracyanoethylene complex. International Journal of Quantum Chemistry, 2003, 94, 23-35.	1.0	2
743	Synthesis and electronic spectra of novel merocyanine dyes bearing a maleimide ring incorporated into the methine chains. Dyes and Pigments, 2003, 56, 167-179.	2.0	6
744	Metal-Metal Interactions in Heterobimetallic d ⁸ d ¹⁰ Complexes. Structures and Spectroscopic Investigation of [M ⁺ M ⁺ (1/4-dcpm) ₂ (CN) ₂] ⁺ (M ⁺ = Pt, Pd; M ⁺ = Cu, Ag, Au) and Related Complexes by UV-vis Absorption and Resonance Raman Spectroscopy and ab Initio Calculations. Journal of the American Chemical Society, 2003, 125, 10362-10374.	6.6	105
745	Neurotransmitters in the gas phase: a computational and spectroscopic study of noradrenaline. Molecular Physics, 2003, 101, 1239-1248.	0.8	78
746	Quantum Chemical Calculation of Excited States of Flavin-Related Molecules. Journal of Physical Chemistry A, 2003, 107, 140-147.	1.1	140
747	Non-Localized Ligand-to-Metal Charge Transfer Excited States in (Cp) ₂ Ti(IV)(NCS) ₂ . Journal of the American Chemical Society, 2003, 125, 5461-5470.	6.6	23
748	Theoretical Study of the pH-Dependent Photophysics Of N1,N6-Ethnoadenine and N3,N4-Ethenocytosine. Journal of Physical Chemistry A, 2003, 107, 8923-8931.	1.1	8
749	Electronic Spectrum of Dicyanoacetylene. 1. Calculations of the Geometries and Vibrations of Ground and Excited States of Diacetylene, Cyanoacetylene, Cyanogen, Triacetylene, Cyanodiacetylene, and Dicyanoacetylene. Journal of Physical Chemistry A, 2003, 107, 10631-10636.	1.1	21
750	Calculation of the Energetics for Oxidation of Gas-Phase Elemental Hg by Br and BrO. Journal of Physical Chemistry A, 2003, 107, 7804-7808.	1.1	86

#	ARTICLE	IF	CITATIONS
751	Ground and Excited-State Acetic Acid Catalyzed Double Proton Transfer in 2-Aminopyridine. Journal of Physical Chemistry A, 2003, 107, 3244-3253.	1.1	47
752	Light-Induced Aminocarbene to Imine Dyotropic Rearrangement in a Chromium(0) Center: An Unprecedented Reaction Pathway. Journal of the American Chemical Society, 2003, 125, 9572-9573.	6.6	37
753	Rational classification of a series of aromatic donor-acceptor systems within the twisting intramolecular charge transfer model, a time-dependent density-functional theory investigation. Journal of Chemical Physics, 2003, 119, 12852-12865.	1.2	32
754	Electronic Spectra, Excited-State Geometries, and Molecular Electrostatic Potentials of Hypoxanthine: A Theoretical Investigation. Journal of Physical Chemistry A, 2003, 107, 5538-5543.	1.1	30
755	Photodissociation Spectroscopy of Zn+ Methanol. Journal of Physical Chemistry A, 2003, 107, 984-989.	1.1	12
756	Gallium and Indium Hydrazides. Molecular and Electronic Structure of In[N(SiMe3)NMe2]3 and Related Compounds. Inorganic Chemistry, 2003, 42, 3431-3437.	1.9	19
757	Theoretical study of the ground and first excited singlet state potential energy surfaces of disulphur monoxide (S2O). Molecular Physics, 2003, 101, 1303-1310.	0.8	14
758	Ab Initio and Density Functional Study of the Electronic Transitions of Indoline and Indoline-2-Carboxylic Acid. Journal of Physical Chemistry A, 2003, 107, 5670-5680.	1.1	15
759	Photochemistry of 1-(N,N-Diethylamino)diazen-1-ium-1,2-diolate: An Experimental and Computational Investigation. Journal of the American Chemical Society, 2003, 125, 14934-14940.	6.6	16
760	Dynamic Helical Chirality of an Intramolecularly Hydrogen-Bonded Bisoxazoline. Journal of Organic Chemistry, 2003, 68, 22-26.	1.7	28
761	Ab Initio Comparative Study of the Structure and Properties of H2-Porphin and H2-Phthalocyanine. The Electronic Absorption Spectra. Journal of Physical Chemistry A, 2003, 107, 8968-8974.	1.1	35
762	An ab Initio Study of the Silicon-Oxygen-Sulfur Oligomers (SiOS)n (n ≤ 6). Journal of Physical Chemistry A, 2003, 107, 6259-6263.	1.1	6
763	Vibrational and Electronic Spectroscopy of Sulfuric Acid Vapor. Journal of Physical Chemistry A, 2003, 107, 1112-1118.	1.1	107
764	Excited state nuclear forces from the Tamm-Dancoff approximation to time-dependent density functional theory within the plane wave basis set framework. Journal of Chemical Physics, 2003, 118, 3928-3934.	1.2	173
765	Calculation of optical absorption spectra of hydrogenated Si clusters: Bethe-Salpeter equation versus time-dependent local-density approximation. Physical Review B, 2003, 68, .	1.1	94
766	Theoretical Study of the Amazing Firefly Bioluminescence: The Formation and Structures of the Light Emitters. Journal of the American Chemical Society, 2003, 125, 6962-6971.	6.6	132
767	LIF excitation spectra of jet-cooled 3,5-dicyanoaniline. Physical Chemistry Chemical Physics, 2003, 5, 4096-4107.	1.3	11
768	Optical properties of functionalized thiophenes: a theoretical and experimental study. Synthetic Metals, 2003, 139, 897-899.	2.1	10

#	ARTICLE	IF	CITATIONS
769	Time-Dependent Density Functional Theory Study on Polyazopyrrole and Polyazothiophene. <i>Macromolecules</i> , 2003, 36, 9585-9593.	2.2	27
770	Activation Barriers in the Homolytic Cleavage of Radicals and Ion Radicals. <i>Journal of the American Chemical Society</i> , 2003, 125, 105-112.	6.6	30
771	Alkali Ion-Controlled Excited-State Ordering of Acetophenones Included in Zeolites: λ Emission, Solid-State NMR, and Computational Studies. <i>Journal of Physical Chemistry A</i> , 2003, 107, 3187-3198.	1.1	19
772	Electronic structure of the trimethylenemethane diradical in its ground and electronically excited states: σ -Bonding, equilibrium geometries, and vibrational frequencies. <i>Journal of Chemical Physics</i> , 2003, 118, 6874-6883.	1.2	90
773	Photodissociation dynamics of enolic-acetylacetone at 266, 248, and 193 nm: Mechanism and nascent state product distribution of OH. <i>Journal of Chemical Physics</i> , 2003, 118, 2590.	1.2	47
774	The Nature and Absolute Hydration Free Energy of the Solvated Electron in Water. <i>Journal of Physical Chemistry B</i> , 2003, 107, 4403-4417.	1.2	107
775	Singlet and Triplet Valence Excited States of Pyrimidine. <i>Journal of Physical Chemistry A</i> , 2003, 107, 3093-3106.	1.1	45
776	Local treatment of electron excitations in the EOM-CCSD method. <i>Journal of Chemical Physics</i> , 2003, 118, 3006-3019.	1.2	273
777	A New, Self-Contained Asymptotic Correction Scheme To Exchange-Correlation Potentials for Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2003, 107, 10154-10158.	1.1	106
778	Vibrational and structural analysis of the radical cation of N,N,N',N'-tetramethylbenzidine based on ab initio calculations and time-resolved resonance Raman spectroscopy. Electronic supplementary information (ESI) available: Potential energy distributions (PED) expressed in terms of the local symmetry coordinates for each isotopomer (Table 1S and 3S); description of the symmetry coordinates (Table 2S) and related internal coordinates (Fig. 1S). See http://www.rsc.org/suppdata/cp/b2/b210837m/ .	1.3	12
779	The Electronic Structure of the Photoexcited Triplet State of Free-Base (Tetraphenyl)porphyrin by Time-Resolved Electron-Nuclear Double Resonance and Density Functional Theory. <i>Journal of the American Chemical Society</i> , 2003, 125, 13861-13867.	6.6	26
780	The vertical spectrum of H ₂ CO revisited: (SC)2-Cl and CC calculations. <i>Molecular Physics</i> , 2003, 101, 483-494.	0.8	15
781	Intramolecular charge transfer in 2-methyl-1,3-dihydrobenz[d,e]isoquinoline: Calculation of the electronic coupling matrix element. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 4556.	1.3	6
782	Analytic gradients for excited states in the coupled-cluster model CC2 employing the resolution-of-the-identity approximation. <i>Journal of Chemical Physics</i> , 2003, 119, 5021-5036.	1.2	372
783	Theoretical study of photoinduced electron transfer from tetramethylethylene to tetracyanoethylene. <i>Journal of Chemical Physics</i> , 2003, 119, 8854-8863.	1.2	9
784	Spectroscopy and dynamics of excited states in maleimide and N-methyl maleimide: Ionic projection and ab initio calculations. <i>Journal of Chemical Physics</i> , 2003, 118, 10944-10955.	1.2	17
785	Ab initio embedded cluster study of optical second-harmonic generation below the gap of a NiO(001) surface. <i>Physical Review B</i> , 2003, 67, .	1.1	16
786	Electronic structure of solid 1,3,5-triamino-2,4,6-trinitrobenzene under uniaxial compression: Possible role of pressure-induced metallization in energetic materials. <i>Physical Review B</i> , 2003, 67, .	1.1	77

#	ARTICLE	IF	CITATIONS
787	Quantum Monte Carlo study of singlet \leftrightarrow triplet transition in ethylene. <i>Journal of Chemical Physics</i> , 2003, 119, 1483-1488.	1.2	26
788	High level ab initio studies of the excited states of sulfuric acid and sulfur trioxide. <i>Journal of Chemical Physics</i> , 2003, 118, 7226.	1.2	29
789	On the inversion of the 1 π -Bu and 2 π -Ag electronic states in $\hat{\pm}$ -diphenylpolyenes. <i>Journal of Chemical Physics</i> , 2003, 119, 1373-1385.	1.2	24
790	Calculation of electric properties using regular approximations to relativistic effects: The polarizabilities of RuO ₄ , OsO ₄ , and HsO ₄ (Z=108). <i>Journal of Chemical Physics</i> , 2003, 119, 1412-1420.	1.2	31
791	Laser-driven electron transfer through metal-insulator-metal contacts: Time-dependent configuration interaction singles calculations for a jellium model. <i>Physical Review B</i> , 2003, 68, .	1.1	86
792	A spin-complete version of the spin-flip approach to bond breaking: What is the impact of obtaining spin eigenfunctions?. <i>Journal of Chemical Physics</i> , 2003, 118, 9084-9094.	1.2	142
793	Electronic excitation and transient defects in As ₂ S ₃ glass. <i>Physical Review B</i> , 2003, 67, .	1.1	6
794	Photodissociation of Mg(CH ₂ =CHCN) _n : Excited electronic states of n=1 and 2 and intracuster electron transfer for n=3 and 4. <i>Journal of Chemical Physics</i> , 2003, 118, 5456-5464.	1.2	8
795	Quantum Energy Flow and trans-Stilbene Photoisomerization: An Example of a Non-RRKM Reaction. <i>Journal of Physical Chemistry A</i> , 2003, 107, 10706-10716.	1.1	94
796	A Generalized Unpaired Electron Spin Density Equation and Organic Hyperconjugation Mechanism. <i>Journal of the Chinese Chemical Society</i> , 2003, 50, 815-822.	0.8	0
797	Theoretical Calculations on Vibrational Frequencies and Absorption Spectra of S ₁ and S ₂ States of Pyridine. <i>Journal of the Chinese Chemical Society</i> , 2003, 50, 735-744.	0.8	7
798	Theoretical Analysis of the Excited State Properties of Wybutine: A Natural Probe for Transfer RNA Dynamics. <i>International Journal of Molecular Sciences</i> , 2004, 5, 75-83.	1.8	6
799	Estimation of Electron Spectra Transitions of Free-Based Porphin and Mg-Porphin Using Various Quantum Chemical Approaches. <i>International Journal of Molecular Sciences</i> , 2004, 5, 196-213.	1.8	10
800	Calculations of static and dynamic polarizabilities of excited states by means of density functional theory. <i>Journal of Chemical Physics</i> , 2004, 121, 7595.	1.2	30
801	Dissociation dynamics of thiolactic acid at 193 nm: Detection of the nascent OH product by laser-induced fluorescence. <i>Journal of Chemical Physics</i> , 2004, 120, 6964-6972.	1.2	16
802	The effects of oxygenation on the optical properties of dimethyl-dithienothiophenes: Comparison between experiments and first-principles calculations. <i>Journal of Chemical Physics</i> , 2004, 121, 3784-3791.	1.2	16
803	Multiple Photofragmentation Pathways with Different Recoil Anisotropy from a Metal-Ion \leftrightarrow Ligand Complex. <i>Physical Review Letters</i> , 2004, 93, 193401.	2.9	11
804	Quantum Monte Carlo for electronic excitations of free-base porphyrin. <i>Journal of Chemical Physics</i> , 2004, 120, 3049-3050.	1.2	54

#	ARTICLE	IF	CITATIONS
805	Optimized Jastrow-Slater wave functions for ground and excited states: Application to the lowest states of ethene. <i>Journal of Chemical Physics</i> , 2004, 120, 10931-10941.	1.2	82
806	Excitonic splitting in conjugated molecular materials: A quantum mechanical model including interchain interactions and dielectric effects. <i>Physical Review B</i> , 2004, 70, .	1.1	10
807	H-bonded N-heterocyclic base-pair phototautomerizational potential barrier and mechanism: The 7-azaindole dimer. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004, 101, 419-422.	3.3	83
808	Synthesis, Crystal Structure and Spectroscopic Studies of a Supramolecular Compound [Cu(IDA)(phen)(H ₂ O)]·4H ₂ O Built from π - π Interactions and Hydrogen Bonds. <i>Transition Metal Chemistry</i> , 2004, 29, 471-476.	0.7	9
809	A theoretical study of the Y ₃ O clusters. <i>European Physical Journal D</i> , 2004, 29, 27-31.	0.6	10
810	Size-Nonextensive Contributions in Singles-Only CI. <i>Structural Chemistry</i> , 2004, 15, 379-384.	1.0	2
811	Quantum Chemical Analysis of the Chemical Bonds in Tris(8-hydroxyquinolinato)aluminum as a Key Emitting Material for OLED. <i>Journal of Physical Chemistry A</i> , 2004, 108, 10296-10301.	1.1	69
812	Time-Dependent Density-Functional Theory Investigation of the Fluorescence Behavior as a Function of Alkyl Chain Size for the 4-(N,N-Dimethylamino)benzonitrile-like Donor-Acceptor Systems 4-(N,N-Diethylamino)benzonitrile and 4-(N,N-Diisopropylamino)benzonitrile. <i>Journal of Physical Chemistry B</i> , 2004, 108, 7132-7141.	1.2	42
813	Ultrafast Excited-State Dynamics in Nucleic Acids. <i>Chemical Reviews</i> , 2004, 104, 1977-2020.	23.0	1,157
814	Electron trapping by excited microvoids (EEM) an explanation of the Staebler-Wronski effect. <i>Physica B: Condensed Matter</i> , 2004, 353, 263-277.	1.3	8
815	Instability of the molecular structure of monobenzoporphin to the alternation of the macrocycle bond lengths and its manifestation in the electronic spectra. <i>Journal of Applied Spectroscopy</i> , 2004, 71, 777-787.	0.3	4
816	Photon-assisted tunneling versus tunneling of excited electrons in metal-insulator-metal junctions. <i>Applied Physics A: Materials Science and Processing</i> , 2004, 78, 189-199.	1.1	29
817	Theoretical and Experimental analysis of ZnPc for its local ordering and electronic structure. <i>Applied Physics A: Materials Science and Processing</i> , 2004, 79, 1913-1918.	1.1	11
818	Calculation of 17 O NMR shieldings in molecular models for crystalline MO, M=Mg, Ca, Sr, and in models for alkaline earth silicates. <i>Physics and Chemistry of Minerals</i> , 2004, 31, 41-44.	0.3	13
819	Theoretical studies of conjugate and substituent effects on the intramolecular proton transfer: an HF/CIS study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2004, 162, 407-414.	2.0	7
820	Gaussian-based computations in molecular science. <i>Computational and Theoretical Chemistry</i> , 2004, 671, 1-21.	1.5	41
821	Theoretical study on the formation mechanism of iso-CH ₂ I-Cl. <i>International Journal of Quantum Chemistry</i> , 2004, 97, 719-724.	1.0	2
822	Electronic structure and molecular orbital study of the first excited state of the high-efficiency blue OLED material bis(2-methyl-8-quinolinolato)aluminum(III) hydroxide complex from ab initio and TD-B3LYP. <i>International Journal of Quantum Chemistry</i> , 2004, 97, 992-1001.	1.0	14

#	ARTICLE	IF	CITATIONS
823	Conformational fluctuations and electronic properties in myoglobin. <i>Journal of Computational Chemistry</i> , 2004, 25, 974-984.	1.5	35
824	Ground and excited state prototropism in 2-(2-methoxyphenyl)-1H-imidazo[4,5-c]pyridine. <i>Journal of Molecular Structure</i> , 2004, 691, 59-70.	1.8	5
825	Theoretical studies on the electronic and spectroscopic properties of Keggin-structure polyoxometalates $[X_{12}O_{40}]^{n-}$ ($X=Si, P; M=Mo, W$). <i>Computational and Theoretical Chemistry</i> , 2004, 676, 55-64.	1.5	23
826	Basis set effects on the ground and excited state of nitrogen containing organic molecules. p-Nitroaniline as a case study. <i>Computational and Theoretical Chemistry</i> , 2004, 681, 57-63.	1.5	15
827	A theoretical investigation on intramolecular hydrogen-atom transfer in curcumin. <i>Computational and Theoretical Chemistry</i> , 2004, 684, 111-116.	1.5	25
828	Electronic absorption and emission spectra and computational studies of some 2-aryl, 2-styryl, and 2-(4-aryl)butadienyl quinazolin-4-ones. <i>Computational and Theoretical Chemistry</i> , 2004, 710, 229-234.	1.5	40
829	Additivity of electron correlation energy and the ab initio MO calculation of $(O^0) S1 \rightarrow S0$ transition energies: polychlorinated dibenzofurans. <i>Computational and Theoretical Chemistry</i> , 2004, 710, 19-23.	1.5	4
830	Gas phase UV and IR absorption spectra of $C_xF_{2x+1}CHO$ ($x = 1-4$). <i>Journal of Fluorine Chemistry</i> , 2004, 125, 1925-1932.	0.9	20
831	Intra- and intermolecular proton transfer in methyl-2-hydroxynicotinate. <i>Journal of Luminescence</i> , 2004, 110, 147-163.	1.5	18
832	Life-time of quasiparticle states in metallic clusters from GW theory. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2004, 327, 241-246.	0.9	20
833	Theoretical investigation on the ground- and excited-state properties of novel octupolar oligothiophene-functionalized truxenes and dipolar analogs. <i>Polymer</i> , 2004, 45, 7747-7757.	1.8	28
834	Solvatochromism and prototropism in methyl 6-aminonicotinate: failure to observe amine-imine phototautomerism in solvents. <i>Journal of Molecular Structure</i> , 2004, 702, 85-94.	1.8	8
835	Theoretical study of the ground and excited electronic states of pyrromethene 546 laser dye and related compounds. <i>Chemical Physics</i> , 2004, 296, 13-22.	0.9	48
836	Prediction of novel complexation of porphine and BF_3 : Is it a 1:1 or 1:2 species?. <i>Chemical Physics</i> , 2004, 301, 1-7.	0.9	11
837	Excited state intramolecular proton transfer in 2-(2-amino-3-pyridyl)-benzimidazole: effect of solvents. <i>Chemical Physics</i> , 2004, 305, 95-103.	0.9	22
838	On photoinduced double-proton transfer reactions: the photophysics of the 9H-imidazo[1,2-a]benzimidazole dimer. <i>Chemical Physics</i> , 2004, 305, 175-185.	0.9	8
839	Calculating electron transfer couplings by the Spin-Flip approach: energy splitting and dynamical correlation effects. <i>Chemical Physics Letters</i> , 2004, 390, 116-123.	1.2	40
840	Theoretical studies on metal-oxo-metal-oxo bond and $\pi \rightarrow \pi^*$ charge transfer (π) transition in binuclear platinum(II) complex. $\langle \text{mml:math altimg="s19.gif" display="inline" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" x="1" y="1" z="1" \rangle$ <i>Chemical Physics Letters</i> , 2004, 394, 155-	1.2	9

#	ARTICLE	IF	CITATIONS
841	Charge separation and charge transfer to solvent in NaClâ€‘water clusters. <i>Chemical Physics Letters</i> , 2004, 399, 200-205.	1.2	17
842	FA1:La2+ and FA2:Sc2+ color center lasers and color image sensitization at the low coordination (001) surface of AgBr by ab initio calculations. <i>Current Applied Physics</i> , 2004, 4, 426-438.	1.1	0
843	Observation of the two triplet state conformations of alkyl phenylglyoxylates Dedicated to Professor Dr J. W. Neckers in honor of his 101st birthday. Electronic supplementary information (ESI) available: Synthetic procedures and characterization of APGs, description of spectra processing procedures, time-resolved FTIR spectra and kinetic traces demonstrating steric and d-isotope effects, 3D structures of cyclohexyl phenylglyoxylate and t-Bu-cyclohexyl glyoxylate conformers. See http://www.rsc.org/suppdata/pp/ . <i>Photochemical and Photobiological Sciences</i> , 2004, 3, 892.	1.6	7
844	Photochemical Stability of Pentacene and a Substituted Pentacene in Solution and in Thin Films. <i>Chemistry of Materials</i> , 2004, 16, 4980-4986.	3.2	389
845	The triplet excited state of ruthenium(ii) bis(2,2â€‘:6â€‘,2â€‘-terpyridine): Comparison between experiment and theory. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 1157-1164.	1.3	63
846	Vibrationally resolved electronic spectroscopy and theoretical studies of deuterated 2-(2â€‘-pyridyl)indole. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 363-367.	1.3	16
847	The role of FA:K+ and FA:Na+ defects in laser light generation and color image formation at the (100) and (110) surface sites of AgCl and AgBr.. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 626.	1.3	14
848	2-(2â€‘-Pyridyl)pyrroles: Part I. Structure and energetics of pyridylpyrroles, their dimers, complexes and excited states. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 3938-3947.	1.3	16
849	Real versus artifactual symmetry-breaking effects in Hartreeâ€‘Fock, density-functional, and coupled-cluster methods. <i>Journal of Chemical Physics</i> , 2004, 120, 7298-7306.	1.2	68
850	Theoretical Modeling of Enzyme Reaction Chemistry: The Electron Transfer of the Reduction Mechanism in CuZn Superoxide Dismutase. <i>Journal of Physical Chemistry B</i> , 2004, 108, 16255-16260.	1.2	31
851	Ab Initio Study on Luminescent Properties and Auophilic Attraction of [Au2(dpm)(i-mnt)] and Its Related Au(I) Complexes (dpm = bis(diphosphino)methane and i-mnt = i-malononitriledithiolate). <i>Organometallics</i> , 2004, 23, 5198-5209.	1.1	21
852	Comprehensive Theoretical Study of the Conversion Reactions of Spiropyrans: Substituent and Solvent Effects. <i>Journal of Physical Chemistry B</i> , 2004, 108, 16233-16243.	1.2	170
853	Theoretical Calculations of the Effects of 2-Heavier Group 14 Element and Substituents on the Singletâ€‘Triplet Energy Gap in Cyclopentane-1,3-diyls and Computational Prediction of the Reactivity of Singlet 2-Silacyclopentane-1,3-diyls. <i>Journal of Organic Chemistry</i> , 2004, 69, 7250-7255.	1.7	27
854	Molecular Dynamics of Excited State Intramolecular Proton Transfer: 2-(2â€‘-Hydroxyphenyl)-4-methyloxazole in Gas Phase, Solution, and Protein Environments. <i>Journal of Physical Chemistry B</i> , 2004, 108, 6616-6623.	1.2	22
855	Hydrogen Atom Formation in the Photolysis of Acetone at 193 nm. <i>Journal of Physical Chemistry A</i> , 2004, 108, 8002-8008.	1.1	12
856	Photophysics of 1,8-Bis(dimethylamino)naphthalene in Solution: Internal Charge Transfer with a Twist. <i>Journal of Physical Chemistry A</i> , 2004, 108, 10623-10631.	1.1	16
857	Electronically Excited States of Methylene cycloalkanes. <i>Journal of Physical Chemistry A</i> , 2004, 108, 9417-9422.	1.1	4
858	Experimental and Theoretical Investigations of Environmentally Sensitive Single-Molecule Fluorophores. <i>Journal of Physical Chemistry B</i> , 2004, 108, 10465-10473.	1.2	76

#	ARTICLE	IF	CITATIONS
859	A Quantum Chemical Study of Intramolecular Charge Transfer in a Closely-Spaced, Donor-acceptor Molecule. <i>Journal of Physical Chemistry A</i> , 2004, 108, 1242-1249.	1.1	10
860	Synthesis and Characterization of Bis(di-2-pyridylmethanamine)ruthenium(II). <i>Inorganic Chemistry</i> , 2004, 43, 1735-1742.	1.9	28
861	Quantum Chemical Determination of the Equilibrium Geometries and Harmonic Vibrational Frequencies of 1,1'-, 1,2'- and 2,2'-Binaphthyl in Their Ground and Excited (1La) Electronic States. <i>Journal of Physical Chemistry A</i> , 2004, 108, 172-184.	1.1	13
862	Direct Observation of the Forbidden Hydrogen Atom Adduct to Acetonitrile: A Neutralization-Reionization Mass Spectrometric and CCSD(T) ab Initio/RRKM Study. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4163-4173.	1.1	11
863	Effects of Spiroconjugation on the Calculated Singlet-Triplet Energy Gap in 2,2-Dialkoxycyclopentane-1,3-diyls and on the Experimental Electronic Absorption Spectra of Singlet 1,3-Diphenyl Derivatives. Assignment of the Lowest-Energy Electronic Transition of Singlet Cyclopentane-1,3-diyls. <i>Journal of the American Chemical Society</i> , 2004, 126, 574-582.	6.6	71
864	Solvent Effects on the Electronic Spectra: An Extension of the Polarizable Continuum Model to the ZINDO Method. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6248-6256.	1.1	55
865	Ab Initio Studies on Metal-Metal Interaction and $3[\text{f}^*(\text{d})\text{f}(\text{s})]$ Excited State of the Binuclear Au(I) Complexes Formed by Phosphine and/or Thioether Ligands. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3650-3661.	1.1	21
866	Ground and Excited State Hydrogen Atom Transfer Reactions and Cyclization of 2-Acetylbenzoic Acid. <i>Journal of Physical Chemistry A</i> , 2004, 108, 9331-9341.	1.1	12
867	Novel isomers of hexasulfur: Prediction of a stable prism isomer and implications for the thermal reactivity of elemental sulfur. <i>Journal of Chemical Physics</i> , 2004, 121, 5899-5907.	1.2	20
868	The electronic properties of polyacetylene-polymethineimine block copolymers. <i>Synthetic Metals</i> , 2004, 143, 229-236.	2.1	12
869	Developing a Structure-Function Model for the Cryptophyte Phycoerythrin 545 Using Ultrahigh Resolution Crystallography and Ultrafast Laser Spectroscopy. <i>Journal of Molecular Biology</i> , 2004, 344, 135-153.	2.0	117
870	Properties of aqueous methanesulfonic acid: complex index of refraction and surface tension. <i>Applied Optics</i> , 2004, 43, 2500.	2.1	10
871	Higher-order equation-of-motion coupled-cluster methods. <i>Journal of Chemical Physics</i> , 2004, 121, 51.	1.2	207
872	ADVENTURES OF QUANTUM CHEMISTRY IN THE REALM OF INORGANIC CHEMISTRY. Comments on <i>Inorganic Chemistry</i> , 2004, 25, 19-74.	3.0	11
873	Conformation of Prion Protein Repeat Peptides Probed by FRET Measurements and Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2004, 86, 2467-2483.	0.2	60
874	Origin of Regioselectivity in Photocycloaddition Reactions of 2-Cyclohexenone with Cycloalkenecarboxylates. <i>Bulletin of the Chemical Society of Japan</i> , 2004, 77, 1209-1215.	2.0	20
875	Tautomerization in the ground and first excited singlet states of phenyl-lapimidazole. <i>Journal of Luminescence</i> , 2004, 109, 207-214.	1.5	2
877	Ab initio and semiempirical study of structure and electronic spectra of hydroxy substituted naphthoquinones. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2005, 61, 777-790.	2.0	41

#	ARTICLE	IF	CITATIONS
878	Photophysics of 1-hydroxy-9-fluorenone: absence of excited state intramolecular proton transfer reaction. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2005, 169, 79-88.	2.0	17
879	Photophysics of 1-hydroxy- and 1-methoxy-9-fluorenone. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2005, 169, 299-307.	2.0	17
880	Quantum study on photophysical and photochemical process of a new photosensitizer: hypomycin B. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2005, 170, 37-43.	2.0	1
881	Spectral characteristics of methyl 2-aminonicotinate: effect of solvents and acid-base concentrations. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2005, 170, 203-213.	2.0	4
882	Spectral characteristics of various prototropic species of 2-(3-aminophenyl)pyrido[3,4-d]imidazole. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2005, 171, 9-20.	2.0	2
883	Excited state prototropism in 2-aminonicotinic acid: effect of solvents and acid-base concentrations. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2005, 171, 281-290.	2.0	5
884	Spectral characteristics of 2-(3,5-diaminophenyl)benzothiazole: effects of solvents and acid-base concentrations. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2005, 172, 185-195.	2.0	12
885	Theoretical study of the photoinduced intramolecular proton transfer and rotational processes in 2-(2-hydroxyphenyl)-4-methyloxazole in gas phase and embedded in β -cyclodextrin. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2005, 173, 365-374.	2.0	17
886	Influence of substituents in the phenyl ring on photophysical properties of 3-[2-(phenyl)benzoxazol-5-yl]alanine derivatives. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2005, 175, 57-68.	2.0	11
887	Excited-state inter- and intramolecular proton transfer in methyl 3-hydroxy-2-quinoxalinate: effects of solvent and acid or base concentrations. <i>Journal of Luminescence</i> , 2005, 114, 101-117.	1.5	6
888	Solvatochromism and prototropism in 6-aminonicotinic acid. <i>Journal of Luminescence</i> , 2005, 114, 213-226.	1.5	3
889	Toward a general mechanism of electron capture dissociation. <i>Journal of the American Society for Mass Spectrometry</i> , 2005, 16, 208-224.	1.2	308
890	Theoretical studies on the electronic and optical properties of two thiophene-fluorene based π -conjugated copolymers. <i>Polymer</i> , 2005, 46, 10970-10981.	1.8	52
891	Spectral characteristics of 2-hydroxynicotinic acid: effects of solvent and acid or base concentrations. <i>Journal of Molecular Structure</i> , 2005, 737, 189-199.	1.8	7
892	Design and development of a fluorescent probe for monitoring hydrogen peroxide using photoinduced electron transfer. <i>Bioorganic and Medicinal Chemistry</i> , 2005, 13, 1131-1139.	1.4	84
893	Theoretical study of the electronic spectra of azobenzene dyes. <i>Computational and Theoretical Chemistry</i> , 2005, 715, 183-189.	1.5	26
894	Isotopic effect of electron excitation in l-[3H]tryptophan. <i>Computational and Theoretical Chemistry</i> , 2005, 724, 53-59.	1.5	3
895	On the electronic excited states of sulfur dioxide. <i>Computational and Theoretical Chemistry</i> , 2005, 717, 231-234.	1.5	2

#	ARTICLE	IF	CITATIONS
896	A CASSCF theoretical study of the vibrational frequencies and structure of formaldehyde, acetaldehyde and acetone valence excited states. Computational and Theoretical Chemistry, 2005, 718, 55-69.	1.5	18
897	On the optical properties of thiophene oligomers: configuration interaction study on their ground (S0) and first singlet excited (S1) states. Computational and Theoretical Chemistry, 2005, 726, 161-169.	1.5	15
898	Theoretical studies of ground and excited electronic states of OLED material bis(2-methyl-8-quinolinolato)gallium(III) chloride. Computational and Theoretical Chemistry, 2005, 722, 161-168.	1.5	5
899	Theoretical investigations on the structure and vibrational spectra of N-(2-hydroxy-1-naphthylidene)threonine. Computational and Theoretical Chemistry, 2005, 723, 159-164.	1.5	1
900	Quantum chemistry of the excited state: 2005 overview. Computational and Theoretical Chemistry, 2005, 729, 99-108.	1.5	185
901	Configuration interaction study on the conformational and optical properties of excited furan oligomers. Computational and Theoretical Chemistry, 2005, 726, 189-196.	1.5	8
902	Dimer complex UV absorption spectra of some nitrogen heterocycles molecules from atom monopole-dipole interaction model. Computational and Theoretical Chemistry, 2005, 726, 125-133.	1.5	1
903	Density functional theory (B3LYP/6-31G*) study of oligothiophenes in their aromatic and polaronic states. Computational and Theoretical Chemistry, 2005, 726, 271-276.	1.5	61
904	Molecular geometry, electronic structure and optical properties study of meridional tris(8-hydroxyquinolinato)gallium(III) with ab initio and DFT methods. Computational and Theoretical Chemistry, 2005, 755, 19-30.	1.5	17
905	Ab initio configuration interaction singles (CIS) study on polycyclic aromatic molecules (II): Predicting fluorescence quantum yields by calculating the excitation energies. Computational and Theoretical Chemistry, 2005, 756, 35-38.	1.5	4
906	Intramolecular proton or hydrogen-atom transfer in the ground- and excited-states of 2-hydroxybenzophenone: A theoretical study. Chemical Physics, 2005, 315, 297-302.	0.9	33
907	Configuration interaction singles method with multilayer fragment molecular orbital scheme. Chemical Physics Letters, 2005, 406, 283-288.	1.2	112
908	A size-extensive modification of super-CI for orbital relaxation. Chemical Physics Letters, 2005, 410, 165-171.	1.2	12
909	DFT and TD-DFT investigation of the ground and excited states for dinuclear and mononuclear copper(I) and silver(I) complexes of 3,5-bis(trifluoromethyl)pyrazole and related bis(pyrazolyl)borate. Chemical Physics Letters, 2005, 410, 302-306.	1.2	13
910	Ab initio studies of the dipole moment and polarizability of azulene in its ground and excited singlet states. Chemical Physics Letters, 2005, 412, 365-368.	1.2	23
911	Single-Reference ab Initio Methods for the Calculation of Excited States of Large Molecules. Chemical Reviews, 2005, 105, 4009-4037.	23.0	2,315
912	Study of electronic spectra of free-base porphyrin and Mg-porphyrin: Comprehensive comparison of variety of ab initio, DFT, and semiempirical methods. Journal of Computational Chemistry, 2005, 26, 294-303.	1.5	18
913	Theoretical studies on the electronic and optical properties of two new alternating fluorene/carbazole copolymers. Journal of Computational Chemistry, 2005, 26, 969-979.	1.5	30

#	ARTICLE	IF	CITATIONS
914	Computational and Experimental Studies on the Mechanism of the Photochemical Carbonylation of Group 6 Fischer Carbene Complexes. <i>Chemistry - A European Journal</i> , 2005, 11, 5988-5996.	1.7	40
915	Simulation of two-photon-photoelectron spectra at a jellium-vacuum interface. <i>Applied Physics A: Materials Science and Processing</i> , 2005, 81, 93-101.	1.1	14
916	Gas phase UV and IR absorption spectra of CF ₃ CH ₂ CH ₂ OH and F(CF ₂ CF ₂) _x CH ₂ CH ₂ OH (x=2, 3, 4). <i>Journal of Fluorine Chemistry</i> , 2005, 126, 1288-1296.	0.9	19
917	A theoretical investigation on the electronic and optical properties of π -conjugated copolymers with an efficient electron-accepting unit bithieno[3,2-b:2'-e]pyridine. <i>Polymer</i> , 2005, 46, 9955-9964.	1.8	30
918	Hydrogen-bond effects on the electronic absorption spectrum and evaluation of nonlinear optical properties of an aminobenzodifuranone derivative that exhibits the largest positive solvatochromism. <i>Journal of Molecular Modeling</i> , 2005, 11, 317-322.	0.8	16
919	Experimental and Theoretical Studies on (p-methoxyphenyl)thiosemicarbazide. <i>Structural Chemistry</i> , 2005, 16, 361-367.	1.0	7
920	Irreducible charge density matrices for analysis of many-electron wave functions. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 582-601.	1.0	39
921	Luminescent compounds diphenylboron analogs of Alq ₃ and its methyl substituents: A theoretical investigation of their electronic and spectroscopic properties. <i>International Journal of Quantum Chemistry</i> , 2005, 103, 775-780.	1.0	24
922	Collectivity, shell openness indices, and complexity measures of multiconfigurational states: Computations within full CI scheme. <i>International Journal of Quantum Chemistry</i> , 2005, 104, 167-180.	1.0	24
923	Theoretical study of laser light generation and color image formation:FA1:Cs ⁺ and FA2:Li ⁺ centers at the low coordination (100) and (110) surfaces of AgCl and AgBr. <i>International Journal of Quantum Chemistry</i> , 2005, 103, 432-448.	1.0	8
924	Understanding complex surface-enhanced Raman scattering, using quantum chemical calculations. <i>International Journal of Quantum Chemistry</i> , 2005, 104, 681-694.	1.0	29
925	Asymmetric structure for the excited S ₁ state of 2,2'-bipyridine evidenced by picosecond time-resolved resonance raman experiments and ab initio calculation. <i>International Journal of Quantum Chemistry</i> , 2005, 104, 794-807.	1.0	5
926	Time-dependent density functional theory (TD-DFT) study of the excited state proton transfer in hypoxanthine. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 387-395.	1.0	22
927	Computational chemistry applied to studies of organic contaminants in the environment: Examples based on benzo[a]pyrene. <i>Numerische Mathematik</i> , 2005, 305, 621-644.	0.7	11
928	Ab Initio Methods for Excited States. <i>Theoretical and Computational Chemistry</i> , 2005, , 35-91.	0.2	38
929	Photodissociation dynamics of acetoxime in gas phase. <i>Journal of Chemical Physics</i> , 2005, 122, 184322.	1.2	2
930	Molecular applications of the intermediate Hamiltonian Fock-space coupled-cluster method for calculation of excitation energies. <i>Journal of Chemical Physics</i> , 2005, 122, 224110.	1.2	78
931	Time-dependent configuration-interaction calculations of laser-pulse-driven many-electron dynamics: Controlled dipole switching in lithium cyanide. <i>Journal of Chemical Physics</i> , 2005, 123, 074105.	1.2	163

#	ARTICLE	IF	CITATIONS
932	Cavity ring-down spectroscopy and theoretical calculations of the S1(B3u1)→S0(Ag1) transition of jet-cooled perylene. <i>Journal of Chemical Physics</i> , 2005, 122, 084318.	1.2	49
933	Potential-energy surface, dynamics of van der Waals motions, and vibronic transitions in p-difluorobenzene-argon complex. <i>Journal of Chemical Physics</i> , 2005, 122, 114312.	1.2	15
934	Solvent effects on the vibronic one-photon absorption profiles of dioxaborine heterocycles. <i>Journal of Chemical Physics</i> , 2005, 123, 194311.	1.2	24
935	Correlated many-electron dynamics: Application to inelastic electron scattering at a metal film. <i>Physical Review A</i> , 2005, 72, .	1.0	33
936	INVESTIGATION OF DOMINANT ELECTRON CONFIGURATIONS IN TIME-DEPENDENT DENSITY FUNCTIONAL THEORY. <i>Journal of Theoretical and Computational Chemistry</i> , 2005, 04, 265-280.	1.8	2
937	Effect of Adiabaticity on Electron Dynamics in Zinc Myoglobin. <i>Journal of Physical Chemistry B</i> , 2005, 109, 5954-5961.	1.2	6
938	Effective conjugation and Raman intensities in oligo(para-phenylene)s: A microscopic view from first-principles calculations. <i>Journal of Chemical Physics</i> , 2005, 122, 114511.	1.2	33
939	Coupled cluster methods including triple excitations for excited states of radicals. <i>Journal of Chemical Physics</i> , 2005, 122, 054110.	1.2	64
940	Third- and fourth-order perturbation corrections to excitation energies from configuration interaction singles. <i>Journal of Chemical Physics</i> , 2005, 122, 094105.	1.2	36
941	Breakdown of the mirror image symmetry in the optical absorption/emission spectra of oligo(para-phenylene)s. <i>Journal of Chemical Physics</i> , 2005, 122, 054501.	1.2	117
942	Theoretical studies on the absorption and luminescent properties of a series of derivatives of 1,3-diphenyl-5-pyrene-2-yl-4,5-dihydro-1H-pyrazole. <i>Canadian Journal of Chemistry</i> , 2005, 83, 166-173.	0.6	1
943	Quantum Monte Carlo: Theory and Application to Molecular Systems. <i>Advances in Quantum Chemistry</i> , 2005, , 209-226.	0.4	6
944	Unusual structural and energetic features of homolytic bond dissociation: from tetrakis(disilyl)diphosphine to tetrakis(di-tert-butylsilyl)hydrazine. <i>Dalton Transactions</i> , 2005, , 2382.	1.6	3
945	Matrix Isolation and Density Functional Theory Study of Bis(trifluoromethyl)dioxodiazine: A Photodimer of Trifluoronitrosomethane. <i>Journal of Physical Chemistry A</i> , 2005, 109, 5307-5315.	1.1	0
946	Light-Induced Structural Changes in the Active Site of the BLUF Domain in AppA by Raman Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2005, 109, 12620-12626.	1.2	91
947	Combinations of chiral and prochiral singlet radical-pairs in reaction cavities of polyethylene films. Control and analysis of radical tumbling and translation. <i>Photochemical and Photobiological Sciences</i> , 2005, 4, 348.	1.6	13
948	First Singlet (n,π*) Excited State of Hydrogen-Bonded Complexes between Water and Pyrimidine. <i>Journal of Physical Chemistry A</i> , 2005, 109, 1576-1586.	1.1	13
949	Effect of Hydration on the Lowest Singlet ππ* Excited-State Geometry of Guanine: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 17333-17339.	1.2	37

#	ARTICLE	IF	CITATIONS
950	Theoretical Investigation of Optical and Electronic Property Modulations of π -Conjugated Polymers Based on the Electron-Rich 3,6-Dimethoxy-fluorene Unit. <i>Journal of Organic Chemistry</i> , 2005, 70, 3009-3020.	1.7	62
951	Comparison of CIS- and EOM-CCSD-Calculated Adiabatic Excited-State Structures. Changes in Charge Density on Going to Adiabatic Excited States. <i>Journal of Physical Chemistry A</i> , 2005, 109, 466-477.	1.1	35
952	α -Cyanine-N Substitutedmer-Ga ₃ andmer-Alq ₃ Derivatives: An Effective Approach for the Tuning of Emitting Color. <i>Journal of Physical Chemistry B</i> , 2005, 109, 17762-17767.	1.2	47
953	Theoretical Study on Electronic Structure and Optical Properties of Phenothiazine-Containing Conjugated Oligomers and Polymers. <i>Journal of Organic Chemistry</i> , 2005, 70, 5987-5996.	1.7	86
954	Intramolecular Nitro-Assisted Proton Transfer in Photoirradiated 2-(2,4-Dinitrobenzyl)pyridine: Polarized Optical Spectroscopic Study and Electronic Structure Calculations. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7264-7275.	1.1	20
955	Isomer-Specific Spectroscopy and Conformational Isomerization Energetics of <i>o</i> -, <i>m</i> -, and <i>p</i> -Ethylnylstyrenes. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4484-4496.	1.1	28
956	A Theoretical, Spectroscopic, and Photophysical Study of 2,7-Carbazolenevinylene-Based Conjugated Derivatives. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6953-6959.	1.1	109
957	An Experimental and Theoretical Investigation of the Photophysics of 1-Hydroxy-2-naphthoic Acid. <i>Journal of Physical Chemistry A</i> , 2005, 109, 2746-2754.	1.1	51
958	Conformation-Specific Spectroscopy of 4-Phenyl-1-butyne and 5-Phenyl-1-pentyne. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8487-8496.	1.1	14
959	Theoretical Studies of the Spectroscopic Properties of [Pt(trpy)Cr]+ (trpy = 2,2',6',2''-Terpyridine; R = H, Me, Et, n-Bu, i-Bu, t-Bu, Ph, CH ₃ , C ₆ H ₅ , C ₆ H ₄ , C ₆ H ₃ , C ₆ H ₂ , C ₆ H, C ₅ H ₄ , C ₅ H ₃ , C ₅ H ₂ , C ₅ H, C ₄ H ₃ , C ₄ H ₂ , C ₄ H, C ₃ H ₂ , C ₃ H, C ₂ H ₂ , C ₂ H, C ₁ H ₂ , C ₁ H). <i>Journal of Physical Chemistry A</i> , 2005, 109, 10784-10794.	1.1	104
960	Excited-State Proton Transfer of 2-(2-Pyridyl)benzimidazole in Microemulsions: Selective Enhancement and Slow Dynamics in Aerosol OT Reverse Micelles with an Aqueous Core. <i>Journal of Physical Chemistry B</i> , 2005, 109, 18895-18901.	1.2	51
961	Optical Properties and Delocalization of Excess Negative Charges on Oligo(Phenylenevinylene)s: A Quantum Chemical Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 5644-5652.	1.2	21
962	Absolute Configuration, Conformation, and Circular Dichroism of Monocyclic Arene Dihydrodiol Metabolites: It is All Due to the Heteroatom Substituents. <i>Journal of the American Chemical Society</i> , 2005, 127, 4308-4319.	6.6	48
963	Tailoring Transition Metal Complexes for Nonlinear Optics Applications. 2. A Theoretical Investigation of the Second-Order Nonlinear Optical Properties of M(CO) ₅ L Complexes (M = Cr, W; L = Py, PyCHO). <i>Journal of Physical Chemistry A</i> , 2005, 109, 7843-7854.	1.1	14
964	Spectroscopy and Femtosecond Dynamics of 7-N,N-Diethylamino-3-hydroxyflavone. The Correlation of Dipole Moments among Various States To Rationalize the Excited-State Proton Transfer Reaction. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11696-11706.	1.1	37
965	Impact of Sulfur vs Oxygen on the Low-Lying Excited States of <i>trans</i> - <i>p</i> -Coumaric Acid and <i>trans</i> - <i>p</i> -Coumaric Thio Acid. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4623-4631.	1.1	52
966	Theoretical Exploration of Ultrafast Dynamics in Atomic Clusters: Analysis and Control. <i>Chemical Reviews</i> , 2005, 105, 11-66.	23.0	110
967	On the Pyrolysis Mechanism of 2-Pyranones and 2-Pyranthiones: Thermally Induced Ground Electronic State Chemistry of Pyran-2-thione. <i>Journal of Organic Chemistry</i> , 2005, 70, 7701-7710.	1.7	14

#	ARTICLE	IF	CITATIONS
968	Theoretical Studies of the Modulation of Polymer Electronic and Optical Properties through the Introduction of the Electron-Donating 3,4-Ethylenedioxythiophene or Electron-Accepting Pyridine and 1,3,4-Oxadiazole Moieties. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7764-7774.	1.1	34
969	Conformation-Specific Spectroscopy of 3-Benzyl-1,5-hexadiyne. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8497-8506.	1.1	2
970	The performance of time-dependent density functional theory based on a noncollinear exchange-correlation potential in the calculations of excitation energies. <i>Journal of Chemical Physics</i> , 2005, 122, 074109.	1.2	121
971	A TDDFT Study of the Optical Response of DNA Bases, Base Pairs, and Their Tautomers in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2005, 109, 2373-2380.	1.1	104
972	Calculation of the UV-visible spectra and the stability of Mo and Re oxysulfides in aqueous solution. <i>Geochimica Et Cosmochimica Acta</i> , 2005, 69, 2497-2503.	1.6	12
973	Calculating the partitioning of the isotopes of Mo between oxidic and sulfidic species in aqueous solution. <i>Geochimica Et Cosmochimica Acta</i> , 2005, 69, 2981-2993.	1.6	202
974	Palladium(II) chloride complexation: Spectrophotometric investigation in aqueous solutions from 5 to 125Å°C and theoretical insight into Pd-Cl and Pd-OH ₂ interactions. <i>Geochimica Et Cosmochimica Acta</i> , 2005, 69, 3773-3789.	1.6	79
975	Electronic properties of alkoxy derivatives of poly(para-phenylenevinylene), investigated by time-dependent density functional theory calculations. <i>Synthetic Metals</i> , 2005, 155, 27-34.	2.1	13
976	Theoretical investigation of electronic structure and spectroscopic properties of functionalized bis-silicon-bridged stilbene homologue. <i>Synthetic Metals</i> , 2005, 152, 269-272.	2.1	0
977	Size-dependent structures of NanIn [~] 1+ cluster ions with a methanol adsorbate: A combined study by photodissociation spectroscopy and density-functional theory calculation. <i>Journal of Chemical Physics</i> , 2005, 123, 161101.	1.2	4
978	Excited state tautomerization of azaindole. <i>Organic and Biomolecular Chemistry</i> , 2005, 3, 3701.	1.5	24
979	Theoretical Study on the Electronic Structure and Optical Properties of Mercury-Containing Diethynylfluorene Monomer, Oligomer, and Polymer. <i>Organometallics</i> , 2005, 24, 385-394.	1.1	30
980	Porphyrin Distortion from Resonance Raman Intensities of Out-of-Plane Modes:â€% Computation and Modeling of N-Methylmesoporphyrin, a Ferrochelatase Transition State Analog. <i>Journal of Physical Chemistry A</i> , 2005, 109, 421-430.	1.1	46
981	Structural, photophysical and lasing properties of pyrromethene dyes. <i>International Reviews in Physical Chemistry</i> , 2005, 24, 339-374.	0.9	137
982	Augmenting basis set for time-dependent density functional theory calculation of excitation energies: Slater-type orbitals for hydrogen to krypton. <i>Molecular Physics</i> , 2005, 103, 749-761.	0.8	116
983	Molecular electronic excitations calculated from a solid-state approach: Methodology and numerics. <i>Physical Review B</i> , 2005, 72, .	1.1	64
984	Femtosecond Dynamics on Excited-State Proton/ Charge-Transfer Reaction in 4â€-N,N-Diethylamino-3-hydroxyflavone. The Role of Dipolar Vectors in Constructing a Rational Mechanism. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3777-3787.	1.1	126
985	Ultrafast Intermolecular Hydrogen Bond Dynamics in the Excited State of Fluorenone. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8693-8704.	1.1	100

#	ARTICLE	IF	CITATIONS
986	Hypervalent ammonium radicals. Competitive N–C and N–H bond dissociations in methyl ammonium and ethyl ammonium. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 912-920.	1.3	35
987	Structure Optimizations for Excited States with Correlated Second-Order Methods: CC2 and ADC(2). <i>Advances in Quantum Chemistry</i> , 2005, 50, 37-60.	0.4	386
988	Excited electronic states of small water clusters. <i>Journal of Chemical Physics</i> , 2005, 122, 044111.	1.2	69
989	Spectroscopic and Theoretical Evidence for the Elusive Intermediate of the Photoinitiated and Thermal Rearrangements of Photochromic Spiropyran. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9605-9616.	1.1	36
990	Excited State Proton Transfer in Guanine in the Gas Phase and in Water Solution: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7775-7780.	1.1	40
991	A simplified relativistic time-dependent density-functional theory formalism for the calculations of excitation energies including spin-orbit coupling effect. <i>Journal of Chemical Physics</i> , 2005, 123, 154102.	1.2	209
992	Role of the Oxyallyl Substructure in the Near Infrared (NIR) Absorption in Symmetrical Dye Derivatives: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 2614-2622.	1.1	40
993	Analyses of In-Cage Singlet Radical-Pair Motions from Irradiations of 1-Naphthyl (R)-1-Phenylethyl Ether and 1-Naphthyl (R)-2-Phenylpropanoate in Alkanes. <i>Journal of Organic Chemistry</i> , 2005, 70, 1243-1252.	1.7	19
994	Theoretical Study of the Benzene Excimer Using Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9174-9182.	1.1	55
995	Fast electron correlation methods for molecular clusters in the ground and excited states. <i>Molecular Physics</i> , 2005, 103, 2255-2265.	0.8	137
996	Toward a Molecular Scale Interpretation of Excitation Energy Transfer in Solvated Bichromophoric Systems. <i>Journal of the American Chemical Society</i> , 2005, 127, 16733-16744.	6.6	85
997	Method of the reduced-added Green function in the calculation of atomic polarizabilities. <i>Physical Review A</i> , 2005, 71, .	1.0	48
998	Theoretical Study of Singlet and Triplet Excitation Energies in Oligothiophenes. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3078-3085.	1.1	73
999	Conical intersections and double excitations in time-dependent density functional theory. <i>Molecular Physics</i> , 2006, 104, 1039-1051.	0.8	557
1000	Evaluation of alternative sum-over-states expressions for the first hyperpolarizability of push-pull π -conjugated systems. <i>Journal of Chemical Physics</i> , 2006, 125, 024101.	1.2	78
1001	Control of Emission by Intermolecular Fluorescence Resonance Energy Transfer and Intermolecular Charge Transfer. <i>Journal of Physical Chemistry A</i> , 2006, 110, 6324-6328.	1.1	52
1002	Intramolecular Hydrogen Bonding in 1,8-Dihydroxyanthraquinone, 1-Aminoanthraquinone, and 9-Hydroxyphenalenone Studied by Picosecond Time-Resolved Fluorescence Spectroscopy in a Supersonic Jet. <i>Journal of Physical Chemistry B</i> , 2006, 110, 19820-19832.	1.2	27
1003	Calculation of the Energetics for the Oligomerization of Gas Phase HgO and HgS and for the Solvolysis of Crystalline HgO and HgS. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2571-2578.	1.1	38

#	ARTICLE	IF	CITATIONS
1004	Early Excited State Dynamics of 6-Styryl-Substituted Pyrylium Salts Exhibiting Dual Fluorescence. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9988-9994.	1.1	27
1005	Mass-analyzed threshold ionization spectroscopy of pyridine. Structural distortion in the first excited state. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 4441.	1.3	28
1006	Protein-bound chromophores astaxanthin and phytochromobilin: excited state quantum chemical studies. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 4053.	1.3	37
1007	Kinetic study of the reactions of the sodium dimer (Na ₂) with a range of atmospheric species. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 3104.	1.3	0
1008	The absorption spectra of anisole-h8, anisole-d3 and anisole-d8. The assignment of fundamental vibrations in the S ₀ and the S ₁ states. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 2360-2377.	1.3	26
1009	Influence of Base Stacking and Hydrogen Bonding on the Fluorescence of 2-Aminopurine and Pyrrolocytosine in Nucleic Acids. <i>Biochemistry</i> , 2006, 45, 9145-9155.	1.2	74
1010	Local CC2 electronic excitation energies for large molecules with density fitting. <i>Journal of Chemical Physics</i> , 2006, 125, 104106.	1.2	166
1011	Time-dependent density functional theory investigation of the absorption, fluorescence, and phosphorescence spectra of solvated coumarins. <i>Journal of Chemical Physics</i> , 2006, 125, 164324.	1.2	115
1012	Theoretical Study on Photophysical and Charge Transport Properties of 1,6-Bis(2-hydroxyphenyl)pyridylboron Bis(4-n-butylphenyl)phenyleneamine Compound. <i>Journal of Physical Chemistry A</i> , 2006, 110, 8758-8762.	1.1	41
1013	Semiempirical (ZINDO-PCM) Approach to Predict the Radiative and Nonradiative Decay Rates of a Molecule Close to Metal Particles. <i>Journal of Physical Chemistry B</i> , 2006, 110, 16652-16659.	1.2	25
1014	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. <i>Journal of Chemical Physics</i> , 2006, 124, 094107.	1.2	1,143
1015	Kohn-Sham Time-Dependent Density Functional Theory with Applications to Linear and Nonlinear Properties. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2006, , 151-209.	0.6	2
1016	Bond Length Alternation and Energy Band Gap of Polyyne. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9771-9774.	1.1	123
1017	Synthesis, Structural Studies, Theoretical Calculations, and Linear and Nonlinear Optical Properties of Terpyridyl Lanthanide Complexes: A New Evidence for the Contribution of f Electrons to the NLO Activity. <i>Journal of the American Chemical Society</i> , 2006, 128, 12243-12255.	6.6	113
1018	Fluorescence Spectroscopic Properties and Crystal Structure of a Series of Donor-Acceptor Diphenylpolyenes. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13379-13387.	1.1	49
1019	Electronic structure and excitations in oligoacenes from ab initio calculations. <i>Journal of Chemical Physics</i> , 2006, 124, 134901.	1.2	103
1020	Electronic Properties of Anthracene Derivatives for Blue Light Emitting Electroluminescent Layers in Organic Light Emitting Diodes: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1152-1162.	1.1	69
1021	Optical and Photophysical Properties of Indolocarbazole Derivatives. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13696-13704.	1.1	50

#	ARTICLE	IF	CITATIONS
1022	Theoretical Study on the Optoelectronic Properties of Electron-Withdrawing Substituted Diethynylfluorenyl Gold(I) Complexes. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13036-13044.	1.1	23
1023	Selection Rules of the Charge Transfer Mechanism of Surface-Enhanced Raman Scattering: The Effect of the Adsorption on the Relative Intensities of Pyrimidine Bonded to Silver Nanoclusters. <i>Journal of Physical Chemistry B</i> , 2006, 110, 14916-14922.	1.2	57
1024	Theoretical Studies on Photophysical Properties and Mechanism of Phosphorescence in [<i>fac</i> -(2-phenylpyridine) ₃]. <i>Journal of the Chinese Chemical Society</i> , 2006, 53, 101-112.	0.8	152
1025	Experimental Probe for Hyperconjugative Resonance Contribution in Stabilizing the Singlet State of 2,2-Dialkoxy-1,3-diyols: Regioselective 1,2-Oxygen Migration. <i>Journal of the American Chemical Society</i> , 2006, 128, 8008-8014.	6.6	34
1026	Excited-State Properties and Transitions of Fluorescent 8-Vinyl Adenosine in DNA. <i>Journal of Physical Chemistry B</i> , 2006, 110, 26327-26336.	1.2	21
1027	Theoretical Study on the Excited-State Intramolecular Proton Transfer in the Aromatic Schiff Base Salicylidene Methylamine: An Electronic Structure and Quantum Dynamical Approach. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4649-4656.	1.1	57
1028	Twisting Dynamics in the Excited Singlet State of Michler's Ketone. <i>Journal of Physical Chemistry A</i> , 2006, 110, 3432-3446.	1.1	38
1029	Optical Excitations in Carbon Architectures Based on Dodecahydrotribenzo[18]annulene. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1305-1318.	1.1	41
1030	Photodissociation of Formyl Fluoride in Rare Gas Matrixes. <i>Journal of Physical Chemistry A</i> , 2006, 110, 6208-6215.	1.1	1
1031	Solvation of Coumarin 153 in Supercritical Fluoroform. <i>Journal of Physical Chemistry B</i> , 2006, 110, 4953-4962.	1.2	38
1032	Two-Dimensional Charge Delocalization in X-Shaped Phenylenevinylene Oligomers. <i>Chemistry of Materials</i> , 2006, 18, 2118-2129.	3.2	23
1033	The role of oxidation states in laser light generation, color image formation and adsorbate-substrate interactions. Comparative study of FA:Tl+1, FB:Tl+1, FA:Tl+3 and FB:Tl+3 color centers at the (100) and (110) surfaces of AgBr crystal. <i>Computational Materials Science</i> , 2006, 38, 144-157.	1.4	3
1034	An ab initio cluster-in-lattice model for the luminescence of K ₂ NbOF ₅ crystal. <i>Computational Materials Science</i> , 2006, 38, 410-417.	1.4	2
1035	Triplet-triplet energy-transfer coupling: Theory and calculation. <i>Journal of Chemical Physics</i> , 2006, 124, 044506.	1.2	110
1036	A state-specific polarizable continuum model time dependent density functional theory method for excited state calculations in solution. <i>Journal of Chemical Physics</i> , 2006, 125, 054103.	1.2	675
1037	Excited state geometry optimizations by analytical energy gradient of long-range corrected time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2006, 124, 144106.	1.2	195
1038	Spectroscopic investigations of copolymers incorporating various thiophene and phenylene monomers. <i>Synthetic Metals</i> , 2006, 156, 318-326.	2.1	22
1039	Quantum Mechanics and Molecular Mechanics Studies of Host-Guest Stabilization and Reactivity in Cyclodextrin Nanocavities. , 2006, , 155-179.		0

#	ARTICLE	IF	CITATIONS
1040	Electronic excitations in anti-aromatic dehydro[12]- and aromatic dehydro[18]annulenes: a time-dependent density functional theory study. <i>Molecular Physics</i> , 2006, 104, 933-941.	0.8	9
1041	Periodane—An unexpectedly stable molecule of unique composition. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1865-1869.	1.0	10
1042	Computational and spectroscopic studies concerning the solvatochromic behavior of 1,3-disubstituted azulenes. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2331-2338.	1.0	7
1043	Novel oligomers based on fluorene and 2,4-difluorobenzene: Correlation between the structures and optical properties. <i>Journal of Polymer Science Part A</i> , 2006, 44, 4346-4353.	2.5	8
1044	A plausible prebiotic synthesis of pyridoxal phosphate: Vitamin B6 — A computational study. <i>Biophysical Chemistry</i> , 2006, 123, 113-121.	1.5	14
1045	Theoretical study on characteristics of structure and vibrational frequency of spiro-linked complex Zn(PyIm) ₂ (PyIm = 2-(2-pyridine)-imidazole) in excited state. <i>Chemical Physics Letters</i> , 2006, 418, 302-306.	1.2	5
1046	Photochemistry of AgCl—water clusters: Comparison with Cl—water clusters. <i>Chemical Physics Letters</i> , 2006, 419, 340-345.	1.2	15
1047	Excited state proton transfer of 2-(2-pyridyl)benzimidazole: A computational study. <i>Chemical Physics Letters</i> , 2006, 422, 446-450.	1.2	5
1048	Substituent effect on the structures and luminescence of binuclear Au(I) complexes: An ab initio study. <i>Chemical Physics Letters</i> , 2006, 426, 257-262.	1.2	2
1049	Spectral origins and ionization potentials of guanine tautomers: Theoretical elucidation of experimental findings. <i>Chemical Physics Letters</i> , 2006, 429, 261-265.	1.2	53
1050	Excited state proton transfer in 2-hydroxypyridine—ammonia clusters: Theoretical investigation. <i>Chemical Physics Letters</i> , 2006, 430, 195-203.	1.2	11
1051	Application of fragment molecular orbital scheme to silicon-containing systems. <i>Chemical Physics Letters</i> , 2006, 430, 361-366.	1.2	15
1052	Excited state properties of novel p- and n-type organic semiconductors with an anthracene unit. <i>Chemical Physics</i> , 2006, 320, 155-163.	0.9	31
1053	The role of oxidation states in FA1 Tln+ (n=1,3) lasers and CO interactions at the (100) surface of NaCl: An ab initio study. <i>Chemical Physics</i> , 2006, 328, 8-16.	0.9	23
1054	A DFT and MP2 study of luminescence of gold(I) complexes. <i>Inorganica Chimica Acta</i> , 2006, 359, 3617-3624.	1.2	18
1055	Interchain interactions in charged diacetylenic oligomers carrying bulk substituents revisited. <i>Materials Science and Engineering C</i> , 2006, 26, 1044-1048.	3.8	0
1056	Theoretical studies on titanium pentafulvene complexes. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4539-4544.	0.8	22
1057	The photo-Fries rearrangement of 9-trimethylsilyl substituted xanthenes. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2006, 182, 17-27.	2.0	3

#	ARTICLE	IF	CITATIONS
1058	The photophysics of cryptophyte light-harvesting. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2006, 184, 1-17.	2.0	88
1059	Fluoride ion detection by 8-hydroxyquinolineâ€“Zr(IV)â€“EDTA complex. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2006, 65, 565-570.	2.0	22
1060	Theoretical modeling of laser light generation and color image formation: FA1:Tl+ and FA2:Ga+ color centers at the low coordination (100) and (110) surfaces of AgCl and AgBr. <i>Optical Materials</i> , 2006, 28, 1197-1208.	1.7	7
1061	Comparison of the Raman spectrum of trans-stilbene in the S1 state calculated by the CIS method and the spectra observed under resonant and off-resonant conditions. <i>Vibrational Spectroscopy</i> , 2006, 42, 176-182.	1.2	9
1062	Turning optical chemosensors into optodes: a quantum chemical and experimental case-study. <i>Tetrahedron Letters</i> , 2006, 47, 5709-5712.	0.7	1
1063	Ab initio study of the structure of aniline in the S1 and S2 $\tilde{\nu}^*$ states. <i>Computational and Theoretical Chemistry</i> , 2006, 758, 17-20.	1.5	16
1064	Structural, electronic and optical properties of a series of oligofluoreneâ€“thiophene oligomers and polymers. <i>Computational and Theoretical Chemistry</i> , 2006, 758, 29-39.	1.5	17
1065	Ab initio configuration interaction singles (CIS) study on polycyclic aromatic molecules (I): Correlation between calculated and observed excitation energies. <i>Computational and Theoretical Chemistry</i> , 2006, 759, 165-169.	1.5	6
1066	Ab initio study on luminescent properties of triangular Au(I) complexes. <i>Computational and Theoretical Chemistry</i> , 2006, 759, 35-39.	1.5	8
1067	Emission energies and photophysical properties of ladder oligo(p-aniline)s. <i>Computational and Theoretical Chemistry</i> , 2006, 760, 147-152.	1.5	14
1068	Quantum computations of the UVâ€“visible spectra of uric acid and its anions. <i>Computational and Theoretical Chemistry</i> , 2006, 761, 203-207.	1.5	11
1069	Origin of regioselectivity in the intramolecular [2+2] photoreaction of $\hat{1}_{\pm}$, $\hat{1}_2$ -unsaturated furanones to a terminal alkene. <i>Computational and Theoretical Chemistry</i> , 2006, 763, 115-121.	1.5	9
1070	A theoretical study of hydration of 4-thiouracil in the electronic singlet excited state. <i>Computational and Theoretical Chemistry</i> , 2006, 771, 149-155.	1.5	10
1071	Density functional study for discoloration reaction of titanylporphyrin. <i>Computational and Theoretical Chemistry</i> , 2006, 766, 41-47.	1.5	12
1072	Potential energy surface of the electron excited states in the state-specific multi-reference coupled cluster theory. Hydrogen fluoride dissociation. <i>Computational and Theoretical Chemistry</i> , 2006, 768, 97-101.	1.5	15
1073	Excited state properties of neutral, anionic and cationic 1,1-disubstituted 2,3,4,5-tetraphenylsiloles: A quantum chemical characterization. <i>Computational and Theoretical Chemistry</i> , 2006, 770, 51-56.	1.5	4
1074	Conformational changes and S1 \rightarrow S0 origin transition energies: Polychlorinated biphenyls (PCBs). <i>Computational and Theoretical Chemistry</i> , 2006, 772, 31-37.	1.5	1
1075	Ab initio MO study on the S1 \rightarrow S0 origin transition energies of polychlorodibenzofurans (PCDFs). <i>Computational and Theoretical Chemistry</i> , 2006, 774, 7-12.	1.5	3

#	ARTICLE	IF	CITATIONS
1076	Heterobimetallic Zn(II)–Ln(III) Phenylene-Bridged Schiff Base Complexes, Computational Studies, and Evidence for Singlet Energy Transfer as the Main Pathway in the Sensitization of Near-Infrared Nd ³⁺ Luminescence. <i>Inorganic Chemistry</i> , 2006, 45, 9315-9325.	1.9	155
1077	Isotopic effects in the electronic spectra of tryptophan. <i>Amino Acids</i> , 2006, 31, 403-407.	1.2	5
1078	Ab initio calculation of molecular chiroptical properties. <i>Theoretical Chemistry Accounts</i> , 2006, 115, 227-245.	0.5	362
1079	Ab initio electronic structure theory as an aid to understanding excited state hydrogen transfer in moderate to large systems. <i>Theoretical Chemistry Accounts</i> , 2006, 116, 355-372.	0.5	8
1080	Time-dependent density functional theory study on electronic and spectroscopic properties for Ph ₂ Bq and its complexes. <i>Theoretical Chemistry Accounts</i> , 2006, 117, 1-5.	0.5	10
1081	Mass-analyzed threshold ionization spectroscopy of pyrimidine: determining the geometry in the first excited and the ionic ground states. <i>Analytical and Bioanalytical Chemistry</i> , 2006, 386, 59-68.	1.9	24
1082	Theoretical investigations on the modulation of the polymer electronic and optical properties by introduction of phenoxazine. <i>Polymer</i> , 2006, 47, 3229-3239.	1.8	11
1083	The role of type II FB (I):Tl ⁺ defect in laser light generation and color image formation at the low coordination surface sites of AgBr: ab initio calculations. <i>Current Applied Physics</i> , 2006, 6, 19-31.	1.1	5
1084	About the photoionization of methyl bromide (CH ₃ Br). Photoelectron and photoionization mass spectrometric investigation. <i>Chemical Physics</i> , 2006, 323, 458-472.	0.9	14
1085	On the intramolecular proton transfer of 3-hydroxyflavone in the first singlet excited state: A theoretical study. <i>Chemical Physics</i> , 2006, 325, 243-250.	0.9	38
1086	An Extremely Long-Lived Singlet 4,4-Dimethoxy-3,5-diphenylpyrazolidine-3,5-diyl Derivative: A Notable Nitrogen-Atom Effect on Intra- and Intermolecular Reactivity. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 7828-7831.	7.2	44
1087	Theoretical Studies on Metal–Metal Interaction and Intrinsic 1,3-[(f*(d))f(s/p)] Excited States of Dinuclear d ¹⁰ Complexes with Bridging Phosphane Ligands. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 1050-1059.	1.0	13
1088	Systematic Studies on Photoluminescence of Oligo(arylene-ethynylene)s: Tunability of Excited States and Derivatization as Luminescent Labeling Probes for Proteins. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 3125-3139.	1.2	17
1089	Computation of vertical excitation energies of retinal and analogs: Scope and limitations. <i>Journal of Computational Chemistry</i> , 2006, 27, 116-123.	1.5	25
1090	Spin-Orbit Ab Initio Investigation of the Photolysis of Bromiodomethane. <i>ChemPhysChem</i> , 2006, 7, 955-963.	1.0	25
1091	Quantum Chemical Methods for the Investigation of Photoinitiated Processes in Biological Systems: Theory and Applications. <i>ChemPhysChem</i> , 2006, 7, 2259-2274.	1.0	69
1093	A Hole-Transporting Material with Controllable Morphology Containing Binaphthyl and Triphenylamine Chromophores. <i>Advanced Functional Materials</i> , 2006, 16, 1343-1348.	7.8	47
1094	On perturbative corrections to excitation energies from configuration interaction singles. <i>Molecular Physics</i> , 2006, 104, 2073-2083.	0.8	9

#	ARTICLE	IF	CITATIONS
1095	Addition by subtraction in coupled-cluster theory: A reconsideration of the CC and CI interface and the nCC hierarchy. <i>Journal of Chemical Physics</i> , 2006, 125, 204105.	1.2	65
1096	Potential-energy surface, van der Waals energy spectrum, and vibronic transitions in s-tetrazine-argon complex. <i>Journal of Chemical Physics</i> , 2006, 124, 044310.	1.2	5
1097	Potential energy surface, van der Waals motions, and vibronic transitions in phenol-argon complex. <i>Journal of Chemical Physics</i> , 2006, 124, 084310.	1.2	24
1098	Photodissociation of Mg+XCH ₃ (X=F, Cl, Br, and I) complexes. I. Electronic spectra and dissociation pathways. <i>Journal of Chemical Physics</i> , 2006, 125, 094309.	1.2	15
1099	Photodissociation of Mg+XCH ₃ (X=F, Cl, Br, and I) complexes. II. Fragment angular and energy distributions. <i>Journal of Chemical Physics</i> , 2006, 125, 094310.	1.2	10
1100	Excitation energies through the locally renormalized equation-of-motion formalism: Singles and doubles model. <i>Journal of Chemical Physics</i> , 2006, 125, 124101.	1.2	7
1101	Hole-particle characterization of coupled-cluster singles and doubles and related models. <i>Journal of Chemical Physics</i> , 2006, 125, 154106.	1.2	13
1102	Optimal control of ultrafast laser driven many-electron dynamics in a polyatomic molecule: N-methyl-6-quinolone. <i>Journal of Chemical Physics</i> , 2006, 124, 144310.	1.2	53
1103	Study of electronic and spectroscopic properties on a newly synthesized red fluorescent material. <i>Journal of Chemical Physics</i> , 2006, 124, 174711.	1.2	10
1104	Towards a photophysical model for 5-hydroxyflavone. <i>Journal of Chemical Physics</i> , 2006, 124, 104506.	1.2	26
1105	Strain-engineered photoluminescence of silicon nanoclusters. <i>Physical Review B</i> , 2006, 74, .	1.1	64
1106	Configuration-interaction-based time-dependent orbital approach forab initiotreatment of electronic dynamics in a strong optical laser field. <i>Physical Review A</i> , 2006, 74, .	1.0	133
1107	Excited states in the multireference state-specific coupled-cluster theory with the complete active space reference. <i>Journal of Chemical Physics</i> , 2006, 124, 184302.	1.2	21
1108	Analysis of multiconfigurational wave functions in terms of hole-particle distributions. <i>Journal of Chemical Physics</i> , 2006, 124, 224109.	1.2	23
1109	Solvent polarity scales revisited: a ZINDO-PCM study of the solvatochromism of betaine-30. <i>Molecular Physics</i> , 2006, 104, 875-887.	0.8	43
1110	Mass-Analyzed-Threshold-Ionization-Spectroscopy of Pyrazine and Pyrazine-Ar. <i>Zeitschrift Fur Physikalische Chemie</i> , 2007, 221, 663-688.	1.4	5
1111	Second- and third-order triples and quadruples corrections to coupled-cluster singles and doubles in the ground and excited states. <i>Journal of Chemical Physics</i> , 2007, 126, 244106.	1.2	57
1112	Adenine Synthesis in Interstellar Space: Mechanisms of Prebiotic Pyrimidine-Ring Formation of Monocyclic HCN-Pentamers. <i>Astrobiology</i> , 2007, 7, 455-470.	1.5	65

#	ARTICLE	IF	CITATIONS
1113	A Computational Strategy for Organic Photochemistry. <i>Reviews in Computational Chemistry</i> , 2007, , 87-146.	1.5	138
1114	Addition by subtraction in coupled cluster theory. II. Equation-of-motion coupled cluster method for excited, ionized, and electron-attached states based on the nCC ground state wave function. <i>Journal of Chemical Physics</i> , 2007, 127, 024106.	1.2	30
1115	Remarkably efficient acid generation in chemically amplified resist from quantum chemistry modeling. <i>Journal of Vacuum Science & Technology B</i> , 2007, 25, 58.	1.3	0
1116	Quadrupole contribution to the third-order optical activity spectroscopy. <i>Journal of Chemical Physics</i> , 2007, 127, 024507.	1.2	10
1117	CNDOL: A fast and reliable method for the calculation of electronic properties of very large systems. Applications to retinal binding pocket in rhodopsin and gas phase porphine. <i>Journal of Chemical Physics</i> , 2007, 127, 145102.	1.2	19
1118	VUV excitation and electronic decay of rubidium halide molecules. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2007, 40, 2261-2275.	0.6	4
1119	High-order electron-correlation methods with scalar relativistic and spin-orbit corrections. <i>Journal of Chemical Physics</i> , 2007, 126, 024104.	1.2	51
1120	Methods and Applications of Combined Quantum Mechanical and Molecular Mechanical Potentials. <i>Reviews in Computational Chemistry</i> , 2007, , 119-185.	1.5	189
1121	Excited-State Dynamics of trans,trans-Distyrylbenzene: Transient Anisotropy and Excitation Energy Dependence. <i>Journal of Physical Chemistry A</i> , 2007, 111, 759-763.	1.1	5
1122	Tetrathiafulvalene-Based Materials for Organic Field Effect Transistors. Inspection of Their Semiconductor Properties by Means of Molecular Spectroscopy and Quantum Chemistry. <i>Journal of Physical Chemistry C</i> , 2007, 111, 10110-10118.	1.5	20
1123	Notable Effect of an Electron-Withdrawing Group at C3 on the Selective Formation of Alkylidenecyclobutanes in the Thermal Denitrogenation of 4-Spirocyclopropane-1-pyrazolines. Nonstatistical Dynamics Effects in the Denitrogenation Reactions. <i>Journal of the American Chemical Society</i> , 2007, 129, 12981-12988.	6.6	42
1124	Electronic structure and optical physical properties of oligothiophenes. <i>Computational Materials Science</i> , 2007, 39, 673-677.	1.4	7
1125	Selective Formation of Triplet Alkyl Nitrenes from Photolysis of \hat{I}^2 -Azido-Propiophenone and Their Reactivity. <i>Journal of the American Chemical Society</i> , 2007, 129, 16263-16272.	6.6	46
1126	Electronic optical response of molecules in intense fields: Comparison of TD-HF, TD-CIS, and TD-CIS(D) approaches. <i>Journal of Chemical Physics</i> , 2007, 126, 244110.	1.2	96
1127	Double-hybrid density functional theory for excited electronic states of molecules. <i>Journal of Chemical Physics</i> , 2007, 127, 154116.	1.2	404
1128	Multiconfigurational Perturbation Theory: Applications in Electronic Spectroscopy. <i>Advances in Chemical Physics</i> , 2007, , 219-331.	0.3	278
1129	Calculations on Open-Shell Molecules: A Beginner's Guide. <i>Reviews in Computational Chemistry</i> , 2007, , 1-97.	1.5	77
1130	Scaled Second-Order Perturbation Corrections to Configuration Interaction Singles: Efficient and Reliable Excitation Energy Methods. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5314-5326.	1.1	185

#	ARTICLE	IF	CITATIONS
1131	Correlation Effects in EOM-CCSD for the Excited States: Evaluated by AIM Localization Index (LI) and Delocalization Index (DI). <i>Journal of Physical Chemistry A</i> , 2007, 111, 3592-3601.	1.1	33
1132	Vibronic transitions in large molecular systems: Rigorous prescreening conditions for Franck-Condon factors. <i>Journal of Chemical Physics</i> , 2007, 127, 234101.	1.2	158
1133	Theoretical Studies of Conjugation Effects on Excited State Intramolecular Hydrogen-Atom Transfer Reactions in Model Systems. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10139-10143.	1.1	11
1134	Radical Cations of the Nucleic Bases and Radiation Damage to DNA: Ab Initio Study. <i>Advances in Quantum Chemistry</i> , 2007, , 121-147.	0.4	26
1135	Theoretical studies on structures and spectroscopic properties of a series of novel mixed-ligand Ir(III) complexes [Ir(Mebib)(ppy)X]. <i>Dalton Transactions</i> , 2007, , 1922.	1.6	21
1136	Conductance Bistability in a Single Porphyrin Molecule in a STM Junction: A Many-Body Simulation Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 9516-9521.	1.5	10
1137	Electron Super-Rich Radicals in the Gas Phase. A Neutralization-Reionization Mass Spectrometric and ab Initio/RRKM Study of Diaminohydroxymethyl and Triaminomethyl Radicals. <i>Journal of Physical Chemistry A</i> , 2007, 111, 8829-8843.	1.1	19
1138	Optical Properties of the Phosphorescent Trinuclear Copper(I) Complexes of Pyrazolates: Insights from Theory. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4965-4973.	1.1	42
1139	Ground- and Excited-State Proton Transfer and Rotamerism in 2-(2-Hydroxyphenyl)-5-phenyl-1,3,4-oxadiazole and Its O-Substituted Derivatives. <i>Journal of Physical Chemistry A</i> , 2007, 111, 6354-6360.	1.1	27
1140	Electronic Structure and Photophysical Properties of 2-(N,N-diethylanilin-4-yl)-4,6-bis(3,5-dimethylpyrazol-1-yl)-1,3,5-triazine. <i>Chinese Journal of Chemical Physics</i> , 2007, 20, 59-64.	0.6	3
1141	Effect of Hexafluorobenzene on the Photophysics of Pyrene. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4884-4889.	1.1	22
1142	Hydrogen Transfer vs Proton Transfer in 7-Hydroxy-quinoline-(NH ₃) ₃ : A CASSCF/CASPT2 Study. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5907-5912.	1.1	29
1143	Theoretical modeling of the O-H stretching IR bands of hydrogen-bonded dimers of benzoic acid in S ₀ and S ₁ electronic states. <i>Journal of Chemical Physics</i> , 2007, 127, 084307.	1.2	22
1144	Competition between C-Cleavage and Energy Transfer in Azidoacetophenones. <i>Journal of Organic Chemistry</i> , 2007, 72, 2757-2768.	1.7	40
1145	Assessment of time-dependent density functional schemes for computing the oscillator strengths of benzene, phenol, aniline, and fluorobenzene. <i>Journal of Chemical Physics</i> , 2007, 127, 084103.	1.2	85
1146	Laser-Induced Fluorescence Spectrum of 3-Vinyl-1H-indene. <i>Journal of Physical Chemistry A</i> , 2007, 111, 3306-3312.	1.1	5
1147	Relative Ground and Excited-State pK _a Values of Phytochromobilin in the Photoactivation of Phytochrome: A Computational Study. <i>Journal of Physical Chemistry B</i> , 2007, 111, 11554-11565.	1.2	38
1148	Predictions of the Geometries and Fluorescence Emission Energies of Oxyluciferins. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4489-4497.	1.1	37

#	ARTICLE	IF	CITATIONS
1149	Photoinduced C-N Bond Cleavage in 2-Azido-1,3-diphenyl-propan-1-one Derivatives: Photorelease of Hydrazoic Acid. <i>Journal of Organic Chemistry</i> , 2007, 72, 6372-6381.	1.7	25
1150	Theoretical Studies on the Excited States, DNA Photocleavage, and Spectral Properties of Complex [Ru(phen) ₂ (6-OH-dppz)] ²⁺ . <i>Journal of Physical Chemistry A</i> , 2007, 111, 273-280.	1.1	32
1151	How the Central Torsion Angle Affects the Rates of Nonradiative Decay in Some Geometrically Restricted p-Quaterphenyls. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2641-2649.	1.1	18
1152	Theoretical Studies on Structures and Spectroscopic Properties of Bis-Cyclometalated Iridium Complexes. <i>Organometallics</i> , 2007, 26, 143-149.	1.1	74
1153	Theoretical Study on Photophysical Properties of Phenolpyridyl Boron Complexes. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2739-2744.	1.1	38
1154	Theoretical Studies on Structures and Spectroscopic Properties of a Series of Novel Cationic [trans-(C ₅ N)2Ir(PH ₃) ₂] ⁺ (C ₅ N = ppy, bzq, ppz, dfppy). <i>Journal of Physical Chemistry A</i> , 2007, 111, 8724-8730.	1.1	76
1155	Luminescent Properties of Mercury-taining Diethynylfluorene Derivatives. <i>Chemical Research in Chinese Universities</i> , 2007, 23, 92-95.	1.3	3
1156	Electronic Spectroscopy of Nonalternant Hydrocarbons Inside Helium Nanodroplets. <i>Journal of Physical Chemistry A</i> , 2007, 111, 12200-12209.	1.1	13
1157	Computational Study of Thioflavin T Torsional Relaxation in the Excited State. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4829-4835.	1.1	206
1158	Fluorinated Diphenylpolyenes: Crystal Structures and Emission Properties. <i>Journal of Physical Chemistry A</i> , 2007, 111, 13441-13451.	1.1	68
1159	Electronically excited water aggregates and the adiabatic band gap of water. <i>Journal of Chemical Physics</i> , 2007, 126, 014509.	1.2	20
1160	On the Electronic Spectra of Small Linear Polyenes. <i>Advances in Chemical Physics</i> , 2007, , 177-214.	0.3	20
1161	Comparison of basis set effects and the performance of ab initio and DFT methods for probing equilibrium fluctuations. <i>Journal of Computational Chemistry</i> , 2007, 28, 478-490.	1.5	19
1162	Hybrid molecular dynamics-quantum mechanics simulations of solute spectral properties in the condensed phase: Evaluation of simulation parameters. <i>Journal of Computational Chemistry</i> , 2007, 28, 1572-1581.	1.5	34
1163	Theoretical Studies of the Electronic Structure and Spectroscopic Properties of [Ru(Htcterpy)(NCS) ₃] ³⁺ . <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 2171-2180.	1.0	17
1164	A Simple One-Pot Synthesis of Solvatofluorescent Push-Pull Thiophenes. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 5404-5409.	1.2	7
1165	The effect of keto defect on the photophysical properties and electronic structure of neutral and charged LOPP. <i>Computational and Theoretical Chemistry</i> , 2007, 803, 1-7.	1.5	0
1166	Ground and excited state properties of naphthazarin: Absorption spectroscopy and theoretical modeling study. <i>Computational and Theoretical Chemistry</i> , 2007, 803, 79-87.	1.5	9

#	ARTICLE	IF	CITATIONS
1167	Intramolecular hydrogen bonding and photoinduced intramolecular proton and electron transfer in 2-(2-hydroxyphenyl)benzothiazole. <i>Computational and Theoretical Chemistry</i> , 2007, 806, 105-112.	1.5	10
1168	Theoretical study on electronic structure and optical properties of novel donor-acceptor conjugated copolymers derived from benzothiadiazole and benzoselenadiazole. <i>Computational and Theoretical Chemistry</i> , 2007, 816, 161-170.	1.5	25
1169	Investigation of the structures and electronic spectra for coumarin 6 through TD-DFT calculations including PCM solvation. <i>Computational and Theoretical Chemistry</i> , 2007, 818, 43-49.	1.5	27
1170	Bonding and aromaticity of cyclic phosphazenes viewed as interaction of Dnh fragments. <i>Computational and Theoretical Chemistry</i> , 2007, 820, 148-158.	1.5	19
1171	Artificial polarization effects on FA1:Sr ²⁺ lasers and NO interactions at NaCl (001) surface: First principles calculations. <i>Computational and Theoretical Chemistry</i> , 2007, 823, 47-58.	1.5	14
1172	Investigation of the structure, the optical properties, and the photophysics of some indolocarbazoles having terminal aromatic rings. <i>Computational and Theoretical Chemistry</i> , 2007, 824, 15-22.	1.5	11
1173	Fragment molecular orbital calculations on red fluorescent protein (DsRed). <i>Chemical Physics Letters</i> , 2007, 433, 360-367.	1.2	33
1174	A fully quantum mechanical simulation study on the lowest $\hat{\nu}^{\ominus}$ state of hydrated formaldehyde. <i>Chemical Physics Letters</i> , 2007, 437, 66-72.	1.2	52
1175	The geometries, absorption and fluorescence wavelengths of solvated fluorescent coumarins: A CIS and TD-DFT comparative study. <i>Chemical Physics Letters</i> , 2007, 438, 208-212.	1.2	63
1176	Ab initio time-resolved density functional theory for lifetimes of excited adsorbate states at metal surfaces. <i>Chemical Physics Letters</i> , 2007, 439, 199-203.	1.2	35
1177	Natural orbitals in CIS and singular-value decomposition. <i>Chemical Physics Letters</i> , 2007, 439, 393-394.	1.2	38
1178	Modification for spin-adapted version of configuration interaction singles with perturbative doubles. <i>Chemical Physics Letters</i> , 2007, 443, 389-397.	1.2	22
1179	Evidence of structural non-planarity in excited state: New findings provided by vibrational analysis of the guanine-cytosine base pair. <i>Chemical Physics Letters</i> , 2007, 447, 330-334.	1.2	6
1180	Simulation of conductance and current-induced fluorescence of conjugated chromophores. <i>Chemical Physics Letters</i> , 2007, 450, 144-150.	1.2	11
1181	Experimental and theoretical study on the structure and electronic spectra of imiquimod and its synthetic intermediates. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2007, 17, 4942-4946.	1.0	11
1182	Photophysical properties of 1-acetoxy-8-hydroxy-1,4,4a,9a-tetrahydroanthraquinone: Evidence for excited state proton transfer reaction. <i>Chemical Physics</i> , 2007, 331, 189-199.	0.9	15
1183	Chain length dependence of singlet and triplet excited states of oligofluorenes: A density functional study. <i>Chemical Physics</i> , 2007, 336, 91-98.	0.9	26
1184	On the molecular conformation of bisaromatic systems the case of 2-phenyl-2H-benzotriazoles. <i>Chemical Physics</i> , 2007, 340, 32-42.	0.9	5

#	ARTICLE	IF	CITATIONS
1185	Theoretical studies on vibrational spectra and nonlinear optical property of l-arginine phosphate monohydrate crystal. <i>Optical Materials</i> , 2007, 29, 1129-1137.	1.7	37
1186	Design and synthesis of 1,4-bis[4-(1,1-dicyanovinyl)styryl]-2,5-bis(alkoxy)benzenes as red organic electroluminescent PPV analogs. <i>Polymer</i> , 2007, 48, 4028-4033.	1.8	7
1187	Electronic structure and optical properties of germanium-bridged platinum(II)-containing diethynylfluorene monomer and oligomers: A theoretical investigation. <i>Polymer</i> , 2007, 48, 6457-6463.	1.8	17
1188	Theoretical studies on the electronic structure and spectral properties of versatile diarylethene-containing 1,10-phenanthroline ligands and their rhenium(I) complexes. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 5368-5374.	0.8	25
1189	Photochemistry of aryl halides: Photodissociation dynamics. <i>Journal of Photochemistry and Photobiology C: Photochemistry Reviews</i> , 2007, 8, 55-66.	5.6	250
1190	Computational study of steric effects on the optical properties of oligomers. <i>Journal of Luminescence</i> , 2007, 126, 278-288.	1.5	3
1191	A water-soluble fluorescent fluoride ion probe based on Alizarin Red S-Al(III) complex. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007, 66, 457-461.	2.0	31
1192	The hydrogen bonding and amino-imino tautomerization of the alkoxy-aminopyridines and amino-methoxypyrimidines with acetic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007, 68, 979-991.	2.0	9
1193	Comparison of ground and excited state polarizabilities of thiophene, cyclopentadiene, and fulvene oligomers and their cyano substituted derivatives-Ab initio study. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2007, 45, 1983-1995.	2.4	5
1194	Synthesis of Hydroxy and Methoxy Perylene Quinones, Their Spectroscopic and Computational Characterization, and Their Antiviral Activity. <i>Photochemistry and Photobiology</i> , 2005, 81, 924-933.	1.3	1
1195	The role of F Al:Ag+ defects in laser light generation and coadsorption of CO and halogen atoms at the KCl and KBr surface sites. First principles calculations. <i>Open Physics</i> , 2007, 5, .	0.8	0
1196	Structure and Medium Effects on the Photochemical Behavior of Nonfluorinated Quinolone Antibiotics. <i>Photochemistry and Photobiology</i> , 2007, 83, 511-519.	1.3	7
1197	Parallelized integral-direct CIS(D) calculations with multilayer fragment molecular orbital scheme. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 541-553.	0.5	71
1198	The localized Hartree-Fock method for a self-interaction free Kohn-Sham potential: applications to closed and open-shell molecules. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 981-989.	0.5	13
1199	Theoretical investigation of excited states of molecules. An application on the nitrogen molecule. <i>Theoretical Chemistry Accounts</i> , 2007, 118, 637-642.	0.5	8
1200	Synthesis, characterization, and quantum chemical calculational studies on 3-p-methylphenyl-4-amino-1, 2, 4-triazole-5-thione. <i>Structural Chemistry</i> , 2007, 18, 993-1000.	1.0	17
1201	Experimental and theoretical spectral properties of ethyl 2-(7-hydroxy-2-oxo-2H-chromen-4-yl)acetate doped sol-gel materials: new materials with potential optical application. <i>Journal of Inclusion Phenomena and Macroscopic Chemistry</i> , 2007, 59, 167-176.	1.6	4
1202	The emission of 1,3-diphenylpolyenes: A model involving several molecular structures. <i>Chemical Physics</i> , 2007, 335, 69-78.	0.9	9

#	ARTICLE	IF	CITATIONS
1203	Theoretical studies on the electronic and optical properties of two blue-emitting fluorene-pyridine-based copolymers. <i>Optical Materials</i> , 2007, 29, 642-650.	1.7	17
1204	The role of artificial polarization in FA2:Ca ²⁺ lasers and NO interactions at RbCl (001) surface: An ab initio study. <i>Physica B: Condensed Matter</i> , 2007, 387, 6-17.	1.3	5
1205	Theoretical studies on the electronic structures and optical properties of the oligomers involving bipyridyl, thiophenyl and ethynyl groups. <i>Polymer</i> , 2007, 48, 502-511.	1.8	40
1206	Understanding the photophysics of 4-nitro-1-hydroxy-2-naphthoic acid: A controlled excited state proton transfer. <i>Chemical Physics</i> , 2008, 352, 175-184.	0.9	15
1207	Synthesis and structure of 1-azo-2-ketomethylquinolines. <i>Dyes and Pigments</i> , 2008, 76, 447-454.	2.0	8
1208	Theoretical studies of the electronic structures and optical properties of stable blue-emitting polymer based on 4H-cyclopenta-[def]-phenanthrene. <i>Polymer</i> , 2008, 49, 2077-2084.	1.8	5
1209	Investigation of the structures and electronic spectra of two coumarins with heterocyclic substituents through TD-DFT calculations. <i>Computational and Theoretical Chemistry</i> , 2008, 859, 73-78.	1.5	14
1210	Theoretical design of blue emitting materials based on symmetric and asymmetric spiroisilabifluorene derivatives. <i>Theoretical Chemistry Accounts</i> , 2008, 119, 489-500.	0.5	12
1211	A charge iteration-corrected extended-Hückel study of the electronic and spectroscopic properties of conjugated heterocycles. <i>Theoretical Chemistry Accounts</i> , 2008, 121, 43-52.	0.5	4
1212	Theoretical studies of the spectroscopic properties of blue emitting iridium complexes. <i>Theoretical Chemistry Accounts</i> , 2008, 121, 155-164.	0.5	22
1213	Path integral renormalization group treatments for many-electron systems with long-range repulsive interactions. <i>Surface and Interface Analysis</i> , 2008, 40, 1071-1074.	0.8	5
1214	Analysis of chemical bonding in electronic excited states using parity function. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1-14.	1.0	5
1215	Improving the TDDFT calculation of low-lying excited states for polycyclic aromatic hydrocarbons using the Tamm-Dancoff approximation. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 430-439.	1.0	62
1216	Quantum mechanical model for Maya Blue. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1664-1673.	1.0	29
1217	The Origin of the Improved Efficiency and Stability of Triphenylamine-Substituted Anthracene Derivatives for OLEDs: A Theoretical Investigation. <i>ChemPhysChem</i> , 2008, 9, 2601-2609.	1.0	93
1218	The Noncarbonylative Photochemistry of Group 6 Fischer Carbene Complexes. <i>European Journal of Inorganic Chemistry</i> , 2008, 2008, 2454-2462.	1.0	20
1219	Investigation of thermodynamic properties of gaseous SiC(X ⁺ and a ⁺) with accurate model chemistry calculations. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2008, 387, 5440-5456.	1.2	14
1220	Sol-gel materials doped with 3-(3-(4-(dimethylamino)phenyl)propenyl)-2H-chromen-2-one: Spectroscopic and structural elucidation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 69, 587-591.	2.0	4

#	ARTICLE	IF	CITATIONS
1221	An experimental and theoretical study of dipole moments of N-[4-(9-acridinylamino)-3-methoxyphenyl]methanesulfonamide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 70, 805-810.	2.0	18
1222	CL-20 photodecomposition: Ab initio foundations for identification of products. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 71, 230-237.	2.0	3
1223	LIF excitation spectra for S0 $\hat{\rightarrow}$ S1 transition of anthranilic acid: Detailed studies. <i>Journal of Molecular Spectroscopy</i> , 2008, 249, 100-112.	0.4	6
1224	Theoretical studies on structures and spectroscopic properties of bis-cyclometalated iridium complexes [Ir(ppy)2X2] $\hat{\rightarrow}$. <i>Journal of Organometallic Chemistry</i> , 2008, 693, 947-956.	0.8	11
1225	Study of the spectroscopic properties and first hyperpolarizabilities of disperse azo dyes derived from 2-amino-5-nitrothiazole. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2008, 199, 23-33.	2.0	8
1226	A practical use of self-energy shift for the description of orbital relaxation. <i>Chemical Physics Letters</i> , 2008, 453, 109-116.	1.2	14
1227	Density functionals for calculating NMR 1JCH coupling constants in electron-rich systems. <i>Chemical Physics Letters</i> , 2008, 454, 129-132.	1.2	7
1228	Theoretical study of absorption and emission spectra of the monomer of PFBT. <i>Chemical Physics Letters</i> , 2008, 456, 206-210.	1.2	14
1229	Theoretical study of 2,5-diphenyl-1,4-distyrylbenzene (A model compound of PPV): A comparison of the electronic structure and photophysical properties of cis- and trans-isomers. <i>Chemical Physics</i> , 2008, 345, 23-31.	0.9	4
1230	Assessment of quantum chemical methods and basis sets for excitation energy transfer. <i>Chemical Physics</i> , 2008, 346, 275-285.	0.9	71
1231	Photovoltaic effect in single-layer organic solar cell devices fabricated with two new imidazolin-5-one molecules. <i>Solar Energy Materials and Solar Cells</i> , 2008, 92, 1043-1046.	3.0	20
1232	Photochemistry of Hantzsch 1,4-dihydropyridines and pyridines. <i>Tetrahedron</i> , 2008, 64, 3190-3196.	1.0	31
1233	Theoretical studies on the structures and spectroscopic properties of rhenium(I) acetylide diimine complexes. <i>Computational and Theoretical Chemistry</i> , 2008, 855, 52-63.	1.5	6
1234	Excited electronic states of dehydro[18]annulene and dehydrobenzo[18]annulene. <i>Computational and Theoretical Chemistry</i> , 2008, 857, 27-32.	1.5	2
1235	Effects of substituents on the electronic properties of polyacetylenes. <i>Computational and Theoretical Chemistry</i> , 2008, 859, 37-45.	1.5	3
1236	Computational study on optical and electronic properties of the $\hat{\rightarrow}$ CH $\hat{\rightarrow}$ N substituted emitting materials based on spiroilabifluorene derivatives. <i>Computational and Theoretical Chemistry</i> , 2008, 862, 85-91.	1.5	25
1237	Theoretical studies upon the electronic structures and spectroscopic properties for a series of luminescent terpyridyl platinum(II) phenylacetylide complexes. <i>Computational and Theoretical Chemistry</i> , 2008, 863, 91-98.	1.5	4
1238	Theoretical studies on the optical properties and substituent effects of osmium (II) complexes Os(N $\hat{\rightarrow}$ N)(CN)2(PH3)2. <i>Computational and Theoretical Chemistry</i> , 2008, 869, 11-18.	1.5	0

#	ARTICLE	IF	CITATIONS
1239	Optical properties of charged : Zn ²⁺ , Cd ²⁺ , Hg ²⁺ centers in the bulk and at the surface of MgO: Theoretical study. <i>Physica B: Condensed Matter</i> , 2008, 403, 3168-3173.	1.3	3
1240	Experimental investigation by UV-VIS and IR spectroscopy to reveal electronic and vibrational properties of pyrrole-2-carboxylaldehyde: A theoretical approach. <i>Journal of Molecular Structure</i> , 2008, 891, 351-356.	1.8	24
1241	Ab initio, DFT, and spectroscopic studies of excited-state structure and dynamics of 9-ethylfluorene. <i>Journal of Molecular Structure</i> , 2008, 892, 110-115.	1.8	17
1242	Substituent Effect on the Optoelectronic Properties of Alternating Fluorene-Cyclopentadithiophene Copolymers. <i>Macromolecules</i> , 2008, 41, 6664-6671.	2.2	71
1243	Theoretical methods of investigation of excited states of organic molecules. <i>Russian Journal of General Chemistry</i> , 2008, 78, 774-783.	0.3	10
1244	On the tautomerism of 1-phenyl-3-substituted-pyrazol-5-ones and their photoinduced products – experimental and theoretical UV spectral analysis. <i>Chemical Papers</i> , 2008, 62, .	1.0	3
1245	Absorption Spectrum of OH Radical in Water. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13372-13381.	1.1	38
1246	Complexes of HNO ₃ and NO ₃ ⁻ with NO ₂ and N ₂ O ₄ , and their potential role in atmospheric HONO formation. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 6019.	1.3	39
1247	Fluorescence Spectroscopy and Amplified Spontaneous Emission (ASE) of Phenylimidazoles: Predicted Vibronic Coupling Along the Excited-State Intramolecular Proton Transfer in 2-(2-Hydroxyphenyl)imidazoles. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5555-5565.	1.1	14
1248	A generalization of the state-specific complete-active-space coupled-cluster method for calculating electronic excited states. <i>Journal of Chemical Physics</i> , 2008, 128, 074101.	1.2	46
1249	A 1,2-Naphthaleneimide-Modified Terthiophene Exhibiting Charge Transfer and Polarization Through the Short Molecular Axis. Joint Spectroscopic and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6732-6740.	1.1	27
1250	Integrated Approach for Modeling the Emission Fluorescence of 4-(<i>N,N</i> -Dimethylamino)benzointrile in Polar Environments. <i>Journal of Physical Chemistry B</i> , 2008, 112, 8106-8113.	1.2	15
1251	Simulation of Structure, Orientation, and Energy Transfer between AlexaFluor Molecules Attached to MscL. <i>Biophysical Journal</i> , 2008, 95, 2711-2721.	0.2	39
1252	DFT/TDDFT Studies on the Electronic Structures and Spectral Properties of Rhenium(I) Pyridinylbenzimidazole Complexes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 11190-11197.	1.1	77
1253	Multireference Fock-space coupled-cluster and equation-of-motion coupled-cluster theories: The detailed interconnections. <i>Journal of Chemical Physics</i> , 2008, 129, 134105.	1.2	75
1254	A Computational Study of the Ground and Excited State Structure and Absorption Spectra of Free-Base N-Confused Porphine and Free-Base N-Confused Tetraphenylporphyrin. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6533-6549.	1.1	45
1255	Theoretical study of excited state proton transfer in pyrrole-2-carboxylic acid. <i>Molecular Physics</i> , 2008, 106, 1441-1449.	0.8	4
1256	Self-Consistent Field Calculations of Excited States Using the Maximum Overlap Method (MOM). <i>Journal of Physical Chemistry A</i> , 2008, 112, 13164-13171.	1.1	435

#	ARTICLE	IF	CITATIONS
1257	Applications and assessment of QM:QM electronic embedding using generalized asymmetric Mulliken atomic charges. <i>Journal of Chemical Physics</i> , 2008, 129, 145101.	1.2	25
1258	Performance of a nonempirical meta- α -generalized gradient approximation density functional for excitation energies. <i>Journal of Chemical Physics</i> , 2008, 128, 084110.	1.2	32
1259	Local configuration interaction single excitation approach: Application to singlet and triplet excited states structure for conjugated chains. <i>Synthetic Metals</i> , 2008, 158, 330-335.	2.1	17
1260	Theoretical studies on the electronic structures and spectroscopic properties for a series of Osmium(II)-2,2',6',2'-terpyridine complexes. <i>Theoretical Chemistry Accounts</i> , 2008, 121, 123-134.	0.5	5
1261	A combined computational and experimental study on DNA-photocleavage of Ru(ii) polypyridyl complexes [Ru(bpy) ₂ (L)] ²⁺ (L = pip, o-mopip and p-mopip). <i>Dalton Transactions</i> , 2008, , 291-301.	1.6	33
1262	Atmospheric photochemical loss of H and H ₂ from formaldehyde: the relevance of ultrafast processes. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 674-680.	1.3	21
1263	Which factors determine the acidity of the phytychromobilin chromophore of plant phytochrome?. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 2528.	1.3	17
1264	Theoretical study of multiphoton ionization of cyclohexadienes and unimolecular decomposition of their mono- and dications. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 2321.	1.3	12
1265	Effect of Chlorin Structure on Theoretical Electronic Absorption Spectra and on the Energy Released by Porphyrin-Based Photosensitizers. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13574-13583.	1.1	29
1266	Hydration-Dependent Structural Deformation of Guanine in the Electronic Singlet Excited State. <i>Journal of Physical Chemistry B</i> , 2008, 112, 5139-5152.	1.2	42
1267	Photophysical Characters of Rationally Designed Hetero-Ring-Expanded Guanine Analogues and Effect of Cytosine Pairing. <i>Journal of Physical Chemistry B</i> , 2008, 112, 10723-10731.	1.2	20
1268	Attractive Tetraceno[2,3- <i>b</i>]thiophene Derivatives for Organic Transistor Applications: A Theoretical Analysis. <i>Journal of Physical Chemistry C</i> , 2008, 112, 16561-16567.	1.5	16
1269	Spectroscopic Characterization of Structural Isomers of Naphthalene: (<i>E</i>)- and (<i>Z</i>)-Phenylvinylacetylene. <i>Journal of Physical Chemistry A</i> , 2008, 112, 9454-9466.	1.1	18
1270	Ultrafast Infrared Spectroscopy of Riboflavin: Dynamics, Electronic Structure, and Vibrational Mode Analysis. <i>Journal of Physical Chemistry B</i> , 2008, 112, 13424-13432.	1.2	79
1271	Mass Analyzed Threshold Ionization Spectroscopy of o-, m-, and p-Dichlorobenzenes. Influence of the Chlorine Position on Vibrational Spectra and Ionization Energy. <i>Journal of Physical Chemistry A</i> , 2008, 112, 425-434.	1.1	24
1272	Heats of Formation of Triplet Ethylene, Ethylidene, and Acetylene. <i>Journal of Physical Chemistry A</i> , 2008, 112, 2082-2087.	1.1	38
1273	Probing Electron Correlations in Molecules by Two-Dimensional Coherent Optical Spectroscopy. <i>Journal of the American Chemical Society</i> , 2008, 130, 3509-3515.	6.6	31
1274	Theoretical Investigation of Perylene Dimers and Excimers and Their Signatures in X-Ray Diffraction. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8179-8187.	1.1	17

#	ARTICLE	IF	CITATIONS
1275	Predicting the UV-Vis Spectra of Tetraarylcyclopentadienones: Using DFT Molecular Orbital Energies to Model Electronic Transitions of Organic Materials. <i>Journal of Organic Chemistry</i> , 2008, 73, 2995-3004.	1.7	24
1276	Theoretical Studies on Structures and Spectroscopic Properties of Photoelectrochemical Cell Ruthenium Sensitizers, [Ru(H ₂ m ₃ tcterpy)(NCS) ₃] ⁿ⁺ (m = 0, 1, 2, and 3; n = 4, 3, 2, and 1). <i>Inorganic Chemistry</i> , 2008, 47, 2312-2324.	1.9	47
1277	Computational Prediction of Absorbance Maxima for a Structurally Diverse Series of Engineered Green Fluorescent Protein Chromophores. <i>Journal of Physical Chemistry B</i> , 2008, 112, 2533-2541.	1.2	29
1278	Radiation Induced Molecular Phenomena In Nucleic Acids: A Brief Introduction. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2008, , 1-14.	0.6	8
1279	Single-Reference Methods for Excited States in Molecules and Polymers. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2008, , 15-64.	0.6	8
1280	INTRAMOLECULAR CHARGE TRANSFER AND PHOTOISOMERIZATION OF THE DCM STYRENE DYE: A THEORETICAL STUDY. <i>Journal of Theoretical and Computational Chemistry</i> , 2008, 07, 719-736.	1.8	12
1281	The C ₃ N ⁻ anion: First detection of its electronic luminescence in rare gas solids. <i>Journal of Chemical Physics</i> , 2008, 128, 164304.	1.2	13
1282	The potential energy curves of low-lying electronic states of S ₂ O. <i>Journal of Chemical Physics</i> , 2008, 128, 184312.	1.2	11
1283	Dipole switching in large molecules described by explicitly time-dependent configuration interaction. <i>Journal of Chemical Physics</i> , 2008, 128, 234307.	1.2	22
1284	State-specific studies of internal mixing in a prototypical flexible bichromophore: Diphenylmethane. <i>Journal of Chemical Physics</i> , 2008, 129, 114301.	1.2	36
1285	Selective calculation of high-intensity vibrations in molecular resonance Raman spectra. <i>Journal of Chemical Physics</i> , 2008, 129, 204103.	1.2	36
1286	QM:QM electronic embedding using Mulliken atomic charges: Energies and analytic gradients in an ONIOM framework. <i>Journal of Chemical Physics</i> , 2008, 128, 034107.	1.2	81
1287	New contributions to the photophysical model for all-trans-polyenes from ttBP4, a nonphotolabile octatetraene. <i>Journal of Chemical Physics</i> , 2008, 128, 104504.	1.2	10
1288	Pseudospectral time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2008, 128, 104103.	1.2	63
1289	Plasma Chemistry of Octafluorocyclopentene/Argon/Oxygen Mixtures. <i>Japanese Journal of Applied Physics</i> , 2008, 47, 6843-6848.	0.8	8
1290	Block correlated coupled cluster method with a complete-active-space self-consistent-field reference function: The implementation for low-lying excited states. <i>Journal of Chemical Physics</i> , 2008, 129, 234106.	1.2	16
1291	Quantum mechanical methods applied to excitation energy transfer: A comparative analysis on excitation energies and electronic couplings. <i>Journal of Chemical Physics</i> , 2008, 129, 034104.	1.2	54
1292	The photophysics of all-trans polyenes from ttBP5, a nonphotolabile pentaene. <i>Journal of Chemical Physics</i> , 2008, 129, 014505.	1.2	6

#	ARTICLE	IF	CITATIONS
1293	First-principles simulation of photoreactions in biological systems. <i>Frontiers in Bioscience - Landmark</i> , 2009, 14, 4862.	3.0	8
1294	Construction of basis sets for time-dependent studies. <i>Journal of Chemical Physics</i> , 2009, 131, 064104.	1.2	3
1295	Absorption and emission properties of phenylene ethynylene oligomers: effect of substitution and π -conjugation length. <i>Molecular Physics</i> , 2009, 107, 1629-1639.	0.8	17
1296	Early events associated with the excited state proton transfer in 2-(2-pyridyl)benzimidazole. <i>Journal of Chemical Physics</i> , 2009, 131, 034504.	1.2	26
1297	Scintillating Metal Organic Frameworks: A New Class of Radiation Detection Materials. <i>Materials Research Society Symposia Proceedings</i> , 2009, 1164, 1.	0.1	3
1298	Photophysical Properties of 1,3,5-Tris(2-naphthyl)benzene and Related Less-Arylated Compounds: Experimental and Theoretical Investigations. <i>Journal of Physical Chemistry A</i> , 2009, 113, 14887-14895.	1.1	4
1299	Nested variant of the method of moments of coupled cluster equations for vertical excitation energies and excited-state potential energy surfaces. <i>Journal of Chemical Physics</i> , 2009, 130, 194110.	1.2	18
1300	Visualization of Metal-to-Ligand and Ligand-to-Ligand Charge Transfer in Metal-Ligand Complexes. <i>Chinese Journal of Chemical Physics</i> , 2009, 22, 269-274.	0.6	4
1301	Double spin-flip approach within equation-of-motion coupled cluster and configuration interaction formalisms: Theory, implementation, and examples. <i>Journal of Chemical Physics</i> , 2009, 130, 044103.	1.2	86
1302	An exploration of electronic structure and nuclear dynamics in tropolone: II. The \tilde{A}^1 excited state. <i>Journal of Chemical Physics</i> , 2009, 130, 144304.	1.2	23
1303	Anharmonic Franck-Condon Simulation of the Absorption and Fluorescence Spectra for the Low-Lying S_1 and S_2 Excited States of Pyridine. <i>Journal of Physical Chemistry A</i> , 2009, 113, 14407-14414.	1.1	21
1304	Ambipolar Organic Field-Effect Transistors from Cross-Conjugated Aromatic Quaterthiophenes; Comparisons with Quinoidal Parent Materials. <i>Advanced Functional Materials</i> , 2009, 19, 386-394.	7.8	71
1305	Thiophene-Diazine Molecular Semiconductors: Synthesis, Structural, Electrochemical, Optical, and Electronic Structural Properties; Implementation in Organic Field-Effect Transistors. <i>Chemistry - A European Journal</i> , 2009, 15, 5023-5039.	1.7	82
1306	Synthesis, Spectroscopy, Nonlinear Optics, and Theoretical Investigations of Thienylethynyl Octopoles with a Tunable Core. <i>Chemistry - A European Journal</i> , 2009, 15, 8223-8234.	1.7	14
1307	Theoretical Study of Origin of Triple Fluorescences of a Squaraine Dye, Bis[4-(dimethylamino)phenyl]squaraine. <i>Chinese Journal of Chemistry</i> , 2009, 27, 2323-2328.	2.6	2
1308	Application of the dressed time-dependent density functional theory for the excited states of linear polyenes. <i>Journal of Computational Chemistry</i> , 2009, 30, 811-817.	1.5	56
1309	Theoretical study of electronic properties of organic photovoltaic materials. <i>Journal of Computational Chemistry</i> , 2009, 30, 1027-1037.	1.5	18
1310	ab initio theory for treating local electron excitations in molecules and its performance for computing optical properties. <i>Journal of Computational Chemistry</i> , 2009, 30, 2213-2230.	1.5	18

#	ARTICLE	IF	CITATIONS
1311	Fragment molecular orbital study of the electronic excitations in the photosynthetic reaction center of <i>Blastochloris viridis</i> . <i>Journal of Computational Chemistry</i> , 2010, 31, 447-454.	1.5	23
1312	Absorption and fluorescence emission spectroscopic characters of naphtho-homologated γ -DNA bases and effect of methanol solution and base pairing. <i>Journal of Computational Chemistry</i> , 2010, 31, 825-836.	1.5	14
1313	Linear and nonlinear optical properties of azobenzene derivatives. <i>Journal of Molecular Modeling</i> , 2009, 15, 581-590.	0.8	24
1314	TCNE-aniline charge transfer complex: ab initio and TDDFT investigations in gas phase. <i>Journal of Molecular Modeling</i> , 2009, 15, 885-895.	0.8	9
1315	Mechanisms for formation, chlorination, dechlorination and destruction of polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/Fs). <i>Progress in Energy and Combustion Science</i> , 2009, 35, 245-274.	15.8	401
1316	Theoretical study of Au(I)-Ag(I) metallophilic attractions and luminescence of $[\text{Au}_2(\text{carb})_2\text{Ag}(\text{1}^{\text{1}}\text{4-3,5-Ph}_2\text{pz})]$ (with Ph=phenyl, pz=pyrazolate) and $[\text{Au}(\text{im})\text{CH}_3(\text{pz})\text{Ag}_2(\text{1}^{\text{1}}\text{4-3,5-H}_2\text{pz})_2]$ (with) TjE5Qq110.784314		
1317	Theoretical investigation of ground- and excited-state properties of fluorenone-alkynyl Hg(II) complexes: The tuning of electronic spectroscopy. <i>Computational and Theoretical Chemistry</i> , 2009, 907, 41-45.	1.5	1
1318	Theoretical study on the electronic structures and optical properties of blue phosphorescent iridium(III) complexes. <i>Journal of Molecular Structure</i> , 2009, 919, 204-209.	1.8	3
1319	Theoretical studies on electronic structures and spectroscopic properties of a series of novel β -diketonate Os(II) complexes. <i>Theoretical Chemistry Accounts</i> , 2009, 122, 31-42.	0.5	4
1320	A theoretical investigation of intermolecular interaction of a phthalimide based α - ω -off-sensor with different halide ions: tuning its efficiency and electro-optical properties. <i>Theoretical Chemistry Accounts</i> , 2009, 122, 77-86.	0.5	33
1321	Theoretical investigation of chemosensor for fluoride anion based on amidophthalimide derivatives. <i>Theoretical Chemistry Accounts</i> , 2009, 124, 225-234.	0.5	10
1322	A theoretical study about the structural, electronic and spectroscopic properties of the ground and singlet excited states of curcuminoidic core. <i>Theoretical Chemistry Accounts</i> , 2009, 124, 235-250.	0.5	10
1323	Substituent effects in the tuning of excited-state intramolecular proton transfer and optical properties of the derivatives of 2-(2-hydroxyphenyl)-5-phenyl-1,3,4-oxadiazole. <i>Theoretical Chemistry Accounts</i> , 2009, 124, 331-338.	0.5	4
1324	Electronic structure and optical properties of chelating heteroatomic conjugated molecules: a SAC-CI study. <i>Theoretical Chemistry Accounts</i> , 2009, 124, 395-408.	0.5	4
1325	Modulation of electronic structures of thienylene vinylene oligomers by substituents and solvents: ground and excited states. <i>Journal of Physical Organic Chemistry</i> , 2009, 22, 670-679.	0.9	4
1326	Modeling excitation properties of iridium complexes. <i>Journal of Physical Organic Chemistry</i> , 2009, 22, 845-856.	0.9	26
1327	Comparative study of electronic structure and optical properties of a series of Pt(II) complexes containing different electron-donating and -withdrawing groups: a DFT study. <i>Journal of Physical Organic Chemistry</i> , 2010, 23, 181-189.	0.9	3
1328	Computational studies on the spectroscopic properties of the 2-pyridylpyrazolate-based platinum(II) complexes with modified pyrazolate fragment. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 308-319.	1.0	6

#	ARTICLE	IF	CITATIONS
1329	Theoretical study on the spectroscopic properties and electronic structures of heteroleptic phosphorescent Ir(III) complexes. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 1167-1176.	1.0	18
1330	Electron invariants and excited state structural analysis for electronic transitions within CIS, RPA, and TDDFT models. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 902-924.	1.0	55
1331	Ground and excited states calculations of 7-phenylamino-substituted coumarins. <i>Journal of Molecular Structure</i> , 2009, 917, 15-20.	1.8	12
1332	Synthesis, structure, spectroscopic properties, and theoretical studies of a new blue/green luminescent complex: $[Cd_2Cl_4(Hbm)_2]_n \cdot nH_2O$ (Hbm=1H-benzimidazol-2-ylmethanol). <i>Journal of Molecular Structure</i> , 2009, 922, 135-139.	1.8	9
1333	Tautomeric forms of N-(5-nitrosalicylidene)-2-butylamine: Experimental and theoretical DFT study. <i>Journal of Molecular Structure</i> , 2009, 928, 25-31.	1.8	13
1334	The computational study of the complex between 4-nitrophenyl[bis(methylsulfonyl)]methane and TBD base in acetonitrile and tetrahydrofuran solution. <i>Journal of Molecular Structure</i> , 2009, 929, 125-127.	1.8	2
1335	Silver(I) complexes with a bulky acridine-based carboxylic ligand: Syntheses, crystal structures, and luminescent properties. <i>Journal of Molecular Structure</i> , 2009, 931, 68-75.	1.8	12
1336	Theoretical analysis of anthracene and its carbonyl and carboxyl derivatives using DFT and TD-DFT. <i>Computational and Theoretical Chemistry</i> , 2009, 894, 64-70.	1.5	22
1337	High-level computational studies of Rhodizonate derivatives: Molecules absorbing in near infrared region due to larger C=C-C angle of the oxyallyl ring. <i>Computational and Theoretical Chemistry</i> , 2009, 904, 1-6.	1.5	19
1338	Theoretical investigation of oligo(fluorene) derivatives containing electron-deficient unit 2-pyran-4-ylidene-malononitrile moiety. <i>Computational and Theoretical Chemistry</i> , 2009, 904, 91-97.	1.5	2
1339	The absorption, emission spectra as well as ground and excited states calculations of some dimethine cyanine dyes. <i>Computational and Theoretical Chemistry</i> , 2009, 906, 50-55.	1.5	21
1340	Structures and excitation energies of Zn tetraarylporphyrin analogues: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2009, 910, 20-26.	1.5	76
1341	The S ₁ →S ₀ transition energies of polychlorinated dibenzofurans (PCDFs) revisited: CIS(D) and MP2 calculations with correction for correlation energies. <i>Computational and Theoretical Chemistry</i> , 2009, 915, 79-85.	1.5	4
1342	Resonance enhanced multiphoton ionization spectroscopy and theoretical calculations of cis and trans p-methoxystyrene rotamers. <i>Journal of Molecular Structure</i> , 2009, 918, 154-159.	1.8	6
1343	Electronic properties of 1-methyl-4-phenyl-1H-tetrazole-5(4H)-thiones: An experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2009, 933, 38-45.	1.8	10
1344	Theoretical investigation on the white-light emission from a single-polymer system with simultaneous blue and orange emission. <i>Polymer</i> , 2009, 50, 6172-6185.	1.8	18
1345	A novel series of iridium complexes with alkenylquinoline ligands: Theoretical study on electronic structure and spectroscopic property. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 150-156.	0.8	8
1346	Triplet-sensitized photolysis of alkoxy carbonyl azides in solution and matrices. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2009, 201, 157-167.	2.0	15

#	ARTICLE	IF	CITATIONS
1347	Photophysical and photochemical properties of the T1 excited state of thioinosine. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2009, 206, 93-101.	2.0	16
1348	Synthesis, characterization, crystal structure and ab initio studies on 5-ethoxycarbonyl-6-methyl-4-phenyl-2-thioxo-1,2,3,4-tetrahydropyrimidine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009, 72, 61-67.	2.0	6
1349	Prediction of molecular properties and molecular spectroscopy with density functional theory: From fundamental theory to exchange-coupling. <i>Coordination Chemistry Reviews</i> , 2009, 253, 526-563.	9.5	927
1350	The vacuum UV photoabsorption spectroscopy of vinyl fluoride (C ₂ H ₃ F): The vibrational fine structure and its analysis. <i>Chemical Physics</i> , 2009, 362, 97-108.	0.9	7
1351	SaX: An open source package for electronic-structure and optical-properties calculations in the GW approximation. <i>Computer Physics Communications</i> , 2009, 180, 1416-1425.	3.0	38
1352	Application of Dyson-corrected second-order perturbation theories. <i>Chemical Physics Letters</i> , 2009, 472, 143-148.	1.2	8
1353	Theoretical study on the excited states of heteroarene chromophores: Comparison of calculated and experimental values. <i>Chemical Physics Letters</i> , 2009, 473, 196-200.	1.2	13
1354	Quantum Monte Carlo for atoms, molecules and solids. <i>Chemical Physics Letters</i> , 2009, 478, 1-10.	1.2	60
1355	Design and photophysical properties of a new molecule with a Na ⁺ -B ⁻ -N linked chromophore. <i>Chemical Physics Letters</i> , 2009, 478, 206-210.	1.2	9
1356	Hydration of guanine: Electronic singlet excited states for complexes with 19 and 27 water molecules. <i>Chemical Physics Letters</i> , 2009, 478, 254-259.	1.2	15
1357	Photoelectron and UV absorption spectroscopy for determination of electronic configurations of negative molecular ions: Chlorophenols. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2009, 171, 37-46.	0.8	12
1358	Quantum-Mechanical Calculations of Resonance Raman Intensities: The Weighted-Gradient Approximation. <i>Journal of Physical Chemistry A</i> , 2009, 113, 2926-2934.	1.1	26
1359	Quantum-chemical investigation of the formation of 1,3-diiodoacetone at the photoinitiated disproportionation of 1-iodoacetone. <i>Russian Journal of Organic Chemistry</i> , 2009, 45, 1610-1615.	0.3	0
1360	Quantum-chemical study of the photochemical addition reaction of dialkyl disulfides with olefins. <i>Petroleum Chemistry</i> , 2009, 49, 240-244.	0.4	1
1361	Time-Dependent Density Functional Theory Study of the Electronic Excitation Spectra of Chlorophyllide a and Pheophorbide a in Solvents. <i>Journal of Physical Chemistry B</i> , 2009, 113, 4817-4825.	1.2	29
1362	Theoretical Study of the Relations between Structure and Photophysical Properties of Model Oligofluorenes with Central Keto Defect. <i>Journal of Physical Chemistry A</i> , 2009, 113, 14141-14149.	1.1	9
1363	Absorption and Fluorescence Emission Spectroscopic Characters of Size-Expanded γ DNA Bases and Effect of Deoxyribose and Base Pairing. <i>Journal of Physical Chemistry B</i> , 2009, 113, 1173-1181.	1.2	24
1364	Benchmarking Second Order Methods for the Calculation of Vertical Electronic Excitation Energies: Valence and Rydberg States in Polycyclic Aromatic Hydrocarbons. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11995-12012.	1.1	51

#	ARTICLE	IF	CITATIONS
1365	Excited-State Forms of 2-Methylamino-6-methyl-4-nitropyridine N-Oxide and 2-Butylamino-6-methyl-4-nitropyridine N-Oxide. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3438-3446.	1.1	6
1366	Volatile Electrical Switching and Static Random Access Memory Effect in a Functional Polyimide Containing Oxadiazole Moieties. <i>Chemistry of Materials</i> , 2009, 21, 3391-3399.	3.2	129
1367	Electron Super-Rich Radicals. III. On the Peculiar Behavior of the Aminodihydroxymethyl Radical in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5855-5864.	1.1	5
1368	Conformation-Specific Spectroscopy and Excited State Photophysics of 5-Phenyl-1-pentene. <i>Journal of Physical Chemistry A</i> , 2009, 113, 118-125.	1.1	3
1369	Theoretical Studies on Structures and Spectroscopic Properties of Cyclometalated Gold(III) Complexes. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9396-9403.	1.1	20
1370	Excited States and Photochemistry of Bicyclo[1.1.0]butane. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1686-1695.	1.1	7
1371	The molecular basis for the behaviour of niobia species in oxidation reaction probed by theoretical calculations and experimental techniques. <i>Molecular Physics</i> , 2009, 107, 171-179.	0.8	20
1372	Beyond 7-Azaindole: Conjugation Effects on Intermolecular Double Hydrogen-Atom Transfer Reactions. <i>Journal of Physical Chemistry A</i> , 2009, 113, 4862-4867.	1.1	16
1373	Quinone-hydroquinone complexes as model components of humic acids: Theoretical studies of their structure, stability and Visible-UV spectra. <i>Geochimica Et Cosmochimica Acta</i> , 2009, 73, 2023-2033.	1.6	24
1374	Theoretical studies on electronic structures, spectra and charge transporting properties of a series of Pt(C ₁ N) ₂ complexes. <i>Synthetic Metals</i> , 2009, 159, 1090-1098.	2.1	7
1375	Triphenylamine-based pH chemosensor: Synthesis, crystal structure, photophysical properties and computational studies. <i>Synthetic Metals</i> , 2009, 159, 2497-2501.	2.1	13
1376	Comparative Theoretical Study of Rotamerism and Excited State Intramolecular Proton Transfer of 2-(2-Hydroxyphenyl)benzimidazole, 2-(2-Hydroxyphenyl)imidazo[4,5-b]pyridine, 2-(2-Hydroxyphenyl)imidazo[4,5-c]pyridine and 8-(2-Hydroxyphenyl)purine. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12063-12070.	1.1	57
1377	Fretting about FRET: Failure of the Ideal Dipole Approximation. <i>Biophysical Journal</i> , 2009, 96, 4779-4788.	0.2	118
1378	High-resolution study of K and resonant Auger decay in KF. <i>Physical Review A</i> , 2009, 80, .		
1379	Relativistic Interactions in the Radical Pair Model of Magnetic Field Sense in CRY-1 Protein of <i>Arabidopsis thaliana</i> . <i>Journal of Physical Chemistry A</i> , 2009, 113, 12276-12284.	1.1	10
1380	Intramolecular H-Atom Abstraction in ¹ 3-Azido-Butyrophenones: Formation of 1,5 Ketyl Iminyl Radicals. <i>Organic Letters</i> , 2009, 11, 2345-2348.	2.4	44
1381	New Type of Dual Solid-State Thermochromism: Modulation of Intramolecular Charge Transfer by Intermolecular H ⁺ Interactions, Kinetic Trapping of the Aci-Nitro Group, and Reversible Molecular Locking. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11354-11366.	1.1	20
1382	Toward a Generalized Treatment of the Solvent Effect Based on Four Empirical Scales: Dipolarity (SdP), Tj ETQq1 1 0.784314 rgBT / Over Chemistry B, 2009, 113, 5951-5960.	1.2	581

#	ARTICLE	IF	CITATIONS
1383	Role of Intramolecular and Intermolecular Hydrogen Bonding in Both Singlet and Triplet Excited States of Aminofluorenones on Internal Conversion, Intersystem Crossing, and Twisted Intramolecular Charge Transfer. <i>Journal of Physical Chemistry A</i> , 2009, 113, 14329-14335.	1.1	221
1384	An ab initio and TD-DFT study of solvent effect contributions to the electronic spectrum of Nile Red. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 4471.	1.3	26
1385	Theoretical Study on the Correlation between Band Gap, Bandwidth, and Oscillator Strength in Fluorene-Based Donor-Acceptor Conjugated Copolymers. <i>Journal of Physical Chemistry B</i> , 2009, 113, 8268-8277.	1.2	70
1386	Quartic-Scaling Analytical Gradient of Quasidegenerate Scaled Opposite Spin Second-Order Perturbation Corrections to Single Excitation Configuration Interaction. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1224-1236.	2.3	23
1387	Performance of Quasi-Degenerate Scaled Opposite Spin Perturbation Corrections to Single Excitation Configuration Interaction for Excited State Structures and Excitation Energies with Application to the Stokes Shift of 9-Methyl-9,10-dihydro-9-silaphenanthrene. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10564-10576.	1.1	22
1388	Jet-cooled vibronic spectroscopy and asymmetric torsional potentials of phenylcyclopentene. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 8330.	1.3	9
1389	Conformational Effects on Excitonic Interactions in a Prototypical H-Bonded Bichromophore: Bis(2-hydroxyphenyl)methane. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5000-5012.	1.1	25
1390	Fragment Molecular Orbital Calculations on Red Fluorescent Proteins (DsRed and mFruits). <i>Journal of Physical Chemistry B</i> , 2009, 113, 1153-1161.	1.2	40
1391	Modulation of Tris(o-phenylenedioxy)cyclotrisphosphazene (TPP) Properties for Zeolite Use: Effect of π -Conjugation Length and CH/N Heterosubstitution. <i>Journal of Physical Chemistry A</i> , 2009, 113, 246-254.	1.1	2
1392	Ultrafast electronic excitations of small sodium clusters and the onset of electron thermalization. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 349-357.	1.3	26
1393	EXCITED-STATE INTRAMOLECULAR ELECTRON TRANSFER COUPLED WITH EXCITED-STATE INTRAMOLECULAR PROTON TRANSFER IN PHOTOINDUCED ENOL TO KETO TAUTOMERIZATION. <i>Journal of Theoretical and Computational Chemistry</i> , 2009, 08, 1073-1086.	1.8	0
1394	Preparation and structural characterization of a series of monoacylhydrazidate-bridged coordination polymers. <i>Dalton Transactions</i> , 2009, , 8248.	1.6	41
1395	Jet-cooled vibronic spectroscopy of potential intermediates along the pathway to PAH: phenylcyclopenta-1,3-diene. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 8316.	1.3	6
1396	Encapsulation of 2-(4-N,N-dimethylamino)phenylimidazo[4,5-b]pyridine in β -cyclodextrin: effect on H-bond-induced intramolecular charge transfer emission. <i>Photochemical and Photobiological Sciences</i> , 2009, 8, 1708.	1.6	28
1397	Franck-Condon analysis of laser-induced fluorescence excitation spectrum of anthranilic acid: Evaluation of geometry change upon $S_0 \rightarrow S_1$ excitation. <i>Journal of Chemical Physics</i> , 2009, 130, 054307.	1.2	14
1398	Injection, Transport, Absorption and Phosphorescence Properties of a Series of Blue-Emitting Ir(III) Emitters in OLEDs: a DFT and Time-Dependent DFT Study. <i>Inorganic Chemistry</i> , 2009, 48, 7740-7749.	1.9	114
1399	Excited State Electronic Structures and Photochemistry of Heterocyclic Annulated Perylene (HAP) Materials Tuned by Heteroatoms: S, Se, N, O, C, Si, and B. <i>Journal of Physical Chemistry A</i> , 2009, 113, 4788-4794.	1.1	119
1400	Computational Study of Environmental Effects in the Adsorption of DMMP, Sarin, and VX on Al_2O_3 : Photolysis and Surface Hydroxylation. <i>Journal of Physical Chemistry C</i> , 2009, 113, 1917-1930.	1.5	73

#	ARTICLE	IF	CITATIONS
1401	Structures and Properties of Electronically Excited Chromophores in Solution from the Polarizable Continuum Model Coupled to the Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3009-3020.	1.1	173
1402	Light-absorbing secondary organic material formed by glyoxal in aqueous aerosol mimics. <i>Atmospheric Chemistry and Physics</i> , 2009, 9, 2289-2300.	1.9	307
1403	Theoretical study of proton tunneling in the excited state of tropolone. <i>Journal of Chemical Physics</i> , 2009, 130, 164306.	1.2	14
1404	<i>Adventures of Quantum Chemistry in the Realm of Inorganic Chemistry.</i> , 2010, , 83-127.		0
1405	Theoretical study of optical properties of gold clusters. <i>Russian Journal of General Chemistry</i> , 2010, 80, 1078-1085.	0.3	6
1406	Solvent-Induced Frequency Shifts: Configuration Interaction Singles Combined with the Effective Fragment Potential Method. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6742-6750.	1.1	74
1407	Theoretical characterization of photoinduced electron transfer in rigidly linked donor-acceptor molecules: the fragment charge difference and the generalized Mulliken-Hush schemes. <i>Molecular Physics</i> , 2010, 108, 2775-2789.	0.8	19
1408	A theoretical investigation on the spectroscopic properties and photosensitizing capability of 5, 10, 15, 20-tetraphenylsapphyrin and 5, 10, 15, 20-tetraphenyl-26,28-diheterosapphyrins with two O, S, or Se Atoms. <i>Theoretical Chemistry Accounts</i> , 2010, 127, 475-484.	0.5	15
1409	Fluorene-based oligomers as red light-emitting materials: a density functional theory study. <i>Theoretical Chemistry Accounts</i> , 2010, 126, 305-314.	0.5	3
1410	Theoretical study on the absorption maxima of real GFPs. <i>Chemical Physics Letters</i> , 2010, 484, 324-329.	1.2	8
1411	Chromophore-specific theoretical spectroscopy: From subsystem density functional theory to mode-specific vibrational spectroscopy. <i>Physics Reports</i> , 2010, 489, 1-87.	10.3	118
1412	DFT and experimental study of N,N-bis(3-carboxy,4-aminophenyl)-1,4-quinonediimine, a carboxyl substituted aniline trimer. <i>Journal of Molecular Structure</i> , 2010, 977, 220-229.	1.8	8
1413	Theoretical insights into the trends in molecular properties of HCY, HSiY and HGeY molecules where Y = N, P, As. <i>Journal of Molecular Modeling</i> , 2010, 16, 1075-1084.	0.8	3
1414	Fluorescent Triphenyl Substituted Maleimide Derivatives: Synthesis, Spectroscopy and Quantum Chemical Calculations. <i>Journal of Fluorescence</i> , 2010, 20, 1077-1085.	1.3	17
1415	A Time-Dependent Density Functional Theory Investigation on the Origin of Red Chemiluminescence. <i>ChemPhysChem</i> , 2010, 11, 251-259.	1.0	30
1419	Stereoselective Triplet-Sensitized Radical Reactions of Furanone Derivatives. <i>Chemistry - A European Journal</i> , 2010, 16, 3341-3354.	1.7	41
1420	Comparison of Thiophene-Pyrrole Oligomers with Oligothiophenes: A Joint Experimental and Theoretical Investigation of Their Structural and Spectroscopic Properties. <i>Chemistry - A European Journal</i> , 2010, 16, 6866-6876.	1.7	27
1421	Experimental and theoretical study of a new carbazole derivative having terminal benzimidazole rings. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010, 75, 525-532.	2.0	9

#	ARTICLE	IF	CITATIONS
1422	Fluorescence emission and enhanced photochemical stability of Zn(II)-5-triethyl ammonium methyl salicylidene ortho-phenylendiimine interacting with native DNA. <i>Journal of Inorganic Biochemistry</i> , 2010, 104, 765-773.	1.5	12
1423	Experimental and theoretical studies of the molecular structure of 1-(2-pyridinylmethyl)-2-methylbenzimidazole. <i>Journal of Molecular Structure</i> , 2010, 968, 6-12.	1.8	9
1424	LIF excitation spectra for S ₀ →S ₁ transition of deuterated anthranilic acid COOD, ND ₂ in supersonic-jet expansion. <i>Journal of Molecular Spectroscopy</i> , 2010, 264, 129-136.	0.4	5
1425	Theoretical and experimental study of the vertical excitation energies in the ionic and tautomeric forms of 4-aminomethylpyridine. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2010, 209, 19-26.	2.0	4
1426	Theoretical studies on DNA-binding, DNA-photocleavage and spectral properties of Co(III) complexes [Co(phen) ₂ (L)] ³⁺ (L=pip, hpip, hnaip). <i>Inorganica Chimica Acta</i> , 2010, 363, 3880-3886.	1.2	5
1427	Density functional theory study on photophysical properties of the porphyrins derivatives with through-bond energy transfer characters. <i>Organic Electronics</i> , 2010, 11, 979-989.	1.4	19
1428	Theoretical studies on the spectral and DNA-photocleavage properties of Co(III) and Ru(II) polypyridyl complexes. <i>Computational and Theoretical Chemistry</i> , 2010, 957, 108-113.	1.5	3
1429	A theoretical study on the substituent effect of DNA-photocleavage by [Ru(phen) ₂ (6-R-dppz)] ²⁺ (R=H, Tj ETQq1 1,0,784314 rgBT /Ove	1.5	4
1430	Structural, electronic, and optical properties of novel indolocarbazole-based conjugated derivatives. <i>Computational and Theoretical Chemistry</i> , 2010, 962, 33-37.	1.5	7
1431	On the geometrical structure and spectral properties of pyrene monomer and sterically constrained intramolecular pyrene dimers. <i>Chemical Physics</i> , 2010, 377, 123-131.	0.9	9
1432	Large-scale FMO-MP3 calculations on the surface proteins of influenza virus, hemagglutinin (HA) and neuraminidase (NA). <i>Chemical Physics Letters</i> , 2010, 493, 346-352.	1.2	44
1433	On the formation of S ₂ O at low energies: An ab initio study. <i>Chemical Physics Letters</i> , 2010, 500, 207-210.	1.2	2
1434	Synthesis of polyimides containing triphenylamine- <i>ε</i> -substituted triazole moieties for polymer memory applications. <i>Journal of Polymer Science Part A</i> , 2010, 48, 5790-5800.	2.5	79
1435	Density functional study on the effect of substituent group for the monomer of donor- <i>ε</i> -acceptor copolymer. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2010, 48, 2099-2107.	2.4	15
1436	Computational study of the cooperative effects of nitrogen and silicon atoms on the singlet- <i>ε</i> -triplet energy spacing in 1,3- <i>ε</i> -diradicals and the reactivity of their singlet states. <i>Journal of Physical Organic Chemistry</i> , 2010, 23, 300-307.	0.9	23
1437	Theoretical study on the influence of ancillary ligand on the spectroscopic properties and electronic structures of phosphorescent Pt(II) complexes. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 1142-1151.	1.0	1
1438	Theoretical studies on the electronic structures and spectroscopic properties of a series of novel N ₂ C ₂ N ₂ - <i>ε</i> -coordinating Pt(II) complexes. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 1605-1614.	1.0	1
1439	Molecular excitation spectra by TDDFT with the nonadiabatic exact exchange kernel. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2202-2220.	1.0	23

#	ARTICLE	IF	CITATIONS
1440	Impact of the ionic forms on the UV-Vis spectra of hydroxybenzylamine. A TD-DFT study. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2179-2191.	1.0	2
1441	Guanine in water solution: Comprehensive study of hydration cage versus continuum solvation model. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 3027-3039.	1.0	13
1442	Charge Transfer in 1,8-Naphthalimide: A Combined Theoretical and Experimental Approach. <i>Photochemistry and Photobiology</i> , 2010, 86, 47-54.	1.3	13
1443	TORSIONAL POTENTIALS AND FULL-DIMENSIONAL SIMULATION OF ELECTRONIC ABSORPTION SPECTRA OF <i>para</i> -PHENYLENEVINYLENE OLIGOMERS USING SEMIEMPIRICAL HAMILTONIANS. <i>Journal of Theoretical and Computational Chemistry</i> , 2010, 09, 249-263.	1.8	13
1444	Competition Between Azido Cleavage and Triplet Nitrene Formation in Azidomethylacetophenones. <i>Australian Journal of Chemistry</i> , 2010, 63, 1645.	0.5	9
1445	ONIOM-based QM:QM electronic embedding method using Löwdin atomic charges: Energies and analytic gradients. <i>Journal of Chemical Physics</i> , 2010, 132, 114107.	1.2	37
1446	Vibrational wave packet induced oscillations in two-dimensional electronic spectra. I. Experiments. <i>Journal of Chemical Physics</i> , 2010, 132, .	1.2	55
1447	Sequential Penning Ionization: Harvesting Energy with Ions. <i>Physical Review Letters</i> , 2010, 105, 243402.	2.9	32
1448	Prediction of Excitation Energies for Conjugated Oligomers and Polymers from Time-Dependent Density Functional Theory. <i>Materials</i> , 2010, 3, 3430-3467.	1.3	3
1449	Ultrafast photochemistry of methyl hydroperoxide on ice particles. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 6600-6604.	3.3	19
1450	A photoelectron spectroscopic investigation of vinyl fluoride (C ₂ H ₃ F): the HeI, threshold and CIS photoelectron spectroscopy. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2010, 43, 015102.	0.6	10
1451	Sorting Out the Relative Contributions of Electrostatic Polarization, Dispersion, and Hydrogen Bonding to Solvatochromic Shifts on Vertical Electronic Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2829-2844.	2.3	45
1452	Fluorescent metal-organic polymers of zinc and cadmium from hydrothermal in situ acylation reaction. <i>Dalton Transactions</i> , 2010, 39, 10617.	1.6	49
1453	Highly Efficient Methyl Ketone Synthesis with Photoactivated Acetone and Olefins Assisted by Mg(II)-Exchanged Zeolite Y. <i>Journal of Organic Chemistry</i> , 2010, 75, 1450-1457.	1.7	17
1454	Multiscale simulation and modelling of adsorptive processes for energy gas storage and carbon dioxide capture in porous coordination frameworks. <i>Energy and Environmental Science</i> , 2010, 3, 1469.	15.6	138
1455	The fragment spin difference scheme for triplet-triplet energy transfer coupling. <i>Journal of Chemical Physics</i> , 2010, 133, 074105.	1.2	58
1456	Fluorescence Quenching by Photoinduced Electron Transfer in the Zn ²⁺ Sensor Zinpyr-1: A Computational Investigation. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10427-10434.	1.1	71
1457	Tautomerization and solvent effects on the absorption and emission properties of the Schiff base <i>N,N'</i> -bis(salicylidene)- <i>p</i> -phenylenediamine: A TDDFT study. <i>Molecular Physics</i> , 2010, 108, 1817-1827.	0.8	18

#	ARTICLE	IF	CITATIONS
1458	Ab Initio Calculations on the Electronically Excited States of Small Helium Clusters. <i>Journal of Physical Chemistry A</i> , 2010, 114, 8023-8032.	1.1	30
1459	Optical Operation by Chromophores Featuring 4,5-Dicyanoimidazole Embedded within Poly(methyl Tj ETQq1 1 0.784314 rgBT /Over	1.1	47
1460	On the Molecular Structure and UV/vis Spectroscopic Properties of the Solvatochromic and Thermochromic Pyridinium- <i>N</i> -Phenolate Betaine Dye B30. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6226-6234.	1.1	64
1461	Excited-State Intramolecular Proton Transfer (ESIPT) Fine Tuned by Quinoline ^π Pyrazole Isomerism: π -Conjugation Effect on ESIPT. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7886-7891.	1.1	67
1462	Probing <i>E</i> / <i>Z</i> Isomerization on the C ₁₀ H ₈ Potential Energy Surface with Ultraviolet Population Transfer Spectroscopy. <i>Journal of the American Chemical Society</i> , 2010, 132, 1611-1620.	6.6	8
1463	Effect of Alkyl Substituents on Photorelease from Butyrophenone Derivatives. <i>Journal of Organic Chemistry</i> , 2010, 75, 1393-1401.	1.7	21
1464	Synthesis and Characterization of the Ground and Excited States of Tripodal-like Oligothieryl-imidazoles. <i>Journal of Physical Chemistry B</i> , 2010, 114, 4964-4972.	1.2	27
1465	Generation and Intermolecular Trapping of 1,2-Diaza-4-silacyclopentane-3,5-diyls in the Denitrogenation of 2,3,5,6-Tetraaza-7-silabicyclo[2.2.1]hept-2-ene: An Experimental and Computational Study. <i>Journal of Organic Chemistry</i> , 2010, 75, 1956-1960.	1.7	24
1466	Substituent and Solvent Effects on Electronic Structure and Spectral Property of ReCl(CO) ₃ (N ⁺ â ⁺ N) (N ⁺ â ⁺ N = Glyoxime): DFT and TDDFT Theoretical Studies. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12251-12257.	1.1	30
1467	Accurate Calculated Optical Properties of Substituted Quaterphenylene Nanofibers. <i>Journal of Physical Chemistry A</i> , 2010, 114, 474-480.	1.1	7
1468	Modeling Photoelectron Spectra of Conjugated Oligomers with Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10997-11007.	1.1	16
1469	Combined Effects of One 8-Hydroxyquinoline/Picolinate and α -CH β /N Substitutions on the Geometry, Electronic Structure and Optical Properties of <i>mer</i> -Alq ₃ . <i>Journal of Physical Chemistry A</i> , 2010, 114, 652-658.	1.1	7
1470	DFT/TD-DFT Study on the Electronic Structures and Optoelectronic Properties of Several Blue-Emitting Iridium(III) Complexes. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6559-6564.	1.1	44
1471	Surface-Enhanced Raman Scattering of Benzoate Anion Adsorbed on Silver Nanoclusters: Evidence of the Transient Formation of the Radical Dianion. <i>Journal of Physical Chemistry C</i> , 2010, 114, 7666-7672.	1.5	24
1472	A Theoretical Investigation of the Photophysical Consequences of Major Plant Light-Harvesting Complex Aggregation within the Photosynthetic Membrane. <i>Journal of Physical Chemistry B</i> , 2010, 114, 15244-15253.	1.2	17
1473	Theoretical Investigation of the Mechanism and Dynamics of Intramolecular Coherent Resonance Energy Transfer in Soft Molecules: A Case Study of Dithia-anthracenophane. <i>Journal of the American Chemical Society</i> , 2010, 132, 16911-16921.	6.6	24
1474	Solid State Isotope Exchange with Spillover Hydrogen in Organic Compounds. <i>Chemical Reviews</i> , 2010, 110, 5425-5446.	23.0	28
1475	Efficient $\dot{\text{I}}_{\pm}$ -(Alkylthio)alkyl-Type Radical Formation in ⁺ OH-Induced Oxidation of $\dot{\text{I}}_{\pm}$ -(Methylthio)acetamide. <i>Journal of Physical Chemistry A</i> , 2010, 114, 105-116.	1.1	11

#	ARTICLE	IF	CITATIONS
1476	Exploration of the Biological Micro-Surrounding Effect on the Excited States of the Size-Expanded Fluorescent Base x-Cytosine in DNA. <i>Journal of Physical Chemistry B</i> , 2010, 114, 3726-3734.	1.2	14
1477	Theoretical study of the photophysical and charge transport properties of novel fluorescent fluorine- ¹⁹ F-boron compounds. <i>Molecular Physics</i> , 2010, 108, 667-674.	0.8	6
1478	Electronic Transition Energies: A Study of the Performance of a Large Range of Single Reference Density Functional and Wave Function Methods on Valence and Rydberg States Compared to Experiment. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 370-383.	2.3	202
1479	A comparative study on the optical properties of indenofluorene and indenopyrazine. <i>Computational Materials Science</i> , 2010, 49, S251-S255.	1.4	4
1480	Theoretical studies on electronic and electron blocking properties of iridium complexes with phenylpyrazolato ligands. <i>Synthetic Metals</i> , 2010, 160, 1015-1021.	2.1	4
1481	Theoretical studies of electronic structure and hole drift mobility of host hole transporting material 4,4'-N,N'-dicarbazol-biphenyl. <i>Synthetic Metals</i> , 2010, 160, 2104-2108.	2.1	9
1482	A benchmark study of the vertical electronic spectra of the linear chain radicals C2H and C4H. <i>Journal of Chemical Physics</i> , 2010, 132, 144303.	1.2	40
1483	Aqueous-based synthesis of atomic gold clusters: Geometry and optical properties. <i>Applied Physics Letters</i> , 2010, 97, 053103.	1.5	14
1484	A parallel implementation of the analytic nuclear gradient for time-dependent density functional theory within the Tamm-Dancoff approximation. <i>Molecular Physics</i> , 2010, 108, 2791-2800.	0.8	58
1485	Fluorescence Spectroscopic and Time-Dependent DFT Studies for Intramolecular Excimer Formation of Di-9H-fluorene-9-yl dimethylsilane: Dynamics and Energetics for Conformational Change. <i>Journal of Physical Chemistry A</i> , 2010, 114, 8969-8974.	1.1	10
1486	Toward highly efficient NLO chromophores: Synthesis and properties of heterocycle-based electronically gradient dipolar NLO chromophores. <i>Journal of Materials Chemistry</i> , 2010, 20, 2369.	6.7	82
1487	Noncentrosymmetric Crystals with Marked Nonlinear Optical Properties. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5099-5103.	1.1	48
1488	Synthesis, Structures, Photoluminescent Behaviors, and DFT Studies of Novel Aluminum Complexes Containing Phenoxybenzotriazole Derivatives. <i>Organometallics</i> , 2010, 29, 347-353.	1.1	16
1489	Double proton transfer in the ground and excited states of the tropolone-HF complex. <i>Molecular Physics</i> , 2010, 108, 1171-1190.	0.8	2
1490	Quantum chemical study of benzimidazole derivatives to tune the second-order nonlinear optical molecular switching by proton abstraction. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 4791.	1.3	106
1491	Theoretical study on the electron transfer and phosphorescent properties of iridium(III) complexes with 2-phenylpyridyl and 8-hydroxyquinolate ligands. <i>Dalton Transactions</i> , 2010, 39, 7733.	1.6	30
1492	Fluorescence Spectroscopic Properties of Nitro-Substituted Diphenylpolyenes: Effects of Intramolecular Planarization and Intermolecular Interactions in Crystals. <i>Journal of Physical Chemistry A</i> , 2010, 114, 172-182.	1.1	50
1493	The influence of the relative position of the thiophene and pyrrole rings in donor-acceptor thienylpyrrolyl-benzothiazole derivatives. A photophysical and theoretical investigation. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 9719.	1.3	31

#	ARTICLE	IF	CITATIONS
1494	Computational and experimental evidence for the first direct spectroscopic detection of the pyryloxy neutral redox partner. <i>Photochemical and Photobiological Sciences</i> , 2010, 9, 796-800.	1.6	6
1495	Computational design of ring-expanded pyrimidine-based DNA motifs with improved conductivity. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 5906.	1.3	18
1496	Electronically excited states of membrane fluorescent probe 4-dimethylaminochalcone. Results of quantum chemical calculations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 9518.	1.3	13
1497	Comparison of photoenolization and alcohol release from alkyl-substituted benzoyl benzoic esters. <i>Canadian Journal of Chemistry</i> , 2011, 89, 331-338.	0.6	6
1498	Modulation of the photophysics of 2-(4- N,N -dimethylaminophenyl)imidazo-[4,5- <i>b</i>]pyridine by long chain <i>N</i> -alkylations. <i>Photochemical and Photobiological Sciences</i> , 2011, 10, 939-946.	1.6	13
1499	Microscopic solvation of NaBO ₂ in water: anion photoelectron spectroscopy and ab initio calculations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 15865.	1.3	23
1500	Multi-Copper-Mediated DNA Base Pairs Acting as Suitable Building Blocks for the DNA-Based Nanowires. <i>Journal of Physical Chemistry C</i> , 2011, 115, 2855-2864.	1.5	16
1501	Ab Initio Study of the Anomalous Solvatochromic Behavior of Large Betaines. <i>Journal of Physical Chemistry A</i> , 2011, 115, 7994-8002.	1.1	8
1502	Theoretical Study on the Electronic Excitations of a Porphyrin-Polypyridyl Ruthenium(II) Photosensitizer. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11988-11997.	1.1	15
1503	Vibrational and Electronic Spectroscopy of the 4-Hydroxystyrene-CO ₂ Cluster and Its Hydrate: A Coumaric Acid Impostor. <i>Journal of Physical Chemistry B</i> , 2011, 115, 1275-1281.	1.2	5
1504	Efficient Blue-Emitting Ir(III) Complexes with Phosphine Carbanion-Based Ancillary Ligand: A DFT Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11689-11695.	1.1	35
1505	Introduction of a New Theory for the Calculation of Magnetic Coupling Based on Spin-Flip Constricted Variational Density Functional Theory. Application to Trinuclear Copper Complexes which Model the Native Intermediate in Multicopper Oxidases. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1858-1866.	2.3	41
1506	Comprehensive Studies on an Overall Proton Transfer Cycle of the <i>ortho</i> -Green Fluorescent Protein Chromophore. <i>Journal of the American Chemical Society</i> , 2011, 133, 2932-2943.	6.6	133
1507	Theoretical Modeling of Peptide α -Helical Circular Dichroism in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2011, 115, 1734-1742.	1.1	31
1508	Vibrational Spectra of the Ground and the Singlet Excited $\tilde{\nu}_1^*$ State of 6,7-Dimethyl-8-ribityllumazine. <i>Journal of Physical Chemistry B</i> , 2011, 115, 3689-3697.	1.2	7
1509	Density Functional and Spin-Orbit Ab Initio Study of CF ₃ Br: Molecular Properties and Electronic Curve Crossing. <i>Journal of Physical Chemistry A</i> , 2011, 115, 1264-1271.	1.1	12
1510	Understanding Optoelectronic Properties of Cyano-Terminated Oligothiophenes in the Context of Intramolecular Charge Transfer. <i>Journal of Physical Chemistry B</i> , 2011, 115, 10573-10585.	1.2	23
1511	TD-DFT Vibronic Couplings in Anthraquinones: From Basis Set and Functional Benchmarks to Applications for Industrial Dyes. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1882-1892.	2.3	113

#	ARTICLE	IF	CITATIONS
1512	Peculiarities of the Environmental Influence on the Optical Properties of Push-Pull Nonlinear Optical Molecules: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12251-12258.	1.1	24
1513	Concentration and Temperature Dependency of Regio- and Stereoselectivity in a Photochemical [2 + 2] Cycloaddition Reaction (the Paternò-Büchi Reaction): Origin of the Hydroxy-Group Directivity. <i>Journal of the American Chemical Society</i> , 2011, 133, 2592-2604.	6.6	30
1514	State-specific multireference coupled-cluster theory of molecular electronic excited states. <i>Annual Reports on the Progress of Chemistry Section C</i> , 2011, 107, 169.	4.4	8
1515	Oscillator Strength: How Does TDDFT Compare to EOM-CCSD?. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 456-466.	2.3	123
1516	Dynamics on the Electronically Excited State Surface of the Bioluminescent Firefly Luciferase-Oxyluciferin System. <i>Journal of the American Chemical Society</i> , 2011, 133, 12040-12049.	6.6	53
1517	Analytical approach for the excited-state Hessian in time-dependent density functional theory: Formalism, implementation, and performance. <i>Journal of Chemical Physics</i> , 2011, 135, 184111.	1.2	107
1518	Electronic promotion effect of double proton transfer on conduction of DNA through improvement of transverse electronic communication of base pairs. <i>Journal of Chemical Physics</i> , 2011, 135, 134315.	1.2	15
1520	Analytical Hessian of electronic excited states in time-dependent density functional theory with Tamm-Dancoff approximation. <i>Journal of Chemical Physics</i> , 2011, 135, 014113.	1.2	74
1521	Structural and Spectral Properties of 4-Bromo-1-naphthyl Chalcones: A Quantum Chemical Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 6594-6602.	1.1	36
1522	Computational Studies of the Luciferase Light-Emitting Product: Oxyluciferin. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 809-817.	2.3	78
1523	Application of Molecular Simulation Techniques to the Study of Factors Affecting the Thin-Film Morphology of Small-Molecule Organic Semiconductors. <i>Chemistry of Materials</i> , 2011, 23, 522-543.	3.2	52
1524	Energy-Specific Linear Response TDHF/TDDFT for Calculating High-Energy Excited States. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3540-3547.	2.3	100
1525	MSINDO-sCIS: A New Method for the Calculation of Excited States of Large Molecules. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3675-3685.	2.3	20
1526	UV/Vis Absorption, Emission Spectra and Two-Photo Absorption Cross Sections of 4-Dihydroquinolinone Derivatives. <i>Advanced Materials Research</i> , 0, 233-235, 2748-2754.	0.3	0
1527	Time-dependent density functional theory study on the hydrogen bonding in electronic excited states of 6-amino-3-((thiophen-2-yl) methylene)-phthalide in methanol solution. <i>Computational and Theoretical Chemistry</i> , 2011, 972, 57-62.	1.1	3
1528	Calculation of the properties of molecules in the pyridine catalyst system for the photochemical conversion of CO ₂ to methanol. <i>Computational and Theoretical Chemistry</i> , 2011, 977, 123-127.	1.1	37
1529	Practical computation of electronic excitation in solution: vertical excitation model. <i>Chemical Science</i> , 2011, 2, 2143.	3.7	202
1530	Theoretical studies on structures and spectroscopic properties of highly efficient phosphorescent iridium(III) complexes with pyrazine and pyrimidine ligands. <i>Synthetic Metals</i> , 2011, 161, 2492-2497.	2.1	4

#	ARTICLE	IF	CITATIONS
1531	Calculation of the exchange coupling constants of copper binuclear systems based on spin-flip constricted variational density functional theory. <i>Journal of Chemical Physics</i> , 2011, 135, 184105.	1.2	24
1532	Excited State Structural Analysis: TDDFT and Related Models. , 2011, , 415-449.		15
1533	Assessing Excited State Methods by Adiabatic Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2376-2386.	2.3	164
1534	Efficient time-dependent density functional theory approximations for hybrid density functionals: Analytical gradients and parallelization. <i>Journal of Chemical Physics</i> , 2011, 134, 054116.	1.2	182
1535	Role of nitrogen substitution in phenyl ring on excited state intramolecular proton transfer and rotamerism of 2-(2-hydroxyphenyl)benzimidazole: A theoretical study. <i>Journal of Chemical Physics</i> , 2011, 134, 104308.	1.2	35
1536	Low-energy Electron Collisions with Gas-phase Thymine Molecule. <i>Medziagotyra</i> , 2011, 17, .	0.1	0
1538	QM:QM embedding using electronic densities within an ONIOM framework: Energies and analytic gradients. <i>Journal of Chemical Physics</i> , 2011, 135, 014105.	1.2	20
1539	Quantum chemical and experimental studies on the structure and vibrational spectra of substituted 2-pyranones. <i>Journal of Structural Chemistry</i> , 2011, 52, 247-256.	0.3	1
1540	Physical optical properties and crystal structures of organic 5-sulfosalicylates – Theoretical and experimental study. <i>Journal of Molecular Structure</i> , 2011, 1003, 1-9.	1.8	20
1541	Conformation, optical properties, and absolute configuration of 2,3-isopropylideneadenosines: Theoretical vs. experimental study. <i>Journal of Molecular Structure</i> , 2011, 1004, 303-312.	1.8	11
1542	Novel quinonediimines derived from amino acid-like structures 1: Characterization and DFT computational study: N,N-bis(5-benzimidazolyl)-1,4-quinonediimine. <i>Journal of Molecular Structure</i> , 2011, 1004, 319-328.	1.8	9
1543	Experimental and theoretical study of three new benzothiazole-fused carbazole derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 730-738.	2.0	19
1544	Experimental and theoretical study of two new pyrazoline derivatives based on dibenzofuran. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 83, 242-249.	2.0	17
1545	The quantified NTO analysis for the electronic excitations of molecular many-body systems. <i>Chemical Physics Letters</i> , 2011, 514, 362-367.	1.2	11
1546	The effect of diphenylamine on the electronic, optical, and charge transport properties of BTD-based derivative: Insights from theory. <i>Chinese Chemical Letters</i> , 2011, 22, 1383-1386.	4.8	2
1547	Influence of Triplet Instabilities in TDDFT. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3578-3585.	2.3	285
1548	Excited-State Electronic Structure with Configuration Interaction Singles and Tamm-Dancoff Time-Dependent Density Functional Theory on Graphical Processing Units. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1814-1823.	2.3	180
1549	Designing of the white-light emission from a single-polymer system: Quantum theoretical study. <i>Polymer Science - Series A</i> , 2011, 53, 1097-1105.	0.4	0

#	ARTICLE	IF	CITATIONS
1550	Photolysis of (3-Methyl-2-azirin-2-yl)-phenylmethanone: Direct Detection of a Triplet Vinylnitrene Intermediate. <i>Journal of Organic Chemistry</i> , 2011, 76, 9934-9945.	1.7	32
1551	Triplet-Sensitized Photoreactivity of a Geminal Diazidoalkane. <i>Journal of Organic Chemistry</i> , 2011, 76, 8177-8188.	1.7	15
1552	Theoretical study on the second-order nonlinear optical properties and reorganization energy of silafluorenes and spirobisilafluorenes derivatives. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 249-256.	0.5	10
1553	Photophysical properties and vibrational structure of ladder-type penta p-phenylene and carbazole derivatives based on SAC-CI calculations. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 161-173.	0.5	4
1554	Thermodynamic limit and size-consistent design. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 727-746.	0.5	50
1555	TD-DFT study on the fluorescent chemosensor for Hg ²⁺ , 2-(Benzo-d-thiazol-2-yl)quinoline. <i>Journal of Molecular Structure</i> , 2011, 991, 73-78.	1.8	1
1556	Fragment molecular orbital calculations for excitation energies of blue- and yellow-fluorescent proteins. <i>Chemical Physics Letters</i> , 2011, 504, 76-82.	1.2	16
1557	Electronic correlations in organometallic complexes. <i>Chemical Physics Letters</i> , 2011, 508, 22-28.	1.2	11
1558	Stereochemical deuterium labeling study on the denitrogenation of 7,7-diethoxy-2,3-diazabicyclo[2.2.1]heptane. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 894-901. ^{0.9}		8
1559	Phenylethanol derivatives as triplet sensitizers for azidoadamantane. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 902-908.	0.9	1
1560	Ab initio and DFT study of the electronic structures and spectroscopic properties of pyrene ligands and their cyclometalated complexes. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2258-2267.	1.0	3
1561	The chemical bond overlap plasmon as a tool for quantifying covalency in solid state materials and its applications to spectroscopy. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1626-1638.	1.0	13
1562	Theoretical investigation on the spectroscopic properties of cyclometallated iridium (III) complexes and the deprotonation influence on them in solution. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 4080-4090.	1.0	5
1563	Effects of the Au(I)-Au(I) closed-shell attraction on the electronic and phosphorescent properties in a series of coordination compounds: A theoretical study. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 4378-4388.	1.0	8
1564	Organic spectroscopy under B ₂ Irn O. Roos. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 3284-3290.	1.0	2
1565	Study of the Structure and Photochemical Decomposition of Azidoadamantanes Entrapped in α - and β -Cyclodextrin. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 1249-1255.	1.2	14
1566	Theoretical Study of Structure, Energetic, Hydrogen Bonds Strength and Intramolecular Proton Transfer of 2-(2-R (R = 3/4 OH, NH ₂ , SH) Phenyl (or Pyridyl)) Benzoxazoles (or Benzothiazoles). <i>Chinese Journal of Chemistry</i> , 2011, 29, 650-654.	2.6	3
1567	Influence of Hydrogen Bonds and Nonspecific Interactions on the Spectral and Photophysical Properties of the Excited Singlet States of 4-Aminophthalimide in Amine Solution. <i>ChemPhysChem</i> , 2011, 12, 322-332.	1.0	18

#	ARTICLE	IF	CITATIONS
1568	Computational Investigation of the Effect of pH on the Color of Firefly Bioluminescence by DFT. ChemPhysChem, 2011, 12, 951-960.	1.0	66
1569	Study on the Effects of Intermolecular Interactions on Firefly Multicolor Bioluminescence. ChemPhysChem, 2011, 12, 3002-3008.	1.0	33
1570	Spin-Orbit Coupling in Phosphorescent Iridium(III) Complexes. ChemPhysChem, 2011, 12, 2429-2438.	1.0	73
1571	The opsin shift and mechanism of spectral tuning in rhodopsin. Journal of Computational Chemistry, 2011, 32, 854-865.	1.5	44
1572	Theoretical study on phosphorescence efficiency and color tuning from orange to blue-green of Ir(III) complexes based on substituted 2-phenylimidazo[1,2-a]pyridine ligand. Journal of Computational Chemistry, 2011, 32, 1033-1042.	1.5	23
1573	Theoretical modulation of the color of light emitted by firefly oxyluciferin. Journal of Computational Chemistry, 2011, 32, 2654-2663.	1.5	30
1574	Density functional theory [B3LYP/6-311G(d,p)] study of a new copolymer based on carbazole and (3,4-ethylenedioxythiophene) in their aromatic and polaronic states. Journal of Applied Polymer Science, 2011, 122, 3351-3360.	1.3	13
1576	Matrix Isolation of Two Isomers of N ₄ CO. Angewandte Chemie - International Edition, 2011, 50, 482-485.	7.2	20
1577	Enhanced Functionality for Donor-Acceptor Oligothiophenes by means of Inclusion of BODIPY: Synthesis, Electrochemistry, Photophysics, and Model Chemistry. Chemistry - A European Journal, 2011, 17, 498-507.	1.7	63
1578	Addition and Redox Reactivity of Hydrogen Sulfides (H ₂ S/HS ⁻) with Nitroprusside: New Chemistry of Nitrososulfide Ligands. Chemistry - A European Journal, 2011, 17, 4145-4156.	1.7	42
1579	Hexaazatriphenylene (HAT) versus tri-HAT: The Bigger the Better?. Chemistry - A European Journal, 2011, 17, 10312-10322.	1.7	40
1580	Theoretical investigation on the white-light emission from a single-polymer system with simultaneous blue and orange emission (Part II). European Polymer Journal, 2011, 47, 208-224.	2.6	21
1581	Theoretical studies on structures and spectroscopic properties of a series of heteroleptic iridium complexes based on tridentate bis(benzimidazolyl)pyridine ligand. Computational and Theoretical Chemistry, 2011, 963, 298-305.	1.1	4
1582	Investigation of the ICT state of DPA-DSB using spectroscopic experiments and quantum chemical calculations. Chemical Physics Letters, 2011, 502, 184-186.	1.2	6
1583	Coulomb and Exchange contributions to electronic excitations of benzene aggregates. Chemical Physics Letters, 2011, 502, 271-276.	1.2	5
1584	Size and hydrogen saturation effects on third-order polarizabilities of Si clusters. Chemical Physics Letters, 2011, 509, 124-128.	1.2	3
1585	N-Heteroaryl-1,8-naphthalimide fluorescent sensor for water: Molecular design, synthesis and properties. Dyes and Pigments, 2011, 88, 307-314.	2.0	109
1586	Synthesis, characterization, and computational study of N,N'-bis(2,4-dihydroxyphenyl)-1,4-quinonediimine, a hydroxyl-capped three-ring quinonediimine with sterically hindered substituent on outer rings. Journal of Molecular Structure, 2011, 985, 299-306.	1.8	7

#	ARTICLE	IF	CITATIONS
1587	A DFT exploration of luminescent rhenium(I) tricarbonyl diimine complex with a triarylboron moiety and its F derivative. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 2943-2948.	0.8	7
1588	Theoretical study on the influence of ancillary ligand on the energy and optical properties of heteroleptic phosphorescent Ir(III) complexes. <i>Journal of Luminescence</i> , 2011, 131, 1158-1163.	1.5	9
1589	Experimental and theoretical study of 10-methoxy-2-phenylbenzo[h]quinoline. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 78, 1143-1148.	2.0	48
1590	A study on quantum chemical calculations of 3-, 4-nitrobenzaldehyde oximes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 1783-1793.	2.0	33
1591	Gas phase solvatochromic effects of phenol and naphthol photoacids. <i>Journal of Chemical Physics</i> , 2011, 134, 244303.	1.2	5
1592	Assessing limitations to the two-level approximation in nonlinear optics for organic chromophores by ab initio methods. <i>Proceedings of SPIE</i> , 2011, , .	0.8	3
1593	Application of an efficient multireference approach to free-base porphyrin and metalloporphyrins: Ground, excited, and positive ion states. <i>Journal of Chemical Physics</i> , 2011, 135, 084118.	1.2	16
1594	Flickering dipoles in the gas phase: Structures, internal dynamics, and dipole moments of \hat{I}^2 -naphthol-H ₂ O in its ground and excited electronic states. <i>Journal of Chemical Physics</i> , 2011, 134, 114304.	1.2	9
1595	Long-range interactions between like homonuclear alkali metal diatoms. <i>Journal of Chemical Physics</i> , 2011, 135, 244307.	1.2	22
1596	Theoretical study of the origin of the large difference in the visible absorption spectra of organic dyes containing a thienylmethine unit and differing by the methine unit position. , 2011, , .		6
1597	DFT Study of Substituted Effect on Absorption and Emission Spectra of Naphthoquinone Derivatives. <i>Advanced Materials Research</i> , 0, 233-235, 1878-1883.	0.3	1
1598	Theoretical Investigation on the Electronic and Optical Properties of Poly(fluorenevinylene) Derivatives as Light-Emitting Materials. <i>International Journal of Photoenergy</i> , 2011, 2011, 1-9.	1.4	9
1599	Theoretical Investigation on the Structure and Optical Properties of Alq ₃ and its Difluorinated Derivatives. <i>Advanced Materials Research</i> , 2011, 287-290, 1526-1531.	0.3	1
1600	ELECTRON-WITHDRAWING SUBSTITUTED BTD-BASED DERIVATIVE: ELECTRONIC AND OPTICAL PROPERTIES, CHARGE TRANSFER, STABILITY STUDY. <i>Journal of Theoretical and Computational Chemistry</i> , 2011, 10, 829-838.	1.8	1
1601	Molecular-orbital-free algorithm for the excited-state force in time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2011, 134, 044114.	1.2	17
1602	Full-Quantum chemical calculation of the absorption maximum of bacteriorhodopsin: a comprehensive analysis of the amino acid residues contributing to the opsin shift. <i>Biophysics (Nagoya-shi, Japan)</i> , 2012, 8, 115-125.	0.4	4
1603	Photo-Absorption Studies on Formaldehyde Using Synchrotron Radiation at Indus I. <i>Spectroscopy Letters</i> , 2012, 45, 65-73.	0.5	2
1605	Electronic, Optical, and Charge Transport Properties of New 2,1,3-Benzothiadiazole-Based Derivative for Organic Light-Emitting Diodes. <i>Spectroscopy Letters</i> , 2012, 45, 17-21.	0.5	7

#	ARTICLE	IF	CITATIONS
1606	Quantum Monte Carlo for the x-ray absorption spectrum of pyrrole at the nitrogen K-edge. <i>Journal of Chemical Physics</i> , 2012, 136, 144301.	1.2	1
1607	Failure of the two-level and sum over states methods in nonlinear optics, demonstrated by ab initio methods. <i>Proceedings of SPIE</i> , 2012, , .	0.8	0
1609	Low-frequency Raman scattering of bioinspired self-assembled diphenylalanine nanotubes/microtubes. <i>Optics Express</i> , 2012, 20, 5119.	1.7	17
1610	Carbon, Nitrogen, and Chalcogen Substitution Effects on 2,1,3-Benzothiadiazole Derivative: Theoretical Investigations of Electronic, Optical, and Charge Transport Properties. <i>Chinese Journal of Chemical Physics</i> , 2012, 25, 25-30.	0.6	0
1611	Theoretical Studies of Dynamic Interactions in Excited States of Hydrogen-Bonded Systems. <i>Journal of Atomic, Molecular, and Optical Physics</i> , 2012, 2012, 1-17.	0.5	3
1612	Experimental and Time-Dependent Density Functional Theory Characterization of the UV-Visible Spectra of Monomeric and 1/4-Oxo Dimeric Ferriprotoporphyrin IX. <i>Inorganic Chemistry</i> , 2012, 51, 10233-10250.	1.9	21
1613	Performance of recent and high-performance approximate density functionals for time-dependent density functional theory calculations of valence and Rydberg electronic transition energies. <i>Journal of Chemical Physics</i> , 2012, 137, 244104.	1.2	165
1614	Development of Calculation and Analysis Methods for the Dynamic First Hyperpolarizability Based on the Ab Initio Molecular Orbital Quantum Master Equation Method. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4371-4380.	1.1	4
1615	Coordination ability of silver(I) with antimycins and actinomycins Properties of the T-shaped chromophores. <i>Polyhedron</i> , 2012, 38, 235-244.	1.0	7
1616	Dipole moment and polarizability of the low-lying excited states of uracil. <i>Chemical Physics Letters</i> , 2012, 546, 24-29.	1.2	25
1617	The effects of H-bonding and sterics on the photoreactivity of a trimethyl butyrophenone derivative. <i>Photochemical and Photobiological Sciences</i> , 2012, 11, 744-751.	1.6	5
1618	Hydrogen bond effects in the ground and excited singlet states of 4H-1-benzopyrane-4-thione in water theory and experiment. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 8842.	1.3	25
1619	A series of coordination polymers constructed from in situ amidation ligands: syntheses, structures and luminescent properties. <i>CrystEngComm</i> , 2012, 14, 4719.	1.3	28
1620	Understanding the absorption and emission spectra of borondipyromethene dye and its substituted analogues. <i>Molecular Physics</i> , 2012, 110, 445-456.	0.8	11
1621	TDDFT and CIS Studies of Optical Properties of Dimers of Silver Tetrahedra. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8260-8269.	1.1	48
1622	Existence of a New Emitting Singlet State of Proflavine: Femtosecond Dynamics of the Excited State Processes and Quantum Chemical Studies in Different Solvents. <i>Journal of Physical Chemistry A</i> , 2012, 116, 37-45.	1.1	26
1623	Impact of Electron Acceptor on Three-Photon Absorption Cross-Section of the Fluorene Derivatives. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7445-7451.	1.1	8
1624	Band structure engineering for low band gap polymers containing thienopyrazine. <i>Journal of Materials Chemistry</i> , 2012, 22, 7331.	6.7	14

#	ARTICLE	IF	CITATIONS
1625	Mode Recognition in UV Resonance Raman Spectra of Imidazole: Histidine Monitoring in Proteins. <i>Journal of Physical Chemistry B</i> , 2012, 116, 9387-9395.	1.2	15
1626	A comparative experimental and quantum chemical study on monomeric and dimeric structures of 3,5-dibromoanthranilic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 96, 644-656.	2.0	2
1627	Electronic structure and optical properties of some anthocyanins extracted from grapes. <i>Optical Materials</i> , 2012, 34, 1644-1650.	1.7	20
1628	Overcoming Low Orbital Overlap and Triplet Instability Problems in TDDFT. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9783-9789.	1.1	190
1629	Derivatives of Ergot-alkaloids: Molecular structure, physical properties, and structure-activity relationships. <i>Journal of Molecular Structure</i> , 2012, 1024, 18-31.	1.8	7
1630	Novel quinonediimines derived from amino acid-like structures 2: Characterization and DFT computational study of N,N'-bis(4-phenylalaninyl)-1,4-quinonediimine. <i>Journal of Molecular Structure</i> , 2012, 1022, 181-188.	1.8	5
1631	Theoretical study on the electronic structures and photophysical properties of a series of dithienylbenzothiazole derivatives. <i>Computational and Theoretical Chemistry</i> , 2012, 981, 14-24.	1.1	24
1632	Theoretical analysis of the color tuning mechanism of oxyluciferin and 5-hydroxyoxyluciferin. <i>Computational and Theoretical Chemistry</i> , 2012, 988, 56-62.	1.1	11
1633	Calculation of the properties of the S3 ⁻ radical anion and its complexes with Cu ⁺ in aqueous solution. <i>Geochimica Et Cosmochimica Acta</i> , 2012, 95, 79-92.	1.6	28
1634	Type-I Dyotropic Reactions: Understanding Trends in Barriers. <i>Chemistry - A European Journal</i> , 2012, 18, 12395-12403.	1.7	79
1635	Water-Sensitive High-Frequency Molecular Vibrations in Self-Assembled Diphenylalanine Nanotubes. <i>Journal of Physical Chemistry C</i> , 2012, 116, 9793-9799.	1.5	29
1636	8.27 Spectroscopic Analysis: Ab initio Calculation of Chiroptical Spectra. , 2012, , 520-544.		4
1637	Transition-density-fragment interaction combined with transfer integral approach for excitation-energy transfer via charge-transfer states. <i>Journal of Chemical Physics</i> , 2012, 137, 034101.	1.2	45
1638	Periodic calculations of excited state properties for solids using a semiempirical approach. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 741-750.	1.3	14
1639	Structure-properties correlation of copolymers derived from poly(phenylene vinylene) (PPV). <i>Synthetic Metals</i> , 2012, 162, 1762-1768.	2.1	9
1640	Synthesis, photophysical and electrochemical properties and theoretical studies on three novel indolo[3,2-b]carbazole derivatives containing benzothiazole units. <i>Tetrahedron</i> , 2012, 68, 9788-9794.	1.0	13
1641	Theoretical characterization of a class of orange dopants for white-light-emitting single polymers. <i>Materials Chemistry and Physics</i> , 2012, 135, 965-972.	2.0	0
1642	Structural Optimization by Quantum Monte Carlo: Investigating the Low-Lying Excited States of Ethylene. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1260-1269.	2.3	46

#	ARTICLE	IF	CITATIONS
1643	TD-DFT/Molecular Mechanics Study of the Photinus pyralis Bioluminescence System. Journal of Physical Chemistry B, 2012, 116, 2008-2013.	1.2	29
1644	Effect of Molecular Symmetry on the Spectra and Dynamics of the Intramolecular Charge Transfer (ICT) State of Peridinin. Journal of Physical Chemistry B, 2012, 116, 10748-10756.	1.2	36
1645	Theoretical studies on DNA-photocleavage efficiencies and mechanisms of Ru(II) polypyridyl complexes. Journal of Biological Inorganic Chemistry, 2012, 17, 1177-1185.	1.1	3
1646	Role of hydrogen bonding in excited state intramolecular proton transfer of Indole-7-Carboxaldehyde: A theoretical and experimental study. Chemical Physics Letters, 2012, 548, 71-79.	1.2	28
1647	Correlation between Photophysical Parameters and Gold-Gold Distances in Gold(I) (4-Pyridyl)ethynyl Complexes. Inorganic Chemistry, 2012, 51, 7636-7641.	1.9	69
1648	Coordination ability of bradykinin with ZnII- and AgI-metal ions - Experimental and theoretical study. Inorganica Chimica Acta, 2012, 392, 211-220.	1.2	8
1649	Seven-membered ring excited-state intramolecular proton-transfer in 2-benzamido-3-(pyridin-2-yl)acrylic acid. Dyes and Pigments, 2012, 92, 619-625.	2.0	19
1650	Theoretical studies of the structural, electronic and optical properties of carbazole-based compounds. Journal of Physical Organic Chemistry, 2012, 25, 334-342.	0.9	5
1651	Basis set and functional effects on excited-state properties: Three bicyclic chromogens as working examples. International Journal of Quantum Chemistry, 2012, 112, 2135-2141.	1.0	36
1652	Excitation Gaps of Finite-Sized Systems from Optimally Tuned Range-Separated Hybrid Functionals. Journal of Chemical Theory and Computation, 2012, 8, 1515-1531.	2.3	765
1653	Elusive Fluoro Sulfinyl Nitrite, FS(O)NO, Produced by Photolysis of Matrix-Isolated FS(O) ₂ N. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2012, 638, 526-533.	0.6	25
1654	Recent Advances in Wave Function-Based Methods of Molecular-Property Calculations. Chemical Reviews, 2012, 112, 543-631.	23.0	549
1655	Benchmarking the performance of time-dependent density functional methods. Journal of Chemical Physics, 2012, 136, 104101.	1.2	295
1656	Quantum chemical comparison of vertical, adiabatic, and 0-0 excitation energies: The PYP and GFP chromophores. Journal of Computational Chemistry, 2012, 33, 1892-1901.	1.5	29
1657	Resonant two-photon ionization of jet-cooled fluorene clusters: elucidation of dimer structures and vibrations. Journal of the Korean Physical Society, 2012, 60, 496-500.	0.3	2
1658	Analytical Gradients for the MSINDO-sCIS and MSINDO-UCIS Method: Theory, Implementation, Benchmarks, and Examples. Journal of Chemical Theory and Computation, 2012, 8, 986-996.	2.3	11
1659	On the Electrochemistry and Spectroelectrochemistry of Small Model Star-Shaped Compounds: 1,3,5-Triaryl-1,3,5-Trimethoxybenzenes and 2,4,6-Triaryl-1,3,5-Trimethoxybenzenes. ChemPhysChem, 2012, 13, 2322-2330.	1.0	7
1660	Rational Design for Building Blocks of DNA-Based Conductive Nanowires through Multi-Copper Incorporation into Mismatched Base Pairs. ChemPhysChem, 2012, 13, 3293-3302.	1.0	4

#	ARTICLE	IF	CITATIONS
1661	Electrical Bistability and WORM Memory Effects in Donor- π -Acceptor Polymers Based on Poly(<i>N,N</i> -vinylcarbazole). <i>ChemPlusChem</i> , 2012, 77, 74-81.	1.3	37
1662	Calculation of Excited States: Molecular Photophysics and Photochemistry on Display. , 2012, , 483-560.		13
1663	Guide to Programs for Non-relativistic Quantum Chemistry Calculations. , 2012, , 611-630.		0
1664	CH ₂ , NH, and O heteroatom substitution effects on the electronic, optical, and charge transport properties of a 2,1,3-benzothiadiazole-based derivative: Insights from theory. <i>Science China Chemistry</i> , 2012, 55, 1364-1369.	4.2	2
1665	Adsorption of croconate dyes on TiO ₂ anatase (101) surface: A periodic DFT study to understand the binding of diketo groups#. <i>Journal of Chemical Sciences</i> , 2012, 124, 301-310.	0.7	15
1666	Theoretical studies of the effect of electron-withdrawing dicyanovinyl group on the electronic and charge-transport properties of fluorene-thiophene oligomers. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	16
1667	Time-dependent density functional theory benchmarking for the calculations of atomic spectra: efficiency of exc-ETDZ basis set. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	7
1668	The first solvation shell of Reichardt's dye in ionic liquids: a semiempirical study. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	12
1669	Ab initio and DFT study of luminescent cyclometalated N-heterocyclic carbene organogold(III) complexes. <i>Journal of Molecular Modeling</i> , 2012, 18, 2543-2551.	0.8	4
1670	Role of cationic size in the optical properties of the LiCl crystal surface: theoretical study. <i>Journal of Molecular Modeling</i> , 2012, 18, 2493-2500.	0.8	0
1671	Excited state calculation for free-base and metalloporphyrins with the partially renormalized polarization propagator approach. <i>Chemical Physics Letters</i> , 2012, 525-526, 144-149.	1.2	6
1672	Theoretical study of the alkoxy groups effect on PPV-ether excited states, a relationship with femtosecond decay. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 88, 23-30.	2.0	21
1673	The effect of zinc ion on the absorption and emission spectra of glutathione derivative: Prediction by ab initio and DFT methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 91, 307-313.	2.0	3
1674	Synthesis, photophysical and electrochemical properties of a carbazole dimer-based derivative with benzothiazole units. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 93, 19-25.	2.0	20
1675	Modeling of a violaxanthin-chlorophyll b chromophore pair in its LHCII environment using CAM-B3LYP. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2012, 109, 12-19.	1.7	17
1676	Progress and Challenges in the Calculation of Electronic Excited States. <i>ChemPhysChem</i> , 2012, 13, 28-51.	1.0	344
1677	Quantum Chemical Description of Absorption Properties and Excited-State Processes in Photosynthetic Systems. <i>ChemPhysChem</i> , 2012, 13, 386-425.	1.0	107
1678	A combined experimental and theoretical study on vibrational and optical properties of copolymer incorporating thienylene-dioxyphenylene-thienylene and bipyridine units. <i>Journal of Applied Polymer Science</i> , 2012, 123, 2684-2696.	1.3	13

#	ARTICLE	IF	CITATIONS
1679	Structure and properties of camptothecin derivatives, their protonated forms, and model interaction with the topoisomerase-DNA complex. <i>Biopolymers</i> , 2012, 97, 134-144.	1.2	31
1680	Electronically excited states and photodynamics: a continuing challenge. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	77
1681	Theoretical study of electronic absorptions in aminopyridines TCNE CT complexes by quantum chemical methods, including solvent. <i>Journal of Molecular Modeling</i> , 2013, 19, 4639-4650.	0.8	5
1682	Analysis of the performance of DFT functionals in the study of light emission by oxyluciferin analogs. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 45-51.	1.0	15
1683	Distinguishing tautomers by their spectroscopic signatures: A theoretical investigation. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1225-1233.	1.0	3
1684	Double Proton Transfer Induced Twisted Intramolecular Charge Transfer Emission in 2-(4-Dimethylaminophenyl)imidazo[4,5-b]pyridine. <i>Journal of Physical Chemistry B</i> , 2013, 117, 9469-9477.	1.2	36
1685	Manipulation of connecting topology in carbazole/benzimidazole universal bipolar host materials for RGB and White PhOLEDs. <i>RSC Advances</i> , 2013, 3, 13891.	1.7	21
1686	A novel dimesitylboron-substituted indolo[3,2-b]carbazole derivative: Synthesis, electrochemical, photoluminescent and electroluminescent properties. <i>Organic Electronics</i> , 2013, 14, 868-874.	1.4	32
1687	On asymptotic behavior of density functional theory. <i>Journal of Chemical Physics</i> , 2013, 139, 024104.	1.2	33
1688	Physical properties and inclusion interactions of new stilbazolium salts: experimental versus theoretical study. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2013, 76, 75-85.	1.6	0
1689	Substituted benzo[<i>i</i>]phenanthridines as promising topoisomerase-I non-camptothecin targeting agents: an experimental and theoretical study. <i>Medicinal Chemistry Research</i> , 2013, 22, 5204-5217.	1.1	5
1690	New Development in the Solid-State Isotope Exchange with Spillover Hydrogen in Organic Compounds. <i>Journal of Physical Chemistry C</i> , 2013, 117, 16878-16884.	1.5	10
1691	Second-order many-body perturbation expansions of vibrational Dyson self-energies. <i>Journal of Chemical Physics</i> , 2013, 139, 034111.	1.2	35
1692	A THEORETICAL STUDY ON SECOND HARMONIC GENERATION HYPERPOLARIZABILITIES OF PHENYLALANINE POLYPEPTIDES. <i>Journal of Theoretical and Computational Chemistry</i> , 2013, 12, 1250118.	1.8	2
1693	Time-dependent density functional theory study of UV/vis spectra of natural styrylpyrones. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 115, 675-682.	2.0	8
1694	Is the Tamm-Dancoff Approximation Reliable for the Calculation of Absorption and Fluorescence Band Shapes?. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4517-4525.	2.3	95
1695	Luminescence of BODIPY and Dipyrrin: An MCSCF Comparison of Excited States. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1665-1669.	1.1	34
1696	Spectroscopic investigations and hydrogen bond interactions of 8-aza analogues of xanthine, theophylline and caffeine: a theoretical study. <i>Journal of Molecular Modeling</i> , 2013, 19, 1835-1851.	0.8	7

#	ARTICLE	IF	CITATIONS
1697	Excited states of aniline by photoabsorption spectroscopy in the 30 000â€“90 000Âcmâˆ’1 region using synchrotron radiation. <i>Journal of Chemical Physics</i> , 2013, 139, 064303.	1.2	20
1698	Determination of conformational and spectroscopic features of ethyl trans- α -cyano-3-indole-acrylate compound: An experimental and quantum chemical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 104, 428-436.	2.0	12
1699	Orthogonality Constrained Density Functional Theory for Electronic Excited States. <i>Journal of Physical Chemistry A</i> , 2013, 117, 7378-7392.	1.1	76
1701	Evaluating pushâ€“pull dye efficiency using TD-DFT and charge transfer indices. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 20210.	1.3	68
1702	Quantum chemical analysis of salenâ€“aluminum complexes for organic light emitting diodes. <i>Chemical Physics Letters</i> , 2013, 585, 143-148.	1.2	6
1703	Pump and Probe of Ultrafast Charge Reorganization in Small Peptides: A Computational Study through Sudden Ionizations. <i>Journal of Physical Chemistry A</i> , 2013, 117, 10513-10525.	1.1	34
1704	Structureâ€“property relationships of soluble poly(2,5-dibutoxyethoxy-1,4-phenylene-alt-2,5-thienylene) (PBuPT) for organic-optoelectronic devices. <i>Journal of Molecular Structure</i> , 2013, 1036, 7-18.	1.8	23
1705	Synthesis and semi-empirical sparkle PM6 study of substituted dithiophosphoric compounds of gadolinium(III). <i>Journal of Coordination Chemistry</i> , 2013, 66, 1016-1030.	0.8	3
1706	A theoretical study of crystallochromy: Spectral tuning of solid-state tetracenes. <i>Journal of Chemical Physics</i> , 2013, 139, 084511.	1.2	19
1707	Photoluminescence Characteristics of Bi ³⁺ -Doped Silica Optical Fiber: Structural Model and Theoretical Analysis. <i>Japanese Journal of Applied Physics</i> , 2013, 52, 122501.	0.8	26
1708	Resonant electron attachment to polar aromatic molecules: consequences for their chemistry in the interstellar medium. <i>European Physical Journal D</i> , 2013, 67, 1.	0.6	5
1709	Cysteamine-Based Cell-Permeable Zn ²⁺ -Specific Molecular Bioimaging Materials: From Animal to Plant Cells. <i>ACS Applied Materials & Interfaces</i> , 2013, 5, 11730-11740.	4.0	17
1710	Exciton Transfer of Azobenzene Derivatives in Self-Assembled Monolayers. <i>Journal of Physical Chemistry C</i> , 2013, 117, 25026-25041.	1.5	16
1711	Molecular design and physical properties of highly functionalized configurationally locked polyenes â€“ an experimental and theoretical study. <i>Journal of Materials Chemistry C</i> , 2013, 1, 6278-6298.	2.7	3
1712	Quantum mechanical/molecular mechanical/continuum style solvation model: Time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2013, 139, 084106.	1.2	6
1713	Brazilwood Reds: The (Photo)Chemistry of Brazilin and Brazilein. <i>Journal of Physical Chemistry A</i> , 2013, 117, 10650-10660.	1.1	28
1714	Electronic structure calculations for the study of D- π -A organic sensitizers: Exploring polythiophene linkers. <i>Chemical Physics</i> , 2013, 423, 157-166.	0.9	6
1715	Theoretical studies on DNA-photocleavage efficiencies of Ru(II) polypyridyl complexes. <i>Dalton Transactions</i> , 2013, 42, 2463-2468.	1.6	10

#	ARTICLE	IF	CITATIONS
1716	Theoretical Study of Photochemical Hydrogen Abstraction by Triplet Aliphatic Carbonyls by Using Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2013, 117, 439-450.	1.1	8
1717	Determination of structural, spectrometric and nonlinear optical features of 2-(4-hydroxyphenylazo)benzoic acid by experimental techniques and quantum chemical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 105, 80-87.	2.0	15
1718	Theoretical Approaches to Excited-State-Related Phenomena in Oxide Surfaces. <i>Chemical Reviews</i> , 2013, 113, 4456-4495.	23.0	80
1719	Characterization of tetraene intermediates formed in the [3+2]-photocycloaddition of 1,4-dicyano-6-methylnaphthalene with styrene. <i>Research on Chemical Intermediates</i> , 2013, 39, 49-59.	1.3	1
1720	The Nature of the Intramolecular Charge Transfer State in Peridinin. <i>Biophysical Journal</i> , 2013, 104, 1314-1325.	0.2	57
1721	Single amino acid mutation in alpha-helical peptide affect second harmonic generation hyperpolarizability. <i>Chemical Physics Letters</i> , 2013, 556, 260-265.	1.2	2
1722	One trinucleus dimethine cyanine dye: Experimental and theoretical studies on molecular structure as well as absorption and fluorescence properties. <i>Journal of Molecular Structure</i> , 2013, 1039, 84-93.	1.8	0
1723	Spectroscopic properties and singlet oxygen production by the compound ethyl 3,12-dioxopyran[3,2-a]xanthone-2-carboxylate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 115, 610-616.	2.0	1
1724	Estimation of ground and excited state dipole moments of quinidine and quinidine dication: Experimental and numerical methods. <i>Journal of Molecular Liquids</i> , 2013, 179, 88-93.	2.3	17
1725	Probing DNA photocleavage efficiencies of Ru(II) polypyridyl complexes: Theoretical calculation of redox potentials. <i>Inorganica Chimica Acta</i> , 2013, 407, 37-40.	1.2	6
1726	Modeling of phytochrome absorption spectra. <i>Journal of Computational Chemistry</i> , 2013, 34, 1363-1374.	1.5	30
1727	Photophysical properties of NIR-emitting fluorescence probes: insights from TD-DFT. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 10019.	1.3	33
1728	Organosilver(Ag^{I}) catalyzed C-N coupling reactions of phenazines. <i>Catalysis Science and Technology</i> , 2013, 3, 1129-1135.	2.1	7
1729	On the triplet instability in TDDFT. <i>Molecular Physics</i> , 2013, 111, 1271-1274.	0.8	50
1730	Ultraviolet-Visible Dual Absorption by Single BODIPY Dye Confined in LTL Zeolite Nanochannels. <i>Journal of Physical Chemistry C</i> , 2013, 117, 13331-13336.	1.5	33
1731	Excited State Properties of Naphtho-Homologated xxDNA Bases and Effect of Methanol Solution, Deoxyribose, and Base Pairing. <i>Journal of Physical Chemistry B</i> , 2013, 117, 3983-3992.	1.2	11
1732	Communication: An efficient analytic gradient theory for approximate spin projection methods. <i>Journal of Chemical Physics</i> , 2013, 138, 101101.	1.2	26
1733	Evolution of Electric Dipole (Hyper)polarizabilities of β^2 -Strand Polyglycine Single Chains: An ab Initio and DFT Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2013, 117, 5184-5194.	1.1	12

#	ARTICLE	IF	CITATIONS
1734	Crystal Structure and Highly Luminescent Properties Studies of Bis- β^2 -diketonate Lanthanide Complexes. <i>Inorganic Chemistry</i> , 2013, 52, 5013-5022.	1.9	112
1735	Solvent Induced Shifts in the UV Spectrum of Amides. <i>Journal of Physical Chemistry A</i> , 2013, 117, 11847-11855.	1.1	16
1736	Excited state behavior of Pyrrole 2-carboxyldehyde: Theoretical and experimental study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 112, 125-131.	2.0	8
1737	Density functional investigation of photo induced Intramolecular Proton Transfer (IPT) in Indole-7-carboxaldehyde and its experimental verification. <i>Journal of Molecular Structure</i> , 2013, 1045, 72-80.	1.8	11
1738	Ab initio studies of the structure, physicochemical properties and behavior of lead chlorides and chloroplumbate anions in gaseous and aqueous phases. <i>Computational and Theoretical Chemistry</i> , 2013, 1004, 61-68.	1.1	1
1739	Thioflavin T and Its Photoirradiative Derivatives: Exploring Their Spectroscopic Properties in the Absence and Presence of Amyloid Fibrils. <i>Journal of Physical Chemistry B</i> , 2013, 117, 3459-3468.	1.2	21
1740	Nonstationarity and related measures for time-dependent hartree-fock and multiconfigurational models. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2489-2505.	1.0	3
1741	Photoexcitation and Charge-Transfer-to-Solvent Relaxation Dynamics of the $(\text{CH}_3)_3\text{CN}$ Complex. <i>Journal of Physical Chemistry A</i> , 2013, 117, 7595-7605.	1.1	8
1742	Excited electronic states from a variational approach based on symmetry-projected Hartree-Fock configurations. <i>Journal of Chemical Physics</i> , 2013, 139, 224110.	1.2	28
1743	Novel Approach to Excited-State Calculations of Large Molecules Based on Divide-and-Conquer Method: Application to Photoactive Yellow Protein. <i>Journal of Physical Chemistry B</i> , 2013, 117, 5565-5573.	1.2	36
1744	Vinylnitrene Formation from 3,5-Diphenyl-isoxazole and 3-Benzoyl-2-phenylazirine. <i>Journal of Organic Chemistry</i> , 2013, 78, 11349-11356.	1.7	31
1745	Jet-Cooled Fluorescence Spectroscopy of a Natural Product: Anethole. <i>Journal of Physical Chemistry A</i> , 2013, 117, 12831-12841.	1.1	3
1746	Improved convergence of Hartree-Fock style excited-state wavefunctions using second-order optimisation with an exact Hessian. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	26
1747	Energetics and Dynamics of the Low-Lying Electronic States of Constrained Polyenes: Implications for Infinite Polyenes. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1449-1465.	1.1	25
1748	Chalcogenide clusters of copper and silver from silylated chalcogenide sources. <i>Chemical Society Reviews</i> , 2013, 42, 1871-1906.	18.7	293
1749	14 Description of excited states in photocatalysis with theoretical methods. , 2013, , 263-294.		2
1750	Mechanisms of H ₂ O desorption from amorphous solid water by 157-nm irradiation: An experimental and theoretical study. <i>Journal of Chemical Physics</i> , 2013, 139, 164702.	1.2	31
1751	Direct \hat{P}^m MBPT(2) method for ionization potentials, electron affinities, and excitation energies using fractional occupation numbers. <i>Journal of Chemical Physics</i> , 2013, 138, 074101.	1.2	15

#	ARTICLE	IF	CITATIONS
1752	Dynamical second-order Bethe-Salpeter equation kernel: A method for electronic excitation beyond the adiabatic approximation. Journal of Chemical Physics, 2013, 139, 154109.	1.2	23
1753	Dissociations of C ₅ F ₈ and C ₅ H ₇ F in Etching Plasma. Japanese Journal of Applied Physics, 2013, 52, 05EB02.	0.8	7
1754	Double, Rydberg and charge transfer excitations from pairing matrix fluctuation and particle-particle random phase approximation. Journal of Chemical Physics, 2013, 139, 224105.	1.2	52
1755	Reducing the propensity for unphysical wavefunction symmetry breaking in multireference calculations of the excited states of semiconductor clusters. Journal of Chemical Physics, 2013, 139, 074102.	1.2	14
1756	Investigation of activated oxygen molecules on the surface of Y ₂ O ₃ nanocrystals by Raman scattering. Journal of Applied Physics, 2013, 114, .	1.1	25
1757	A multi-state fragment charge difference approach for diabatic states in electron transfer: Extension and automation. Journal of Chemical Physics, 2013, 139, 154104.	1.2	44
1758	Theoretical study on the influence of different N ₂ ligands on the electronic structures and optoelectronic properties of heteroleptic Iridium(III) complexes. Molecular Physics, 2013, 111, 3716-3725.	0.8	4
1759	Analytic energy gradients for constrained DFT-configuration interaction. Journal of Chemical Physics, 2014, 140, 18A503.	1.2	13
1760	Synthesis of Bright Alkenyl-1,2,4-triazoles: A Theoretical and Photophysical Study. ChemPlusChem, 2014, 79, 1489-1497.	1.3	4
1761	Electronic coupling calculations with transition charges, dipoles, and quadrupoles derived from electrostatic potential fitting. Journal of Chemical Physics, 2014, 141, 214105.	1.2	27
1762	A combined resonance enhanced multiphoton ionization and ab initio study of the first absorption band of 1,2,4,5-tetrafluorobenzene, pentafluorobenzene, and hexafluorobenzene. Journal of Chemical Physics, 2014, 141, 154310.	1.2	4
1763	Probing ground and low-lying excited states for HIO ₂ isomers. Journal of Chemical Physics, 2014, 141, 234303.	1.2	8
1764	Electronic Structures, DNA-binding, SAR, and Spectral Properties of Ruthenium Methylimidazole Complexes [Ru(Melm) ₄ L] ²⁺ (L=iip, tip, 2ntz). Chinese Journal of Chemical Physics, 2014, 27, 159-167.	0.6	3
1765	Analytic derivative couplings for spin-flip configuration interaction singles and spin-flip time-dependent density functional theory. Journal of Chemical Physics, 2014, 141, 064104.	1.2	89
1766	Simulations of the dissociation of small helium clusters with <i>ab initio</i> molecular dynamics in electronically excited states. Journal of Chemical Physics, 2014, 140, 134306.	1.2	35
1767	Correlation correction to configuration interaction singles from coupled cluster perturbation theory. Journal of Chemical Physics, 2014, 140, 234108.	1.2	4
1768	Communication: Smoothing out excited-state dynamics: Analytical gradients for dynamically weighted complete active space self-consistent field. Journal of Chemical Physics, 2014, 141, 171102.	1.2	19
1769	Normal-ordered second-quantized Hamiltonian for molecular vibrations. Journal of Chemical Physics, 2014, 141, 184111.	1.2	12

#	ARTICLE	IF	CITATIONS
1770	A systematic approach to vertically excited states of ethylene using configuration interaction and coupled cluster techniques. <i>Journal of Chemical Physics</i> , 2014, 141, 104302.	1.2	41
1771	Nonuniform Continuum Model for Solvatochromism Based on Frozen-Density Embedding Theory. <i>ChemPhysChem</i> , 2014, 15, 3291-3300.	1.0	10
1772	Rational design of outer-expanded purine analogues as building blocks of DNA-based nanowires with enhanced electronic properties. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 911-919.	1.0	0
1773	Strong-field ionization rates of linear polyenes simulated with time-dependent configuration interaction with an absorbing potential. <i>Journal of Chemical Physics</i> , 2014, 141, 174104.	1.2	37
1774	Theoretical study on absorption and emission spectra of size-expanded Janus-type AT nucleobases and effect of base pairing. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 121, 670-677.	2.0	12
1775	Attaching electrons to a 3-ring acene: Structures and dynamics of anions in gas-phase anthracene. <i>International Journal of Mass Spectrometry</i> , 2014, 365-366, 377-383.	0.7	5
1776	Structural, optical, and charge transport properties of cyclopentadithiophene derivatives: a theoretical study. <i>Structural Chemistry</i> , 2014, 25, 715-731.	1.0	18
1777	Luminol: Extended hydrogen bond network in water solution. <i>Computational and Theoretical Chemistry</i> , 2014, 1028, 81-86.	1.1	3
1778	On the mutual exclusion of variationality and size consistency. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	5
1779	Tunable Fluorophores Based on N -Arylimino)pyrrolyl Chelates of Diphenylboron: Synthesis, Structure, Photophysical Characterization, and Application in OLEDs. <i>Chemistry - A European Journal</i> , 2014, 20, 4126-4140.	1.7	36
1780	Theoretical studies on electronic structures and photophysical properties of anthracene derivatives as hole-transporting materials for OLEDs. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 125, 36-45.	2.0	27
1781	Hetero-Wolff Rearrangement of an $\hat{\pm}$ -Sulfinyl Carbene: Thermally Activated Intersystem Crossing of the Lowest Excited Triplet State of a Ground-State Singlet Carbene. <i>European Journal of Organic Chemistry</i> , 2014, 2014, 2297-2304.	1.2	13
1782	Tunable single and dual emission behavior of imidazole fluorophores based on D-A architecture. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2014, 284, 36-48.	2.0	20
1783	Computational Tests of Quantum Chemical Models for Excited and Ionized States of Molecules with Phosphorus and Sulfur Atoms. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3514-3524.	1.1	5
1784	A star-shaped bipolar host material based on carbazole and dimesitylboron moieties for fabrication of highly efficient red, green and blue electrophosphorescent devices. <i>Journal of Materials Chemistry C</i> , 2014, 2, 2160-2168.	2.7	25
1785	Synthesis, characterization and DFT calculation of 4-fluorophenyl substituted tris(8-hydroxyquinoline)aluminum(III) complexes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 118, 66-72.	2.0	20
1786	Synthesis, characterisation and electroluminescence behaviour of π -conjugated imidazole-isoquinoline derivatives. <i>Dyes and Pigments</i> , 2014, 102, 180-188.	2.0	25
1787	Electronic structure and reactivity in water splitting of the iron oxide dimers and their hexacarbonyls: A density functional study. <i>Journal of Chemical Physics</i> , 2014, 140, 024303.	1.2	5

#	ARTICLE	IF	CITATIONS
1788	The Triplet–Singlet Gap in the <i>m</i> -Xylylene Radical: A Not So Simple One. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 335-345.	2.3	56
1789	Dye chemistry with time-dependent density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14334-14356.	1.3	294
1790	Analytical derivative techniques for TDDFT excited-state properties: Theory and application. <i>Science China Chemistry</i> , 2014, 57, 48-57.	4.2	16
1791	Efficient Implementation of Local Excitation Approximation for Treating Excited States of Molecules in Condensed Phase. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5308-5317.	2.3	7
1792	Diabatic Population Matrix Formalism for Performing Molecular Mechanics Style Simulations with Multiple Electronic States. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5238-5253.	2.3	9
1793	Computational evaluation of optoelectronic and photophysical properties of unsymmetrical distyrylbiphenyls. <i>RSC Advances</i> , 2014, 4, 53060-53071.	1.7	19
1794	Ab Initio Implementation of the Frenkel–Davydov Exciton Model: A Naturally Parallelizable Approach to Computing Collective Excitations in Crystals and Aggregates. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5366-5376.	2.3	74
1795	Strong field ionization rates simulated with time-dependent configuration interaction and an absorbing potential. <i>Journal of Chemical Physics</i> , 2014, 140, 174113.	1.2	89
1796	From Ordinary to Blue Emission in Peralkylated <i>n</i> -Oligosilanes: The Calculated Structure of Delocalized and Localized Singlet Excitons. <i>Journal of Physical Chemistry A</i> , 2014, 118, 10538-10553.	1.1	1
1797	Photophysical characteristics of two novel coumarin derivatives: Experimental and theoretical estimation of dipole moments using the solvatochromic shift method. <i>Canadian Journal of Physics</i> , 2014, 92, 1330-1336.	0.4	5
1798	Structural, electronic, and photophysical properties of thieno-expanded tricyclic purine analogs: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 4338.	1.3	6
1799	Computational study of the working mechanism and rate acceleration of overcrowded alkene-based light-driven rotary molecular motors. <i>RSC Advances</i> , 2014, 4, 10240.	1.7	21
1800	Trans–Cis Isomerization of Vinylketones through Triplet 1,2-Biradicals. <i>Journal of Physical Chemistry A</i> , 2014, 118, 10433-10447.	1.1	14
1801	Quenching of the Photoisomerization of Azobenzene Self-Assembled Monolayers by the Metal Substrate. <i>Journal of Physical Chemistry C</i> , 2014, 118, 25906-25917.	1.5	14
1802	Improved description of the orbital relaxation effect by practical use of the self-energy. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 577-586.	1.0	0
1803	Electron-correlated fragment-molecular-orbital calculations for biomolecular and nano systems. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 10310-10344.	1.3	251
1804	Triplet Sensitized Photolysis of a Vinyl Azide: Direct Detection of a Triplet Vinyl Azide and Nitrene. <i>Journal of Organic Chemistry</i> , 2014, 79, 9325-9334.	1.7	20
1805	High Efficiency Light Harvesting by Carotenoids in the LH2 Complex from Photosynthetic Bacteria: Unique Adaptation to Growth under Low-Light Conditions. <i>Journal of Physical Chemistry B</i> , 2014, 118, 11172-11189.	1.2	16

#	ARTICLE	IF	CITATIONS
1806	How Method-Dependent Are Calculated Differences between Vertical, Adiabatic, and $0\text{--}0$ Excitation Energies?. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4157-4171.	1.1	74
1807	Assessment of Various Electronic Structure Methods for Characterizing Temporary Anion States: Application to the Ground State Anions of N_2 , C_2H_2 , C_2H_4 , and C_6H_6 . <i>Journal of Physical Chemistry A</i> , 2014, 118, 7489-7497.	1.1	52
1808	The Variationally Orbital-Adapted Configuration Interaction Singles (VOA-CIS) Approach to Electronically Excited States. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1004-1020.	2.3	36
1809	Two novel indolo[3,2-b]carbazole derivatives containing dimesitylboron moieties: synthesis, photoluminescent and electroluminescent properties. <i>New Journal of Chemistry</i> , 2014, 38, 2368-2378.	1.4	37
1810	Inclusion behaviour of Indole-7-Carboxaldehyde inside β -cyclodextrin: A nano cage. <i>Chemical Physics</i> , 2014, 441, 93-100.	0.9	5
1811	Investigation of the structures, potential energy surface, transition states and vibrational frequencies of a vitamin E precursor-chroman in S_0 and S_1 states: DFT based computational study. <i>Computational and Theoretical Chemistry</i> , 2014, 1049, 115-121.	1.1	9
1812	Excited-State Dynamics of Bis(9-fluorenyl)methane and its Derivative 9-(9-Ethylfluorenyl)-9 $\text{--}9$ -fluorenylmethane: Steric Effect on Energetics and Dynamics of Ground- and Excited-State Conformations. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2269-2278.	1.1	1
1813	Theoretical study of the structural and optical properties of cytosine analogues. <i>Computational and Theoretical Chemistry</i> , 2014, 1049, 75-81.	1.1	10
1814	Theoretical studies of the excited states of p-cyanophenylalanine and comparisons with the natural amino acids phenylalanine and tyrosine. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	4
1815	Theoretical study on absorption and emission spectra of adenine analogues. <i>Journal of Molecular Modeling</i> , 2014, 20, 2100.	0.8	8
1816	Accurate simulation of geometry, singlet-singlet and triplet-singlet excitation of cyclometalated iridium(III) complex. <i>Journal of Molecular Modeling</i> , 2014, 20, 2108.	0.8	5
1817	Regioregular electrochromic polymers based on thienyl derivatives of fluorescent pyrene monomers: Optical properties, spectroelectrochemistry and quantum chemical study. <i>Electrochimica Acta</i> , 2014, 122, 57-65.	2.6	9
1818	Comparison of the Photochemistry of 3-Methyl-2-phenyl-2 <i>H</i> -azirine and 2-Methyl-3-phenyl-2 <i>H</i> -azirine. <i>Journal of Organic Chemistry</i> , 2014, 79, 653-663.	1.7	30
1819	Unrestricted density functional theory based on the fragment molecular orbital method for the ground and excited state calculations of large systems. <i>Journal of Chemical Physics</i> , 2014, 140, 144101.	1.2	19
1820	Introducing many-body physics using atomic spectroscopy. <i>American Journal of Physics</i> , 2014, 82, 113-122.	0.3	27
1821	Ab Initio Nonadiabatic Dynamics of Multichromophore Complexes: A Scalable Graphical-Processing-Unit-Accelerated Exciton Framework. <i>Accounts of Chemical Research</i> , 2014, 47, 2857-2866.	7.6	83
1822	Photophysics, Excited-State Double-Proton Transfer and Hydrogen-Bonding Properties of 5-Deazaalloxazines. <i>Photochemistry and Photobiology</i> , 2014, 90, 972-988.	1.3	5
1823	Density Relaxation in Time-Dependent Density Functional Theory: Combining Relaxed Density Natural Orbitals and Multireference Perturbation Theories for an Improved Description of Excited States. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4014-4024.	2.3	41

#	ARTICLE	IF	CITATIONS
1824	In silico assessment of the HPLC-UV response coefficients. Computational and Theoretical Chemistry, 2014, 1040-1041, 1-5.	1.1	5
1825	Resonance enhanced multiphoton ionization spectroscopy and theoretical calculations of cis- and trans-m-aminostyrene rotamers. Journal of Molecular Structure, 2014, 1058, 205-212.	1.8	4
1826	Enhancement of fluorescence in anthracene by chlorination: Vibronic coupling and transition dipole moment density analysis. Chemical Physics, 2014, 430, 47-55.	0.9	40
1827	A theoretical study on elementary building blocks for organic solar cells – Influence of a donor molecule on electronic spectrum of PCBM. Computational and Theoretical Chemistry, 2014, 1040-1041, 243-258.	1.1	8
1828	Ultrafast X-ray Auger probing of photoexcited molecular dynamics. Nature Communications, 2014, 5, 4235.	5.8	140
1829	The effect of conjugation length distribution on the properties of modified PPV. Journal of Physics and Chemistry of Solids, 2014, 75, 752-758.	1.9	6
1830	Analytical gradients for MP2, double hybrid functionals, and TD- \hat{E} -DFT with polarizable embedding described by fluctuating charges. Journal of Computational Chemistry, 2015, 36, 2271-2290.	1.5	43
1831	Approximating electronically excited states with equation-of-motion linear coupled-cluster theory. Journal of Chemical Physics, 2015, 143, 164103.	1.2	18
1832	Analytic first derivatives of floating occupation molecular orbital-complete active space configuration interaction on graphical processing units. Journal of Chemical Physics, 2015, 143, 014111.	1.2	44
1833	The consequences of improperly describing oscillator strengths beyond the electric dipole approximation. Journal of Chemical Physics, 2015, 143, 234103.	1.2	34
1834	Density function theory study on structures and electronic properties of 2Meq2AlOPh and its derivatives. IOP Conference Series: Materials Science and Engineering, 2015, 87, 012104.	0.3	1
1835	B800-B850 coherence correlates with energy transfer rates in the LH2 complex of photosynthetic purple bacteria. Physical Chemistry Chemical Physics, 2015, 17, 30805-30816.	1.3	12
1836	The somatic autosomal mutation matrix in cancer genomes. Human Genetics, 2015, 134, 851-864.	1.8	16
1837	Identification of vibrational excitations and optical transitions of the organic electron donor tetraphenyldibenzoperiflanthene (DBP). Physical Chemistry Chemical Physics, 2015, 17, 30404-30416.	1.3	16
1838	Distortions of the Xanthophylls Caused by Interactions with Neighboring Pigments and the LHCII Protein Are Crucial for Studying Energy Transfer Pathways within the Complex. Journal of Physical Chemistry B, 2015, 119, 15550-15560.	1.2	5
1839	Modeling electric field-induced quenching in conjugated polymers and oligomers. Proceedings of SPIE, 2015, , .	0.8	1
1840	Application of Time-Dependent Density Functional and Natural Bond Orbital Theories to the UV-vis Absorption Spectra of Some Phenolic Compounds. Journal of Physical Chemistry A, 2015, 119, 9352-9362.	1.1	40
1841	NTChem: A high-performance software package for quantum molecular simulation. International Journal of Quantum Chemistry, 2015, 115, 349-359.	1.0	55

#	ARTICLE	IF	CITATIONS
1842	Two-Photon Spectroscopy of the Q-Bands of <i>meso</i> -Tetraphenyl-Porphyrin and -Chlorin Framework Derivatives. <i>Journal of Physical Chemistry C</i> , 2015, 119, 3711-3724.	1.5	9
1843	New developments in first-principles excited-state dynamics simulations: unveiling the solvent specificity of excited anionic cluster relaxation and electron solvation. <i>Molecular Simulation</i> , 2015, 41, 156-167.	0.9	4
1844	New size-expanded RNA nucleobase analogs: A detailed theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 140, 407-415.	2.0	3
1845	Solvent effect on absorption and fluorescence spectra of cinchonine and cinchonidine dications: Estimation of ground and excited state dipole moments by experimental and numerical studies. <i>Journal of Molecular Liquids</i> , 2015, 206, 159-164.	2.3	10
1846	Theories of phosphorescence in organo-transition metal complexes – From relativistic effects to simple models and design principles for organic light-emitting diodes. <i>Coordination Chemistry Reviews</i> , 2015, 295, 46-79.	9.5	93
1847	Quantum Properties of Small Systems at Equilibrium: First Principle Calculations. , 2015, , 61-110.		0
1848	Synthesis, aggregation-induced emission and electroluminescence properties of a novel compound containing tetraphenylethene, carbazole and dimesitylboron moieties. <i>Journal of Materials Chemistry C</i> , 2015, 3, 9095-9102.	2.7	17
1849	Angle-Dependent Ionization of Small Molecules by Time-Dependent Configuration Interaction and an Absorbing Potential. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 2140-2146.	2.1	56
1850	Experimental and Theoretical Study of O-Substituent Effect on the Fluorescence of 8-Hydroxyquinoline. <i>International Journal of Molecular Sciences</i> , 2015, 16, 3804-3819.	1.8	4
1851	3(2H)-Furanone as a promising scaffold for the synthesis of novel fluorescent organic dyes: an experimental and theoretical investigation. <i>New Journal of Chemistry</i> , 2015, 39, 6667-6676.	1.4	12
1852	Optical properties and electronic transitions of DNA oligonucleotides as a function of composition and stacking sequence. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 4589-4599.	1.3	17
1853	Transfer of Frequency-Dependent Polarizabilities: A Tool To Simulate Absorption and Circular Dichroism Molecular Spectra. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2210-2220.	2.3	4
1854	Why Do TD-DFT Excitation Energies of BODIPY/Aza-BODIPY Families Largely Deviate from Experiment? Answers from Electron Correlated and Multireference Methods. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2619-2632.	2.3	166
1855	Modeling Field-Induced Quenching in Poly(<i>p</i> -phenylene vinylene) Polymers and Oligomers. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7625-7634.	1.2	4
1856	Experimental and theoretical study: Determination of dipole moment of synthesized coumarin-triazole derivatives and application as turn off fluorescence sensor: High sensitivity for iron(III) ions. <i>Sensors and Actuators B: Chemical</i> , 2015, 220, 1266-1278.	4.0	51
1857	Laser-Driven Hole Trapping in a Ge/Si Core-Shell Nanocrystal: An Atomistic Configuration Interaction Perspective. <i>Journal of Physical Chemistry C</i> , 2015, 119, 25606-25614.	1.5	15
1858	Polyazomethine as a component of solar cells-theoretical and optical study. <i>Journal of Physics and Chemistry of Solids</i> , 2015, 86, 186-193.	1.9	13
1859	Configuration interaction singles natural orbitals: An orbital basis for an efficient and size intensive multireference description of electronic excited states. <i>Journal of Chemical Physics</i> , 2015, 142, 024102.	1.2	43

#	ARTICLE	IF	CITATIONS
1860	An atomic orbital-based formulation of the complete active space self-consistent field method on graphical processing units. <i>Journal of Chemical Physics</i> , 2015, 142, 224103.	1.2	98
1861	Experimental and theoretical studies of acetatodi(methylcyano)bis(O, O ² -dialkyl and alkylene) Tj ETQq1 1 0.784314 rgBT /Qoverlock 10	1.0	3
1862	Relay proton transfer triggered twisted intramolecular charge transfer. <i>Photochemical and Photobiological Sciences</i> , 2015, 14, 2225-2237.	1.6	26
1863	A computational study of the interaction between dopamine and DNA/RNA nucleosides. <i>Journal of Molecular Modeling</i> , 2015, 21, 241.	0.8	3
1864	Energy-Specific Equation-of-Motion Coupled-Cluster Methods for High-Energy Excited States: Application to <i>K</i> -edge X-ray Absorption Spectroscopy. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4146-4153.	2.3	92
1865	Integration Approach at the Second-Order Perturbation Theory: Applications to Ionization Potential and Electron Affinity Calculations. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4677-4688.	2.3	14
1866	Highly accurate excited-state energies from direct computation of the 2-electron reduced density matrix by the anti-Hermitian contracted Schrödinger equation. <i>Molecular Physics</i> , 0, , 1-9.	0.8	6
1867	An ab initio molecular dynamics analysis of lignin as a potential antioxidant for hydrocarbons. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 62, 325-341.	1.3	11
1868	Theoretical Calculations of Excitation Energy Transfer. , 2015, , 761-777.		3
1869	Superposition of Fragment Excitations for Excited States of Large Clusters with Application to Helium Clusters. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5791-5803.	2.3	18
1870	Photolysis of acetophenone derivatives with $\hat{\pm}$ cyclopropyl substituents. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 137-146.	0.9	1
1871	Synthesis and nonvolatile memristive switching effect of a donor-acceptor structured oligomer. <i>Journal of Materials Chemistry C</i> , 2015, 3, 664-673.	2.7	29
1872	Theoretical study on absorption and emission spectra of pyrrolo-C analogues. <i>Journal of Molecular Structure</i> , 2015, 1079, 321-326.	1.8	5
1873	TD-DFT Assessment of the Excited State Intramolecular Proton Transfer in Hydroxyphenylbenzimidazole (HBI) Dyes. <i>Journal of Physical Chemistry B</i> , 2015, 119, 2180-2192.	1.2	55
1874	Chemical linkage functions of poly(ether imide)s on the resistive switching memory effects. <i>Organic Electronics</i> , 2015, 16, 148-163.	1.4	9
1875	Synthesis, spectroscopic characterization and photophysics of a novel environmentally sensitive dye 3-naphthyl-1-phenyl-5-(4-carboxyphenyl)-2-pyrazoline. <i>Journal of Luminescence</i> , 2015, 159, 9-16.	1.5	26
1876	Phototautomerization on the Singlet and Triplet Surface in <i>o</i> -Hydroxyacetophenone Derivatives in Polar Solvents. <i>Journal of Physical Chemistry B</i> , 2015, 119, 2668-2676.	1.2	9
1877	Analytic gradients, geometry optimization and excited state potential energy surfaces from the particle-particle random phase approximation. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 1025-1038.	1.3	21

#	ARTICLE	IF	CITATIONS
1878	Effects of Electronic-State-Dependent Solute Polarizability: Application to Solute-Pump/Solvent-Probe Spectra. <i>Journal of Physical Chemistry B</i> , 2015, 119, 9129-9139.	1.2	8
1879	Theoretical Study of the Nontraditional Enol-Based Photoacidity of Firefly Oxyluciferin. <i>ChemPhysChem</i> , 2015, 16, 455-464.	1.0	18
1880	Thioflavin T derivatives for the characterization of insulin and lysozyme amyloid fibrils in vitro: Fluorescence and quantum-chemical studies. <i>Journal of Luminescence</i> , 2015, 159, 284-293.	1.5	19
1881	Photochemistry of Matrix Isolated (Trifluoromethyl)sulfonyl Azide, CF ₃ SO ₂ N ₃ . <i>Journal of Physical Chemistry A</i> , 2015, 119, 2281-2288.	1.1	27
1882	Chemexcitation Induced Proton Transfer: Enolate Oxyluciferin as the Firefly Bioluminophore. <i>Journal of Physical Chemistry B</i> , 2015, 119, 2140-2148.	1.2	27
1883	Electronic Excitations in Nonpolar Solvents: Can the Polarizable Continuum Model Accurately Reproduce Solvent Effects?. <i>Journal of Physical Chemistry B</i> , 2015, 119, 8984-8991.	1.2	23
1884	Electronic Absorption Spectra and Solvatochromic Shifts by the Vertical Excitation Model: Solvated Clusters and Molecular Dynamics Sampling. <i>Journal of Physical Chemistry B</i> , 2015, 119, 958-967.	1.2	68
1886	Interaction of Radiation and Matter and Electronic Spectra. , 2016, , 291-337.		1
1887	Development of massive multilevel molecular dynamics simulation program, platypus (PLATform for) Tj ETQqO O O rgBT /Overlock 10 Tf s Computational Chemistry, 2016, 37, 1125-1132.	1.5	7
1888	Methanesulfonyl Azide: Molecular Structure and Photolysis in Solid Noble Gas Matrices. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5590-5597.	1.1	16
1889	Dexter energy transfer pathways. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 8115-8120.	3.3	105
1890	Celebrating Our 120th Anniversary. <i>Journal of Physical Chemistry B</i> , 2016, 120, 12417-12419.	1.2	1
1891	Celebrating Our 120th Anniversary. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4977-4979.	2.1	0
1892	Ultrafast photoelectron migration in dye-sensitized solar cells: Influence of the binding mode and many-body interactions. <i>Journal of Chemical Physics</i> , 2016, 145, 174704.	1.2	19
1893	Dual hydrogen-bonding motifs in complexes formed between tropolone and formic acid. <i>Journal of Chemical Physics</i> , 2016, 145, 204303.	1.2	7
1894	Implementation of INDO/SCI with COSMO Implicit Solvation and Benchmarking for Solvatochromic Shifts. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9878-9885.	1.1	6
1895	Celebrating Our 120th Anniversary. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9679-9681.	1.1	3
1896	Celebrating Our 120th Anniversary. <i>Journal of Physical Chemistry C</i> , 2016, 120, 27731-27733.	1.5	0

#	ARTICLE	IF	CITATIONS
1897	A new approach to approximate equation-of-motion coupled cluster with triple excitations. <i>Journal of Chemical Physics</i> , 2016, 145, 124102.	1.2	70
1898	Assessment of a composite CC2/DFT procedure for calculating 0 $\hat{=}$ 0 excitation energies of organic molecules. <i>Molecular Physics</i> , 2016, 114, 3448-3463.	0.8	20
1899	Multi-state extrapolation of UV/Vis absorption spectra with QM/QM hybrid methods. <i>Journal of Chemical Physics</i> , 2016, 144, 184102.	1.2	5
1900	Accelerating molecular property calculations with nonorthonormal Krylov space methods. <i>Journal of Chemical Physics</i> , 2016, 144, 174105.	1.2	50
1901	Targeting excited states in all-trans polyenes with electron-pair states. <i>Journal of Chemical Physics</i> , 2016, 145, 234105.	1.2	35
1902	Switching between cis and trans anions of 2-(2 $\hat{=}$ -hydroxyphenyl)benzimidazole: a molecular rotation perturbed by chemical stabilization. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11081-11090.	1.3	14
1903	Ultraviolet vision: photophysical properties of the unprotonated retinyl Schiff base in the Siberian hamster cone pigment. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	5
1904	Controlling charge separation and recombination by chemical design in donor $\hat{=}$ acceptor dyads. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 18536-18548.	1.3	16
1905	Electronic spectroscopy of some isoelectronic MM $\hat{=}$ (CO)10 (M, M $\hat{=}$ = Mn, Cr, Tc, Mo, Re, W) from time-dependent density functional theory. <i>Molecular Physics</i> , 2016, 114, 1794-1805.	0.8	3
1906	Origin of the Red-Shifted Optical Spectra Recorded for Aza-BODIPY Dyes. <i>Journal of Physical Chemistry A</i> , 2016, 120, 2537-2546.	1.1	44
1907	MN15: A Kohn $\hat{=}$ Sham global-hybrid exchange $\hat{=}$ correlation density functional with broad accuracy for multi-reference and single-reference systems and noncovalent interactions. <i>Chemical Science</i> , 2016, 7, 5032-5051.	3.7	858
1908	New low band-gap conjugated organic materials based on fluorene, thiophene and phenylene for photovoltaic applications: Theoretical study. <i>Materials Today: Proceedings</i> , 2016, 3, 2578-2586.	0.9	5
1909	Experimental and theoretical study of stereochemistry for new pseurotin A3 with an unusual hetero-spirocyclic system. <i>Tetrahedron</i> , 2016, 72, 7194-7199.	1.0	7
1910	An Effective Procedure for Analyzing Molecular Vibrations in Terms of Local Fragment Modes. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4768-4777.	2.3	12
1911	An unusual deprotonation trend in 2-(2 $\hat{=}$ -hydroxyphenyl)pyridoimidazoles. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 29905-29913.	1.3	5
1912	Overlapping Electronic States with Nearly Parallel Transition Dipole Moments in Reduced Anionic Flavin Can Distort Photobiological Dynamics. <i>Journal of the American Chemical Society</i> , 2016, 138, 14880-14889.	6.6	12
1913	A Multichannel Least-Squares B-Spline Approach to Molecular Photoionization: Theory, Implementation, and Applications within the Configuration $\hat{=}$ Interaction Singles Approximation. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4996-5008.	2.3	34
1914	Extending Hexaazatriphenylene with Mono-/Bithiophenes in Acceptor $\hat{=}$ Donor Diads and Acceptor $\hat{=}$ Donor $\hat{=}$ Acceptor Triads. <i>Journal of Physical Chemistry C</i> , 2016, 120, 23276-23285.	1.5	5

#	ARTICLE	IF	CITATIONS
1915	Synthesis, aggregation-induced emission and electroluminescence properties of two new tetraphenylethene derivatives. <i>Tetrahedron Letters</i> , 2016, 57, 4428-4434.	0.7	14
1916	Using Molecular Architecture to Control the Reactivity of a Triplet Vinylnitrene. <i>Journal of the American Chemical Society</i> , 2016, 138, 14905-14914.	6.6	28
1917	Theoretical study of selenium and tellurium impurities in (ZnO) ₆ clusters using DFT and TDDFT. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1862-1871.	1.0	5
1918	Synthesis, aggregation-induced emission, and electroluminescence properties of a novel emitter comprising tetraphenylethene and carbazole moieties. <i>Synthetic Metals</i> , 2016, 220, 356-361.	2.1	3
1919	Generalized Energy-Based Fragmentation Approach for Localized Excited States of Large Systems. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9667-9677.	1.1	28
1920	TD-M06-2X insights into the absorption and emission spectra of dichlorvos and its molecularly imprinted recognition by methacrylic acid. <i>Journal of Molecular Modeling</i> , 2016, 22, 282.	0.8	5
1921	Computational calculations of substitution pattern effects on the optical properties of benzobis(thiadiazole) derivatives as near-infrared-emitting organic compounds. <i>Computational and Theoretical Chemistry</i> , 2016, 1098, 31-40.	1.1	4
1922	Analytic formulation of derivative coupling vectors for complete active space configuration interaction wavefunctions with floating occupation molecular orbitals. <i>Journal of Chemical Physics</i> , 2016, 145, 174110.	1.2	35
1923	Controlling the high frequency response of H ₂ by ultra-short tailored laser pulses: A time-dependent configuration interaction study. <i>Journal of Chemical Physics</i> , 2016, 144, 044301.	1.2	11
1924	Photoenolization of <i>cis</i> -Methylvalerophenone Ester Derivative. <i>Photochemistry and Photobiology</i> , 2016, 92, 388-398.	1.3	6
1925	Brianyoungite/Graphene Oxide Coordination Composites for High-Performance Cu ²⁺ Adsorption and Tunable Deep-Red Photoluminescence. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 15848-15854.	4.0	19
1926	A DFT study of solvent effects on the kinetics and mechanism of the [3,3] hetero-Cope rearrangement of 1-butene thiobenzoate. <i>Progress in Reaction Kinetics and Mechanism</i> , 2016, 41, 153-158.	1.1	3
1927	Absorption and emission spectroscopic characteristics of dipterex and its molecularly imprinted recognition: A TD-DFT investigation. <i>Chemical Physics Letters</i> , 2016, 652, 93-97.	1.2	6
1928	Complementary study based on DFT to describe the structure and properties relationship of diblock copolymer based on PVK and PPV. <i>Physica B: Condensed Matter</i> , 2016, 497, 45-50.	1.3	11
1929	“Balancing” the Block Davidson–Liu Algorithm. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3003-3007.	2.3	23
1930	Cyclometalated gold(III) trioxadiborin complexes: studies of the bonding and excited states. <i>Dalton Transactions</i> , 2016, 45, 3820-3830.	1.6	10
1931	DFT Study on the Mechanism and Stereoselectivity of NHC-Catalyzed Synthesis of Substituted Trifluoromethyl Dihydropyranones with Contiguous Stereocenters. <i>Journal of Organic Chemistry</i> , 2016, 81, 868-877.	1.7	28
1932	Photochemical dissociation of HOBr. A nonadiabatic dynamics study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2016, 324, 8-13.	2.0	4

#	ARTICLE	IF	CITATIONS
1933	Analytical gradients for excitation energies from frozen-density embedding. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20955-20975.	1.3	15
1934	Two novel phenylethene-carbazole derivatives containing dimesitylboron groups: Aggregation-induced emission and electroluminescence properties. <i>Dyes and Pigments</i> , 2016, 128, 304-313.	2.0	10
1935	Quantum Mechanical Studies on the Photophysics and the Photochemistry of Nucleic Acids and Nucleobases. <i>Chemical Reviews</i> , 2016, 116, 3540-3593.	23.0	375
1936	Emission shaping in fluorescent proteins: role of electrostatics and π -stacking. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 3944-3955.	1.3	24
1937	Energy transfer upconversion dynamics in YVO ₄ :Yb ³⁺ ,Er ³⁺ . <i>Journal of Luminescence</i> , 2016, 170, 560-570.	1.5	44
1938	Quantum and classical dynamics of reactive scattering of H ₂ from metal surfaces. <i>Chemical Society Reviews</i> , 2016, 45, 3658-3700.	18.7	137
1939	The decomposition of benzenesulfonyl azide: a matrix isolation and computational study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 3792-3799.	1.3	20
1940	Conformational landscape, stability, potential energy curves and vibrations of 1,2,3,4 tetrahydroquinoline. <i>Journal of Molecular Structure</i> , 2017, 1136, 80-89.	1.8	11
1941	Theoretical investigation of oligomer structure and optoelectronic properties for [4-(methoxyphenyl)acetonitrile] _n (n=1-5). <i>Journal of Molecular Modeling</i> , 2017, 23, 41.	0.8	4
1942	Calculation of Excited States: Molecular Photophysics and Photochemistry on Display. , 2017, , 639-725.		1
1943	Guide to Programs for Nonrelativistic Quantum Chemistry Calculations. , 2017, , 861-883.		1
1944	Improved Complete Active Space Configuration Interaction Energies with a Simple Correction from Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1130-1146.	2.3	26
1945	Reproduction and interpretation of the UV-vis spectra of some flavonoids. <i>Chemical Papers</i> , 2017, 71, 543-552.	1.0	19
1946	Can Förster Theory Describe Stereoselective Energy Transfer Dynamics in a Protein-Ligand Complex?. <i>Journal of Physical Chemistry B</i> , 2017, 121, 2265-2278.	1.2	10
1947	Singlet Photoreactivity of 3-Methyl-2-phenyl-2H-azirine. <i>Australian Journal of Chemistry</i> , 2017, 70, 413.	0.5	10
1948	Rational Design of Advanced Photosensitizers Based on Orthogonal BODIPY Dimers to Finely Modulate Singlet Oxygen Generation. <i>Chemistry - A European Journal</i> , 2017, 23, 4837-4848.	1.7	87
1949	Simulating the absorption spectra of helium clusters (N=70, 150, 231, 300) using a charge transfer correction to superposition of fragment single excitations. <i>Journal of Chemical Physics</i> , 2017, 146, 044111.	1.2	11
1950	Photodissociation of FONO: an excited state nonadiabatic dynamics study. <i>Journal of Molecular Modeling</i> , 2017, 23, 77.	0.8	0

#	ARTICLE	IF	CITATIONS
1951	A new efficient method for the calculation of interior eigenpairs and its application to vibrational structure problems. <i>Journal of Chemical Physics</i> , 2017, 146, 124101.	1.2	32
1952	An open-source framework for analyzing <i>N</i> -electron dynamics. I. Multideterminantal wave functions. <i>Journal of Computational Chemistry</i> , 2017, 38, 1515-1527.	1.5	47
1953	Efficient and accurate modeling of electron photoemission in nanostructures with TDDFT. <i>European Physical Journal B</i> , 2017, 90, 1.	0.6	32
1954	Experimental and theoretical studies on fluvastatin primary photoproduct formation. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21946-21954.	1.3	4
1955	Capturing Conformation-Dependent Photoreactivity of Crystalline 3-Azido-1,3-diphenylisobutyrophenone. <i>ChemPhotoChem</i> , 2017, 1, 408-414.	1.5	0
1956	Photophysical properties of the isomorphous emissive RNA nucleobase analogues and effect of water solution, ribose, and base pairing: A theoretical study. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25377.	1.0	7
1957	Investigating cyclic sotolon, maple furanone and their dimers in solution using optical rotation, electronic circular dichroism and vibrational circular dichroism. <i>Tetrahedron</i> , 2017, 73, 2432-2438.	1.0	5
1958	TD-DFT benchmark: Excited states of atoms and atomic ions. <i>Computational and Theoretical Chemistry</i> , 2017, 1108, 50-56.	1.1	12
1959	Contrasting Photolytic and Thermal Decomposition of Phenyl Azidoformate: The Curtius Rearrangement Versus Intramolecular C-H Amination. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8604-8613.	1.1	12
1960	Oxidation of Trialkylamines by BrCCl ₃ : Scope, Applications and Mechanistic Aspects. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 6966-6974.	1.2	21
1961	A low-cost approach to electronic excitation energies based on the driven similarity renormalization group. <i>Journal of Chemical Physics</i> , 2017, 147, 074107.	1.2	12
1962	Cryogenic Photochemical Synthesis and Electronic Spectroscopy of Cyanotetracetylene. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7374-7384.	1.1	11
1963	Correlated natural transition orbital framework for low-scaling excitation energy calculations (CorNFLEX). <i>Journal of Chemical Physics</i> , 2017, 146, 214114.	1.2	20
1964	The hypothiocyanite radical OSCN and its isomers. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 16713-16720.	1.3	6
1965	Synthesis, Linear, and Nonlinear Optical Properties of Phosphonato-Substituted Bithiophenes Derived from 2,2-Dimethyl-1,3-propanediol. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 4077-4093.	1.0	0
1966	An open-source framework for analyzing <i>N</i> -electron dynamics. II. Hybrid density functional theory/configuration interaction methodology. <i>Journal of Computational Chemistry</i> , 2017, 38, 2378-2387.	1.5	45
1967	Laser flash photolysis of nanocrystalline \pm -azido-p-methoxy-acetophenone. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 7380-7386.	1.5	6
1968	Two trans-1-(9-anthryl)-2-phenylethene derivatives as blue-green emitting materials for highly bright organic light-emitting diodes application. <i>Organic Electronics</i> , 2017, 50, 228-238.	1.4	11

#	ARTICLE	IF	CITATIONS
1969	Electronic Properties and Electroluminescent OLED Performance of Panchromatic Emissive <i>N</i> -Aryl-2,3-naphthalimides. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9708-9719.	1.1	10
1970	Complete active space configuration interaction from state-averaged configuration interaction singles natural orbitals: Analytic first derivatives and derivative coupling vectors. <i>Journal of Chemical Physics</i> , 2017, 147, 094104.	1.2	25
1971	The quest for best suited references for configuration interaction singles calculations of core excited states. <i>Journal of Computational Chemistry</i> , 2017, 38, 116-126.	1.5	12
1972	\tilde{f} -SCF: A direct energy-targeting method to mean-field excited states. <i>Journal of Chemical Physics</i> , 2017, 147, 214104.	1.2	50
1973	DFT and TD-DFT study on the optical and electronic properties of derivatives of 1,4-bis(2-substituted-1,3,4-oxadiazole)benzene. <i>Arabian Journal of Chemistry</i> , 2017, 10, S2988-S2993.	2.3	33
1974	Surface Adsorption. , 2017, , 387-416.		4
1975	Theoretical study of chromophores for biological sensing: Understanding the mechanism of rhodol based multi-chromophoric systems. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 198, 123-135.	2.0	1
1976	Near-IR luminescence characteristics of monovalent bismuth in Bi-doped pure silica optical fiber: First-principle study. <i>Journal of Luminescence</i> , 2018, 198, 384-388.	1.5	21
1977	Development of the Fragment Molecular Orbital Method for Calculating Nonlocal Excitations in Large Molecular Systems. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3886-3898.	1.1	28
1978	Energy decomposition analysis for exciplexes using absolutely localized molecular orbitals. <i>Journal of Chemical Physics</i> , 2018, 148, 064105.	1.2	36
1979	Atomic Structures and Electronic States of Divalent Bismuth in Bi-Doped Silica Optical Fiber. <i>IEEE Journal of Selected Topics in Quantum Electronics</i> , 2018, 24, 1-5.	1.9	6
1980	Simple Models for Difficult Electronic Excitations. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1501-1509.	2.3	133
1981	A combined theoretical and experimental investigation on the influence of the bromine substitution pattern on the photophysics of conjugated organic chromophores. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 3768-3783.	1.3	17
1982	Using Density Based Indexes and Wave Function Methods for the Description of Excited States: Excited State Proton Transfer Reactions as a Test Case. <i>Journal of Physical Chemistry A</i> , 2018, 122, 375-382.	1.1	12
1983	Benchmarking Excited-State Calculations Using Exciton Properties. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 710-725.	2.3	128
1984	Photochemically Induced Intramolecular Radical Cyclization Reactions with Imines. <i>Journal of Organic Chemistry</i> , 2018, 83, 1867-1875.	1.7	16
1985	Serenity: A subsystem quantum chemistry program. <i>Journal of Computational Chemistry</i> , 2018, 39, 788-798.	1.5	57
1986	Experimental and theoretical study of donor-acceptor compounds based on malononitrile. <i>Chemistry Central Journal</i> , 2018, 12, 26.	2.6	12

#	ARTICLE	IF	CITATIONS
1987	A study on excited-state properties of conjugated polymers using the Pariser-Parr-Pople-Peierls model combined with configuration-interaction-singles. <i>Organic Electronics</i> , 2018, 57, 277-284.	1.4	6
1988	Influence of Ring Structures on Optical Properties of Trivalent Bismuth in Bi-Doped Silica Optical Fiber. <i>Journal of Cluster Science</i> , 2018, 29, 861-865.	1.7	10
1989	A Novel <i>trans</i> -1-(9-Anthryl)-2-phenylethene Derivative Containing a Phenanthroimidazole Unit for Application in Organic Light-Emitting Diodes. <i>Chemistry - an Asian Journal</i> , 2018, 13, 81-88.	1.7	14
1990	The role of the π -holes in stability of non-bonded chalcogenide π -benzene interactions: the ground and excited states. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 299-306.	1.3	10
1991	Photophysical properties of acetylene-linked <i>syn</i> bimane oligomers: a molecular photonic wire. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 1150-1163.	1.3	1
1992	Comparison between the Bethe-Salpeter Equation and Configuration Interaction Approaches for Solving a Quantum Chemistry Problem: Calculating the Excitation Energy for Finite 1D Hubbard Chains. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 527-542.	2.3	8
1993	Chloro- and Dichloro-methylsulfonyl Nitrenes: Spectroscopic Characterization, Photoisomerization, and Thermal Decomposition. <i>Molecules</i> , 2018, 23, 3312.	1.7	4
1994	Thousand-atom <i>ab initio</i> calculations of excited states at organic/organic interfaces: toward first-principles investigations of charge photogeneration. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 26443-26452.	1.3	7
1995	Communication: Becke's virial exciton model gives accurate charge-transfer excitation energies. <i>Journal of Chemical Physics</i> , 2018, 149, 231101.	1.2	9
1996	Order and disorder in (<i>E</i>)-[1-(biphenyl-4-yl)ethylidene]hydrazine: a structural, spectroscopic and theoretical study. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2018, 74, 1459-1468.	0.2	0
1997	A model hamiltonian tuned toward high level <i>ab initio</i> calculations to describe the character of excitonic states in perylenebisimide aggregates. <i>Journal of Computational Chemistry</i> , 2018, 39, 1979-1989.	1.5	14
1998	Decomposition of Sulfonyl Azide Isocyanate and Sulfonyl Diazide: The Oxygen-Shifted Curtius Rearrangement via Sulfonyl Nitrenes. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8511-8519.	1.1	9
1999	Management of transition dipoles in organic hole-transporting materials under solar irradiation for perovskite solar cells. <i>Nature Communications</i> , 2018, 9, 4537.	5.8	64
2000	Energy Decomposition Analysis for Excimers Using Absolutely Localized Molecular Orbitals within Time-Dependent Density Functional Theory and Configuration Interaction with Single Excitations. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5156-5168.	2.3	22
2001	Excited-State Spectra of Strongly Correlated Molecules from a Reduced-Density-Matrix Approach. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 5373-5378.	2.1	14
2002	Pendular alignment and strong chemical binding are induced in helium dimer molecules by intense laser fields. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E9058-E9066.	3.3	7
2003	Unraveling substituent effects on frontier orbitals of conjugated molecules using an absolutely localized molecular orbital based analysis. <i>Chemical Science</i> , 2018, 9, 8598-8607.	3.7	46
2004	Modeling the effects of molecular disorder on the properties of Frenkel excitons in organic molecular semiconductors. <i>Journal of Chemical Physics</i> , 2018, 149, 094110.	1.2	14

#	ARTICLE	IF	CITATIONS
2005	A new fundamental type of conformational isomerism. <i>Nature Chemistry</i> , 2018, 10, 615-624.	6.6	33
2006	Sulfamoyl nitrenes: singlet or triplet ground state?. <i>Chemical Communications</i> , 2018, 54, 6136-6139.	2.2	10
2007	Syntheses, density functional and sparkle PM6 semi empirical theoretical studies of O, π -dialkyl/alkylenedithiophosphate derivatives of tin(IV) phthalocyanine adducts. <i>Journal of Molecular Structure</i> , 2018, 1167, 294-304.	1.8	3
2008	Linear-Response Density Cumulant Theory for Excited Electronic States. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4097-4108.	2.3	8
2009	A Mountaineering Strategy to Excited States: Highly Accurate Reference Energies and Benchmarks. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4360-4379.	2.3	211
2010	Time-Dependent Configuration Interaction Using the Graphical Unitary Group Approach: Nonlinear Electric Properties. <i>Advances in Quantum Chemistry</i> , 2018, 76, 295-313.	0.4	19
2012	Non-orthogonal configuration interaction with single substitutions for the calculation of core-excited states. <i>Journal of Chemical Physics</i> , 2018, 149, 044116.	1.2	44
2013	The effect of substituents on energy splitting in organic radicals: Quantitative cognizance from ab initio studies. <i>Chemical Physics</i> , 2018, 513, 230-240.	0.9	0
2014	Triplet \leftrightarrow Triplet Coupling in Chromophore Dimers: Theory and Experiment. <i>Journal of Physical Chemistry A</i> , 2018, 122, 6713-6723.	1.1	7
2015	Multireference Approaches for Excited States of Molecules. <i>Chemical Reviews</i> , 2018, 118, 7293-7361.	23.0	287
2016	Excitation energies from diffusion Monte Carlo using selected configuration interaction nodes. <i>Journal of Chemical Physics</i> , 2018, 149, 034108.	1.2	50
2017	Combining Wave Function Methods with Density Functional Theory for Excited States. <i>Chemical Reviews</i> , 2018, 118, 7249-7292.	23.0	166
2018	Phenylsulfinyl Radical: Gas-Phase Generation, Photoisomerization, and Oxidation. <i>Journal of the American Chemical Society</i> , 2018, 140, 9972-9978.	6.6	18
2019	Quantitative modeling of energy dissipation in <i>Arabidopsis thaliana</i> . <i>Environmental and Experimental Botany</i> , 2018, 154, 99-109.	2.0	9
2020	Excitation energies of embedded open-shell systems: Unrestricted frozen-density-embedding time-dependent density-functional theory. <i>Journal of Chemical Physics</i> , 2018, 149, 074102.	1.2	12
2021	Synthesis and Electronic Phosphorescence of Dicyanooctatetrayne (NC ₁₀ N) in Cryogenic Matrixes. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5580-5588.	1.1	3
2022	General Approach for Multireference Ground and Excited States Using Nonorthogonal Configuration Interaction. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4851-4861.	2.3	15
2023	Analytic gradients for the single-reference driven similarity renormalization group second-order perturbation theory. <i>Journal of Chemical Physics</i> , 2019, 151, 044118.	1.2	7

#	ARTICLE	IF	CITATIONS
2024	Formation and Reactivity of Triplet Vinylnitrenes as a Function of Ring Size. <i>Journal of Organic Chemistry</i> , 2019, 84, 9215-9225.	1.7	4
2025	Dibenzo-p-dioxin. Twisted and puckered excited state molecular geometries. <i>Computational and Theoretical Chemistry</i> , 2019, 1164, 112551.	1.1	1
2026	Combined Density Functional and Algebraic-Diagrammatic Construction Approach for Accurate Excitation Energies and Transition Moments. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4440-4453.	2.3	21
2027	Coupled Cluster Theory with Induced Dipole Polarizable Embedding for Ground and Excited States. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4485-4496.	2.3	13
2028	Photodecomposition of Thienylsulfonyl Azides: Generation and Spectroscopic Characterization of Triplet Thienylsulfonyl Nitrenes and 3-Thienylnitrene. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9311-9320.	1.1	7
2029	Photochemistry of (η^3 -allyl)Ru(CO) ₃ X Precursors for Photoassisted Chemical Vapor Deposition. <i>Organometallics</i> , 2019, 38, 4363-4370.	1.1	4
2030	Multi-copper incorporation into ring-expanded base pairs: An ab initio study. <i>Chemical Physics Letters</i> , 2019, 734, 136704.	1.2	0
2031	The electronically excited states of cyclooctatetraene—An analysis of the vacuum ultraviolet absorption spectrum by <i>ab initio</i> configuration interaction methods. <i>Journal of Chemical Physics</i> , 2019, 151, 084304.	1.2	11
2032	Calculation of Free-Energy Barriers with TD-DFT: A Case Study on Excited-State Proton Transfer in Indigo. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8485-8495.	1.1	16
2033	Modelling the absorption properties of polycyclic aromatic hydrocarbons and derivatives over three European cities by TD-DFT calculations. <i>Science of the Total Environment</i> , 2019, 695, 133881.	3.9	10
2034	Synthesis and photophysical properties of conjugated (dodecyl)benzoateethynylene macromolecules: staining of <i>Bacillus subtilis</i> and <i>Escherichia coli</i> rhizobacteria. <i>New Journal of Chemistry</i> , 2019, 43, 3332-3340.	1.4	5
2035	Reduced-Scaling Approach for Configuration Interaction Singles and Time-Dependent Density Functional Theory Calculations Using Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1690-1704.	2.3	10
2036	Reference Energies for Double Excitations. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1939-1956.	2.3	116
2037	Optical absorption of Bi ²⁺ -ODC(II) active center in Bi-doped silica optical fiber. <i>Journal of Luminescence</i> , 2019, 213, 304-309.	1.5	13
2038	Discriminating organic isomers by high harmonic generation: A time-dependent configuration interaction singles study. <i>Journal of Chemical Physics</i> , 2019, 150, 234114.	1.2	21
2039	Geometric and Optical Properties of Cluster Model of Yb-doped Silica Optical Fiber. <i>Journal of Cluster Science</i> , 2019, 30, 1205-1210.	1.7	7
2040	Electronic Excitations of Polythiophene within Many-Body Perturbation Theory with and without the Tamm-Dancoff Approximation. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4547-4554.	2.3	14
2041	Computational Investigation of the Pseudo Jahn-Teller Effect on the Structure and Chemical Properties of Perhaloethene Anions. <i>Journal of Structural Chemistry</i> , 2019, 60, 736-745.	0.3	2

#	ARTICLE	IF	CITATIONS
2042	QM/MM Benchmarking of Cyanobacteriochrome Slr1393g3 Absorption Spectra. <i>Molecules</i> , 2019, 24, 1720.	1.7	24
2043	Applications of molecular modeling to flavoproteins: Insights and challenges. <i>Methods in Enzymology</i> , 2019, 620, 277-314.	0.4	9
2044	Non-Orthogonal Configuration Interaction with Single Substitutions for Core-Excited States: An Extension to Doublet Radicals. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2966-2973.	2.3	39
2045	Half-Projected $\tilde{I}f$ Self-Consistent Field For Electronic Excited States. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2954-2965.	2.3	25
2046	Excited-State Potential Energy Surfaces, Conical Intersections, and Analytical Gradients from Ground-State Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2538-2545.	2.1	23
2047	Quantum-chemical characterization of ion-pairing effect on the linear and third-order nonlinear optical response in cyanine dyes. <i>Journal of Molecular Structure</i> , 2019, 1186, 127-136.	1.8	6
2048	Spectroscopic Characterization of Nicotinoyl and Isonicotinoyl Nitrenes and the Photointerconversion of 4-Pyridylnitrene with Diazacycloheptatetraene. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3793-3801.	1.1	5
2049	Multifunctional Copper(I) Coordination Polymers with Aromatic Mono- and Ditopic Thioamides. <i>Inorganic Chemistry</i> , 2019, 58, 3290-3301.	1.9	42
2050	Vibrational Relaxation in Carotenoids as an Explanation for Their Rapid Optical Properties. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2203-2209.	1.2	15
2051	Absorption-emission symmetry breaking and the different origins of vibrational structures of the 1Qy and 1Qx electronic transitions of pheophytin $\langle i \rangle a \langle /i \rangle$. <i>Journal of Chemical Physics</i> , 2019, 151, 165102.	1.2	17
2052	Rank reduced coupled cluster theory. II. Equation-of-motion coupled-cluster singles and doubles. <i>Journal of Chemical Physics</i> , 2019, 151, 164121.	1.2	13
2053	Beyond the Coulsonâ€™Fischer point: characterizing single excitation CI and TDDFT for excited states in single bond dissociations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21761-21775.	1.3	20
2054	High-Index Optimization-Based Shrinking Dimer Method for Finding High-Index Saddle Points. <i>SIAM Journal of Scientific Computing</i> , 2019, 41, A3576-A3595.	1.3	32
2055	Fluorescence enhancement of fungicide thiabendazole by van der Waals interaction with transition metal dichalcogenide nanosheets for highly specific sensors. <i>Nanoscale</i> , 2019, 11, 23156-23164.	2.8	6
2056	Photodecomposition of 1 $\langle i \rangle H \langle /i \rangle$ â€™Pyrrole Carbonyl Azides: Direct Observation of Singlet 1 $\langle i \rangle H \langle /i \rangle$ â€™Pyrrole Carbonyl Nitrenes and Triplet 1 $\langle i \rangle H \langle /i \rangle$ â€™3â€™Pyrrolylnitrene. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 401-411.	1.2	5
2057	Effect of the alkali metal (Li, Na, K) substitution on the geometric, electronic and optical properties of the smallest diamondoid: First principles calculations. <i>Chinese Journal of Chemical Engineering</i> , 2019, 27, 476-482.	1.7	3
2058	Steric Demand and Rateâ€™determining Step for Photoenolization of Diâ€™orthoâ€™substituted Acetophenone Derivatives. <i>Photochemistry and Photobiology</i> , 2019, 95, 154-162.	1.3	4
2059	R2PI and MATI spectroscopy of 3-fluoro-5-methylanisole: Combined effect of meta-substituents on molecular conformation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 224, 117398.	2.0	2

#	ARTICLE	IF	CITATIONS
2060	Calculating nuclear magnetic resonance chemical shifts in solvated systems. <i>Magnetic Resonance in Chemistry</i> , 2020, 58, 611-624.	1.1	17
2061	A Projective Method for the Calculation of Excited-State Electronic Coupling: Isolating Charge Transfer/Recombination Processes in Organic Photovoltaics. <i>Journal of Physical Chemistry A</i> , 2020, 124, 591-600.	1.1	9
2062	Cunning defects: emission control by structural point defects on Cu(<i>scp</i>)I double chain coordination polymers. <i>Journal of Materials Chemistry C</i> , 2020, 8, 1448-1458.	2.7	11
2063	Experimental and quantum chemical studies of the structural enhancement of three-photon absorption in two symmetrical fluorene derivatives. <i>Optik</i> , 2020, 207, 163761.	1.4	3
2064	Benchmarking the Performance of Time-Dependent Density Functional Theory Methods on Biochromophores. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 587-600.	2.3	69
2065	Substituent Effect on Conformational Preferences in Ground and Excited States of Selected Schiff Bases: An Insight from Theoretical Calculations. <i>Journal of Physical Chemistry A</i> , 2020, 124, 63-73.	1.1	6
2066	Excited state structures projected onto two dimensions: correlations with luminescent behavior. <i>Journal of Mathematical Chemistry</i> , 2020, 58, 2254-2272.	0.7	2
2067	Theoretical investigation of non-Förster exciton transfer mechanisms in perylene diimide donor, phenylene bridge, and terylene diimide acceptor systems. <i>Journal of Chemical Physics</i> , 2020, 153, 144305.	1.2	7
2068	Cherry-picking resolvents: A general strategy for convergent coupled-cluster damped response calculations of core-level spectra. <i>Journal of Chemical Physics</i> , 2020, 153, 141104.	1.2	13
2069	Probing the electronic structure of [Ru(L1)2]Z (z = 0, 1+ and 2+) (H2L1: a tridentate 2-aminophenol) Tj ETQq1 1 0.784314 rgBT /Overlo	1.6	8
2070	Vibronic Dynamics of Photodissociating ICN from Simulations of Ultrafast X-ray Absorption Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 20044-20048.	7.2	5
2071	Exploring interchain polaron pair formation in neat conjugated polymers. <i>European Physical Journal B</i> , 2020, 93, 1.	0.6	2
2073	Vibronic Dynamics of Photodissociating ICN from Simulations of Ultrafast X-ray Absorption Spectroscopy. <i>Angewandte Chemie</i> , 2020, 132, 20219-20223.	1.6	3
2074	Conformers of 1,2,3,4-tetrahydroisoquinoline in S0 and S1: An analysis through potential energy surface, hardness principles and vibrational spectroscopy. <i>Journal of Molecular Structure</i> , 2020, 1207, 127836.	1.8	13
2075	Massively Parallel Quantum Chemistry: A high-performance research platform for electronic structure. <i>Journal of Chemical Physics</i> , 2020, 153, 044120.	1.2	25
2076	Comparison of the Photochemistry of Acyclic and Cyclic 4-(4-Methoxy-phenyl)-4-oxo-but-2-enoate Ester Derivatives. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7346-7354.	1.1	7
2077	Oxygen migration and optical properties of coronene oxides and their persulfurated derivatives: insight into the electric field effect and the oxygen-site dependence. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 20078-20086.	1.3	2
2078	Simulation of time-resolved x-ray absorption spectroscopy of ultrafast dynamics in particle-hole-excited 4-(2-thienyl)-2,1,3-benzothiadiazole. <i>Structural Dynamics</i> , 2020, 7, 044101.	0.9	6

#	ARTICLE	IF	CITATIONS
2079	<i>Uncaria tomentosa</i> (cat's claw): a promising herbal medicine against SARS-CoV-2/ACE-2 junction and SARS-CoV-2 spike protein based on molecular modeling. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 2227-2243.	2.0	29
2080	<sc>DFT</sc> and <sc>CIS</sc>(D) theoretical study on the ground and excited states of pentanitrogen cation. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26393.	1.0	4
2081	Quantum chemical calculation of intrinsic reaction coordinates from trans to cis structure of fluvoxamine. <i>Computational and Theoretical Chemistry</i> , 2020, 1192, 113051.	1.1	0
2082	NWChem: Past, present, and future. <i>Journal of Chemical Physics</i> , 2020, 152, 184102.	1.2	425
2083	Multistate QM/QM Extrapolation of UV/Vis Absorption Spectra with Point Charge Embedding. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4361-4372.	2.3	12
2084	Tautomers of homophthalic anhydride in the ground and excited electronic states: analysis through energy, hardness and vibrational signatures. <i>Journal of Molecular Modeling</i> , 2020, 26, 173.	0.8	7
2085	TeraChem: Accelerating electronic structure and <i>ab initio</i> molecular dynamics with graphical processing units. <i>Journal of Chemical Physics</i> , 2020, 152, 224110.	1.2	87
2086	Fragment Quantum Mechanical Method for Excited States of Proteins: Development and Application to the Green Fluorescent Protein. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5174-5188.	2.3	26
2087	Extremely solvent-enhanced absorbance and fluorescence of carbazole interpreted using a damped Franck-Condon simulation. <i>Journal of Chemical Physics</i> , 2020, 152, 104106.	1.2	5
2088	Computational Protocol To Predict Anti-Kasha Emissions: The Case of Azulene Derivatives. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7228-7237.	1.1	35
2089	16. Description of excited states in photochemistry with theoretical methods. , 2020, , 379-414.		0
2090	Photophysical and electrochemical properties of two <i>trans</i> -A ₂ B-corroles: differences between phenyl or pyrenyl groups at the <i>meso</i> -10 position. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16965-16977.	1.3	11
2091	State-Targeted Energy Projection: A Simple and Robust Approach to Orbital Relaxation of Non-Aufbau Self-Consistent Field Solutions. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5067-5082.	2.3	62
2092	Benchmark of Simplified Time-Dependent Density Functional Theory for UV-Vis Spectral Properties of Porphyrinoids. <i>Advanced Theory and Simulations</i> , 2020, 3, 1900192.	1.3	13
2093	Double hybrids and time-dependent density functional theory: An implementation and benchmark on charge transfer excited states. <i>Journal of Computational Chemistry</i> , 2020, 41, 1242-1251.	1.5	42
2094	The MRCC program system: Accurate quantum chemistry from water to proteins. <i>Journal of Chemical Physics</i> , 2020, 152, 074107.	1.2	264
2095	Simulating the Nonadiabatic Relaxation Dynamics of 4-(<i>N,N</i> -Dimethylamino)benzotrile (DMABN) in Polar Solution. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2193-2206.	1.1	21
2097	A comprehensive, self-contained derivation of the one-body density matrices from single-reference excited-state calculation methods using the equation-of-motion formalism. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26110.	1.0	3

#	ARTICLE	IF	CITATIONS
2098	Extended Koopmans' theorem at the second-order perturbation theory. <i>Journal of Computational Chemistry</i> , 2020, 41, 1165-1174.	1.5	17
2099	Photolysis of 5-Azido-3-Phenylisoxazole at Cryogenic Temperature: Formation and Direct Detection of a Nitrosoalkene. <i>Molecules</i> , 2020, 25, 543.	1.7	5
2100	Excited-State Turn-On of Auophilicity and Tunability of Relativistic Effects in a Series of Digold Triazolates Synthesized via iClick. <i>Journal of the American Chemical Society</i> , 2020, 142, 8331-8341.	6.6	26
2101	Generalized single excitation configuration interaction: an investigation into the impact of the inclusion of non-orthogonality on the calculation of core-excited states. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 8182-8192.	1.3	16
2102	How accurate are TD-DFT excited-state geometries compared to DFT ground-state geometries?. <i>Journal of Computational Chemistry</i> , 2020, 41, 1718-1729.	1.5	57
2103	Investigating the conformers of 1, 2, 3, 4-tetrahydroquinoxaline: A combined theoretical and experimental investigation through potential energy surface studies, FT-IR and UV-Vis absorption measurements. <i>Journal of Molecular Structure</i> , 2020, 1211, 128064.	1.8	7
2104	3-Nitrene-2-formylthiophene and 3-Nitrene-2-formylfuran: Matrix Isolation, Conformation, and Rearrangement Reactions. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3786-3794.	1.1	4
2105	Description of excited states in photochemistry with theoretical methods. <i>ChemistrySelect</i> , 2021, 6, .	0.7	2
2106	<scp>TeraChem</scp>: A graphical processing unit<scp>-accelerated</scp> electronic structure package for <scp>large-scale</scp> ab initio molecular dynamics. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1494.	6.2	143
2107	Phenanthroline chromophore as efficient antenna for Tb ³⁺ green luminescence: A theoretical study. <i>Dyes and Pigments</i> , 2021, 185, 108890.	2.0	18
2108	Mountaineering Strategy to Excited States: Highly Accurate Oscillator Strengths and Dipole Moments of Small Molecules. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 416-438.	2.3	28
2109	UV polarisation spectroscopy of 1,4-diethynylbenzene. <i>Molecular Physics</i> , 2021, 119, .	0.8	1
2110	Benchmarking Quantum Mechanical Methods for the Description of Charge-Transfer States in π -Stacked Nucleobases. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 376-387.	2.3	13
2111	Many-electron dynamics in laser-driven molecules: wavefunction theory vs. density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13544-13560.	1.3	19
2112	The ABINIT-MP Program. , 2021, , 53-67.		10
2113	An effective potential for Frenkel excitons. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1923-1935.	1.3	2
2114	Spectroscopic characterization and photochemistry of the vinylsulfinyl radical. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16307-16315.	1.3	4
2115	Unravelling the nature of a toluene-fumaronitrile complex. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16128-16141.	1.3	2

#	ARTICLE	IF	CITATIONS
2116	FMO-Based Investigations of Excited-State Dynamics in Molecular Aggregates. , 2021, , 547-566.		2
2117	Computational approaches to dissociative chemisorption on metals: towards chemical accuracy. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 8962-9048.	1.3	47
2118	Ion-Induced Molecule Charge Exchange Reactions between Ar ⁺ and <i>cis</i> -Dichloroethylene. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2573-2580.	1.1	2
2120	CAS without SCF-Why to use CASCI and where to get the orbitals. <i>Journal of Chemical Physics</i> , 2021, 154, 090902.	1.2	24
2121	Synthesis and exploring the excited-state PES of photochromic hydrogen bond-assembled [2]rotaxane based on 1,3-Diazabicyclo-[3.1.0]hex-3-enes. <i>Research on Chemical Intermediates</i> , 2021, 47, 2557-2572.	1.3	3
2122	Progress and challenges in understanding of photoluminescence properties of carbon dots based on theoretical computations. <i>Applied Materials Today</i> , 2021, 22, 100924.	2.3	57
2124	A novel quinoline derivative containing a phenanthroimidazole moiety: Synthesis, physical properties and light-emitting diodes application. <i>Dyes and Pigments</i> , 2021, 188, 109198.	2.0	10
2125	Multi-replica biased sampling for photoswitchable π -conjugated polymers. <i>Journal of Chemical Physics</i> , 2021, 154, 174108.	1.2	6
2126	Simulation of photoexcitation dynamics in conjugated polymer using Ehrenfest method with configuration interaction singles. <i>European Physical Journal B</i> , 2021, 94, 1.	0.6	1
2127	Quantum Chemistry Calculations for Metabolomics. <i>Chemical Reviews</i> , 2021, 121, 5633-5670.	23.0	47
2128	Rifampicin as an example of beyond-rule-of-5 compound: Ionization beyond water and lipophilicity beyond octanol/water. <i>European Journal of Pharmaceutical Sciences</i> , 2021, 161, 105802.	1.9	6
2129	Optical and structural properties of the new triblock copolymer (A-B-C) based on p-terphenyl, PVK and MEH-PPV for organic electronics: Experimental and theoretical study. <i>Materials Research Express</i> , 2021, 8, 075304.	0.8	1
2130	Determining Factor of the Quantum Yield of the Cyclization Reaction via Triplet States for Dye-Attached Diarylethene. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5895-5902.	1.1	7
2131	Initial Maximum Overlap Method for Large Systems by the Quantum Mechanics/Extremely Localized Molecular Orbital Embedding Technique. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4169-4182.	2.3	10
2132	Theoretical Investigation of the 4,5-Dibromorodamine Methyl Ester (TH9402) Photosensitizer Used in Photodynamic Therapy: Photophysics, Reactions in the Excited State, and Interactions with DNA. <i>Journal of Physical Chemistry B</i> , 2021, 125, 8932-8943.	1.2	4
2133	Self-Consistent Field Methods for Excited States in Strong Magnetic Fields: a Comparison between Energy- and Variance-Based Approaches. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5492-5508.	2.3	16
2134	Mild Open-Shell Character of BODIPY and Its Impact on Singlet and Triplet Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5825-5838.	2.3	12
2135	Surface hopping simulations on photoexcitation dynamics of conjugated polymer. <i>Synthetic Metals</i> , 2021, 279, 116841.	2.1	6

#	ARTICLE	IF	CITATIONS
2136	Electronic Excitations in Crystalline Solids through the Maximum Overlap Method. Journal of Chemical Theory and Computation, 2021, 17, 6073-6079.	2.3	4
2137	Luminescent excited-state intramolecular proton-transfer dyes based on 4-functionalized 6,6'-dimethyl-3,3'-dihydroxy-2,2'-bipyridine (BP(OH) ₂ -Rs); DFT simulation study. Journal of Molecular Graphics and Modelling, 2021, 107, 107948.	1.3	2
2139	NWChem: New Functionality. Lecture Notes in Computer Science, 2003, , 168-177.	1.0	7
2140	Relativistic Effects on Magnetic Resonance Parameters and Other Properties of Inorganic Molecules and Metal Complexes. Challenges and Advances in Computational Chemistry and Physics, 2010, , 521-598.	0.6	19
2141	Computational Spectroscopy, Dynamics, and Photochemistry of Photosensory Flavoproteins. Methods in Molecular Biology, 2014, 1146, 191-228.	0.4	6
2142	Cluster Investigations in Cyclodextrin Inclusion Compounds: Theory and Experiment. Springer Series in Cluster Physics, 2002, , 109-131.	0.3	8
2143	Local Approximations for an Efficient and Accurate Treatment of Electron Correlation and Electron Excitations in Molecules. Challenges and Advances in Computational Chemistry and Physics, 2011, , 345-407.	0.6	27
2144	Electronic Excited States in the State-Specific Multireference Coupled Cluster Theory with a Complete-Active-Space Reference. Challenges and Advances in Computational Chemistry and Physics, 2010, , 219-249.	0.6	2
2145	Theoretical Studies of the Electronic Spectra of Organic Molecules. , 1995, , 357-438.		102
2146	Study of Stilbene Molecule Trans \rightarrow CIS Isomerization in First Excited State and Design of Molecular Random-Walkers. , 2000, , 437-450.		1
2147	Developments and applications of ABINIT-MP software based on the fragment molecular orbital method. , 2006, , 39-52.		36
2148	Molecular attochemistry: Correlated electron dynamics driven by light. Advances in Quantum Chemistry, 2020, 81, 15-50.	0.4	15
2150	Full configuration interaction benchmarks for the 3B_1 , \tilde{A}_1 $1A_1$, 1B_1 and 1A_1 states of methylene. Computational and Theoretical Chemistry, 1997, 400, 139-156.	1.5	4
2151	Cracking under Internal Pressure: Photodynamic Behavior of Vinyl Azide Crystals through N ₂ Release. Journal of the American Chemical Society, 2020, 142, 18565-18575.	6.6	23
2152	Vibronic structure and predissociation dynamics of 2-methoxythiophenol (S1): The effect of intramolecular hydrogen bonding on nonadiabatic dynamics. Journal of Chemical Physics, 2019, 151, 244305.	1.2	7
2153	Theory of analytical energy derivatives for the variational quantum eigensolver. Physical Review Research, 2020, 2, .	1.3	51
2154	Franck-Condon Dominated Chemistry. Formation and Dissociations of the Dimethylhydroxysulfuranyl Radical. Collection of Czechoslovak Chemical Communications, 2000, 65, 455-476.	1.0	21
2155	The Fragment Molecular Orbital-Based Time-Dependent Density Functional Theory for Excited States in Large Systems. , 2009, , 91-118.		3

#	ARTICLE	IF	CITATIONS
2156	Synthesis of Hydroxy and Methoxy Perylene Quinones, Their Spectroscopic and Computational Characterization, and Their Antiviral Activity. <i>Photochemistry and Photobiology</i> , 2005, 81, 924.	1.3	14
2157	Excitation Energies of Stacked DNA Base Pair. <i>Journal of Computer Aided Chemistry</i> , 2010, 11, 25-35.	0.3	1
2158	An ab initio Study of the amidine formed by tacrine and saccharin: Structural, Electronic and Spectroscopic Investigation. <i>Turkish Computational and Theoretical Chemistry</i> , 2019, 3, 25-37.	0.5	1
2159	Ab Initio and Experimental Studies on Dibenzothiazyl-Disulfide. <i>Bulletin of the Korean Chemical Society</i> , 2006, 27, 1048-1052.	1.0	4
2160	Quantum Chemical Studies on Nicotinato Lead(II) Complex [Pb(II)(C ₅ H ₄ NCOO) ₂]. <i>Bulletin of the Korean Chemical Society</i> , 2008, 29, 546-550.	1.0	6
2162	Recent Advances in Fragment Molecular Orbital-Based Molecular Dynamics (FMO-MD) Simulations. , 0, , .		11
2163	Isomerization Pathways of Azobenzene. , 2002, , 289-292.		0
2167	The Design of Blue Emitting Materials Based on Spirosilabifluorene Derivatives. <i>Lecture Notes in Computer Science</i> , 2007, , 319-326.	1.0	0
2168	Excited States of Photoactive Proteins by Configuration Interaction Studies. , 2009, , 63-90.		0
2169	Theoretical calculation of valence shell ionization potentials of XF ₃ (X=N, P, As) using the equation-of-motion coupled cluster method. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2011, 60, 053301.	0.2	0
2170	DFT and Time-dependant DFT Investigation of eElectronic Structure, Phosphorescence and Electroluminescence Properties of Iridium (III) Quinoxaline Complexes. <i>Journal of the Korean Chemical Society</i> , 2011, 55, 354-363.	0.2	0
2171	Quantum Mechanical Insights into Biological Processes at the Electronic Level. <i>Biological and Medical Physics Series</i> , 2012, , 117-164.	0.3	0
2172	Electronically excited states and photodynamics: a continuing challenge. , 2012, , 147-160.		1
2173	The first solvation shell of Reichardt's dye in ionic liquids: a semiempirical study. <i>Highlights in Theoretical Chemistry</i> , 2013, , 299-305.	0.0	0
2174	Theoretical Studies on 2-Hexylthieno[3,2-b]thiophene End-Capped Oligomers for Organic Semiconductor Materials. <i>Bulletin of the Korean Chemical Society</i> , 2012, 33, 1213-1219.	1.0	0
2175	Theoretical study of the ground and excited state properties of newly designed size-expanded adenine analogue x-adenine. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2013, 62, 107102.	0.2	1
2177	Valence and Inner Shell Multipole Electronic Excitations in Chlorofluorocarbons by Momentum-Transfer-Resolved Electron Energy Loss Spectroscopy. , 1994, , 141-150.		0
2178	A Coupled MCSCF-perturbation Treatment for Electronic Spectra. <i>Topics in Molecular Organization and Engineering</i> , 1996, , 39-53.	0.1	0

#	ARTICLE	IF	CITATIONS
2179	Theoretical Studies of the Models of Self-Trapped Excitons and Holes in Ionic Crystals. Springer Series in Solid-state Sciences, 1997, , 203-211.	0.3	0
2180	Quantum Mechanical Modelling of Exciton and Hole Self-Trapping in Ionic Crystals. , 1997, , 231-239.		0
2181	An Extended INDO-CI Theory of the General Relation between Bond Length and Bond Order. Journal of the Physical Society of Japan, 1998, 67, 1939-1947.	0.7	0
2182	Beyond the Hartree-Fock Method. , 1999, , 147-171.		0
2183	Ionization potentials of hypervalent LinC (2 ≤ n ≤ 10). , 1999, , 289-295.		0
2186	Guide to Programs for Nonrelativistic Quantum Chemistry Calculations. , 2015, , 1-23.		0
2187	Calculation of Excited States: Molecular Photophysics and Photochemistry on Display. , 2015, , 1-88.		0
2188	Effects of Water Molecules and Configurations of Neighboring Amino Acid Residues Surrounding DsRed Chromophore on Its Excitation Energy. Journal of Computer Chemistry Japan, 2015, 14, 155-163.	0.0	0
2189	Theoretical study on the photophysical properties of the newly designed guanine analog γ -guanine and its tautomers. Wuli Xuebao/Acta Physica Sinica, 2015, 64, 077101.	0.2	0
2190	Absorption and Microstructure Properties Calculated of Er-doped Silica Fiber Based on DFT Theory. , 2016, , .		1
2191	Novel Dipstick model for Portable Bio-sensing Application. , 0, 7, 36-41.		4
2193	Rotameric Isomers of La ₂ @C ₈₀ & Dodecafluoro-Subphthalocyanine Conjugate: Computational Characterization. ECS Journal of Solid State Science and Technology, 2020, 9, 061014.	0.9	6
2194	Actual Potentials of Theoretical Chemistry: What Can Be Obtained. , 2020, , 3-99.		0
2195	The role of π -donors/acceptors in molecular rotors towards development of ambient blue light sensors - A density functional theory study. Materials Chemistry and Physics, 2022, 277, 125563.	2.0	0
2196	Quantifying Fluctuations of Average Solvent Environments for Embedding Calculations. Journal of Chemical Theory and Computation, 2022, 18, 1072-1088.	2.3	4
2197	Accurate Spectral Properties within Double-Hybrid Density Functional Theory: A Spin-Scaled Range-Separated Second-Order Algebraic-Diagrammatic Construction-Based Approach. Journal of Chemical Theory and Computation, 2022, 18, 865-882.	2.3	14
2198	Fragment-Based Excited-State Calculations Using the GW Approximation and the Bethe-Salpeter Equation. Journal of Physical Chemistry A, 2021, 125, 10580-10592.	1.1	11
2199	Fluoromethylsulfinyl radicals: spectroscopic characterization and photoisomerization via intramolecular hydrogen shift. Physical Chemistry Chemical Physics, 2022, 24, 8881-8889.	1.3	2

#	ARTICLE	IF	CITATIONS
2200	Charge-Transfer Excitation within a Hybrid-(G)KS Framework through Cartesian Grid DFT. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1448-1457.	1.1	3
2201	Energy Landscape of State-Specific Electronic Structure Theory. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1512-1526.	2.3	13
2202	Nanoarchitecture of PANI/CNT/GO hybrid nanocomposites with enhanced dielectric and gas sensing properties. <i>Polymer Bulletin</i> , 0, , 1.	1.7	0
2203	The anthocyanin's role on the food metabolic pathways, color and drying processes: An experimental and theoretical approach. <i>Food Bioscience</i> , 2022, 47, 101700.	2.0	7
2204	Improving Results by Improving Densities: Density-Corrected Density Functional Theory. <i>Journal of the American Chemical Society</i> , 2022, 144, 6625-6639.	6.6	45
2205	A theoretical and experimental analysis of the luminescent properties of Europium(III) complex sensitized by tryptophan. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 428, 113875.	2.0	0
2206	Fragment-Based Quantum Mechanical Calculation of Excited-State Properties of Fluorescent RNAs. <i>Frontiers in Chemistry</i> , 2021, 9, 801062.	1.8	4
2207	Robust \hat{T}^2 SCF calculations with direct energy functional minimization methods and STEP for molecules and materials. <i>Journal of Chemical Physics</i> , 2022, 156, 154104.	1.2	3
2208	Calculation of the visible-UV absorption spectra of hydrogen sulfide, bisulfide, polysulfides, and As and Sb sulfides, in aqueous solution. <i>Geochemical Transactions</i> , 2003, 4, 28.	1.8	1
2210	Quantum Chemical Approaches to the Calculation of NMR Parameters: From Fundamentals to Recent Advances. <i>Magnetochemistry</i> , 2022, 8, 50.	1.0	20
2211	Revisiting the Performance of Time-Dependent Density Functional Theory for Electronic Excitations: Assessment of 43 Popular and Recently Developed Functionals from Rungs One to Four. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3460-3473.	2.3	61
2212	Transition orbital projection approach for excited state tracking. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	2
2213	Computing x-ray absorption spectra from linear-response particles atop optimized holes. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	7
2214	Interactive Molecular Dynamics: Exploring Excited States in Virtual Reality with <i>Ab Initio</i> Interactive Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 0, , .	2.3	3
2215	Influence of the monovalent bismuth on optical properties in Bi-doped silica optical fiber. <i>Optical Materials</i> , 2022, 131, 112720.	1.7	0
2216	Recent Advances in Cartesian-Grid DFT in Atoms and Molecules. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	0
2217	Computational study of optoelectronic properties of oxadiazole-based compounds for organic light emitting diodes. <i>Molecular Physics</i> , 2022, 120, .	0.8	1
2218	Theoretical transient absorption spectroscopy of trans-1,3-butadiene in intense laser fields. <i>Chemical Physics Letters</i> , 2022, 806, 140004.	1.2	0

#	ARTICLE	IF	CITATIONS
2219	Photochemistry of phosphenic chloride (ClPO ₂): isomerization with chlorine metaphosphite (ClOPO) and reduction by carbon monoxide. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 20828-20836.	1.3	2
2220	Dot-Size Dependent Excitons in Droplet-Etched Cone-Shell GaAs Quantum Dots. <i>Nanomaterials</i> , 2022, 12, 2981.	1.9	6
2221	ONIOM Method with Charge Transfer Corrections (ONIOM-CT): Analytic Gradients and Benchmarking. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 6052-6064.	2.3	3
2222	Beyond the Ground State: Predicting Electron Ionization Mass Spectra Using Excited-State Molecular Dynamics. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 4403-4410.	2.5	4
2223	Second quantisation for unrestricted references: formalism and quasi-spin-adaptation of excitation and spin-flip operators. <i>Molecular Physics</i> , 0, , .	0.8	1
2224	On the choice of reference orbitals for linear-response calculations of solution-phase K-edge X-ray absorption spectra. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 26170-26179.	1.3	5
2225	Electron-Affinity Time-Dependent Density Functional Theory: Formalism and Applications to Core-Excited States. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 9664-9672.	2.1	10
2226	MOLECULAR AND MULTISCALE MODELING: REVIEW ON THE THEORIES AND APPLICATIONS IN CHEMICAL ENGINEERING. <i>CTyF - Ciencia, Tecnologia Y Futuro</i> , 2009, 3, 205-223.	0.3	6
2227	Comparative performance of theoretical tools in order to quantify the effect of the electric potential on the vibrational wavenumbers and intensities of the SERS of 2-methylpyrazine adsorbed on a nanostructured silver electrode. <i>Journal of Raman Spectroscopy</i> , 2023, 54, 150-158.	1.2	0
2228	Generalized Energy-Based Fragmentation Approach for the Electronic Emission Spectra of Large Systems. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 7630-7638.	2.3	4
2229	Coupled-Cluster Theories for Excited States. , 2024, , 116-140.		0
2230	Developing electron dynamics into a tool for 21st century chemistry simulations. <i>Chemical Modelling</i> , 2022, , 91-152.	0.2	1
2231	The vertical excitation energies and a lifetime of the two lowest singlet excited states of the conjugated polyenes from C ₂ to C ₂₂ : Ab initio, DFT, and semiclassical MNDO-MD simulations. <i>Journal of Computational Chemistry</i> , 2023, 44, 777-787.	1.5	4
2232	Multi-action of a Fluorophore in the Sight of Light: Release of NO, Emergence of FONs, and Organelle Switching. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 55957-55970.	4.0	3
2233	Assessment of State-Averaged Driven Similarity Renormalization Group on Vertical Excitation Energies: Optimal Flow Parameters and Applications to Nucleobases. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 122-136.	2.3	3
2234	Phosphorus-Boron Multiple Bonding in the Ā Radical HBP. <i>Chemistry - A European Journal</i> , 0, , .	1.7	0
2235	Libkrylov: A modular open-source software library for extremely large on-the-fly matrix computations. <i>Journal of Computational Chemistry</i> , 2023, 44, 1105-1118.	1.5	0
2236	Synthesis, Quantum Computational Analysis and Molecular Docking of 3-(2-Hydroxyphenyl)-1-Phenyl Propanone: A Combined Experimental and Theoretical Analysis. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 8903-8932.	1.4	1

#	ARTICLE	IF	CITATIONS
2237	Double-Hybrid Density Functional Theory for Core Excitations: Theory and Benchmark Calculations. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 1310-1321.	2.3	3
2238	Machine-Learned Electronically Excited States with the MolOrblmage Generated from the Molecular Ground State. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 1955-1961.	2.1	2
2239	Why Is Quantum Chemistry So Complicated?. <i>Journal of the American Chemical Society</i> , 2023, 145, 4343-4354.	6.6	6
2240	Blue-Emitting 2-Fluoroaryl-1,2,3-Triazole Fluorophores: Synthesis, Theoretical Calculations, and Optical Properties. <i>Asian Journal of Organic Chemistry</i> , 2023, 12, .	1.3	1
2241	Simulation workflows to predict the circular dichroism and circularly polarized luminescence of chiral materials. <i>Chirality</i> , 2023, 35, 673-680.	1.3	4
2242	Excited-State Intramolecular Proton Transfer in Salicylidene- β -Hydroxy Carboxylate Derivatives: Direct Detection of the Triplet Excited State of the <i>cis</i> -Keto Tautomer. <i>Journal of Physical Chemistry A</i> , 2023, 127, 2765-2778.	1.1	0
2243	Performance of Common Density Functionals for Excited States of Tetraphenyldibenzoperiflanthene. <i>Journal of Physical Chemistry A</i> , 2023, 127, 3265-3273.	1.1	1
2244	Adiabatic extraction of nonlinear optical properties from real-time time-dependent electronic-structure theory. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	2
2245	Theoretical FRET Efficiency of an Antenna Material Containing Natural Dyes and Zeolite L. <i>ACS Omega</i> , 0, , .	1.6	0
2247	Spectroscopic Analysis: Calculations of Chiroptical Spectra. , 2022, , .		0
2252	Density-functional theory for electronic excited states. , 2023, , 69-118.		7
2268	Visualizing and characterizing excited states from time-dependent density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2024, 26, 3755-3794.	1.3	2
2276	ATR-far-ultraviolet spectroscopy: a challenge to new IR chemistry. <i>Chemical Society Reviews</i> , 2024, 53, 1730-1768.	18.7	0