Cheol-Ho Choi

List of Publications by Year in Descending Order

151 papers	3,457 citations	27 h-index	53 g-index
156 ext. papers	3,781 ext. citations	4.9 avg, IF	5.55 L-index

#	Paper	IF	Citations
151	Manifestations of strong electron correlation in polyacene: Fundamental gap, density of states, and photoconductivity. *Carbon Trends*, **2022**, 7, 100146	0	0
150	Exploring Dyson's Orbitals and Their Electron Binding Energies for Conceptualizing Excited States from Response Methodology. *Journal of Physical Chemistry Letters*, **2021**, 12, 9963-9972	6.4	2
149	Optimization of Three State Conical Intersections by Adaptive Penalty Function Algorithm in Connection with the Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory Method (MRSF-TDDFT). *Journal of Physical Chemistry A*, **2021**, 125, 1994-2006	2.8	6
148	Signatures of Conical Intersection Dynamics in the Time-Resolved Photoelectron Spectrum of Furan: Theoretical Modeling with an Ensemble Density Functional Theory Method. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	1
147	Impact of the Dynamic Electron Correlation on the Unusually Long Excited-State Lifetime of Thymine. *Journal of Physical Chemistry Letters*, **2021**, 12, 4339-4346	6.4	9
146	Fast and Accurate Computation of Nonadiabatic Coupling Matrix Elements Using the Truncated Leibniz Formula and Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory. *Journal of Physical Chemistry Letters*, **2021**, 12, 4722-4728	6.4	6
145	Oxidative denitrogenation of liquid fuel over W2N@carbon catalyst derived from a phosphotungstinic acid encapsulated metal□zolate framework. *Applied Catalysis B: Environmental*, **2021**, 285, 119842	21.8	13
144	Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT) as a Simple yet Accurate Method for Diradicals and Diradicaloids. *Journal of Chemical Theory and Computation*, **2021**, 17, 848-859	6.4	8
143	How neutral nitrogen-containing compounds are oxidized in oxidative-denitrogenation of liquid fuel with TiO@carbon. *Physical Chemistry Chemical Physics*, **2021**, 23, 8368-8374	3.6	1
142	Description of Sudden Polarization in the Excited Electronic States with an Ensemble Density Functional Theory Method. *Journal of Chemical Theory and Computation*, **2021**, 17, 5123-5139	6.4	2
141	Internal Conversion between Bright (1) and Dark (2) States in s--Butadiene and s--Hexatriene. *Journal of Physical Chemistry Letters*, **2021**, 12, 9720-9729	6.4	4
140	Relief of excited-state antiaromaticity enables the smallest red emitter. *Nature Communications*, **2021**, 12, 5409	17.4	3
139	How Beneficial Is the Account of Doubly-Excited Configurations in Linear Response Theory?. *Journal of Chemical Theory and Computation*, **2021**, 17, 975-984	6.4	6
138	Computation of Molecular Ionization Energies Using an Ensemble Density Functional Theory Method. *Journal of Chemical Theory and Computation*, **2020**, 16, 4489-4504	6.4	7
137	Low-dimensional projection approach for efficient sampling of molecular recognition and polymer aggregation. *Physical Chemistry Chemical Physics*, **2020**, 22, 6953-6963	3.6	0
136	Green's function of the Smoluchowski equation with reaction sink: Application to geminate and bulk recombination reactions. *Journal of Chemical Physics*, **2020**, 152, 134102	3.9	4
135	A solvent-solute cooperative mechanism for symmetry-breaking charge transfer. *Physical Chemistry Chemical Physics*, **2020**, 22, 1115-1121	3.6	12

134	Entangled iodine and hydrogen peroxide formation in ice. *Physical Chemistry Chemical Physics*, **2020**, 22, 16532-16535	3.6	
133	Structural or population dynamics: what is revealed by the time-resolved photoelectron spectroscopy of 1,3-cyclohexadiene? A study with an ensemble density functional theory method. *Physical Chemistry Chemical Physics*, **2020**, 22, 17567-17573	3.6	3
132	Diboron- and Diaza-Doped Anthracenes and Phenanthrenes: Their Electronic Structures for Being Singlet Fission Chromophores. *Journal of Physical Chemistry A*, **2020**, 124, 8159-8172	2.8	10
131	Computation of Molecular Electron Affinities Using an Ensemble Density Functional Theory Method. *Journal of Physical Chemistry A*, **2020**, 124, 7795-7804	2.8	7
130	Performance Analysis and Optimization of Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT) for Vertical Excitation Energies and Singlet-Triplet Energy Gaps. *Journal of Physical Chemistry A*, **2019**, 123, 7991-8000	2.8	17
129	Sulfuric Acid Formation via HSO Oxidation by HO in the Atmosphere. *Journal of Physical Chemistry A*, **2019**, 123, 8385-8390	2.8	5
128	Symmetry-breaking charge transfer dynamics of 9,9Ebianthracene revealed by experiment and theory. *EPJ Web of Conferences*, **2019**, 205, 09008	0.3	
127	Theoretical modelling of the dynamics of primary photoprocess of cyclopropanone. *Physical Chemistry Chemical Physics*, **2019**, 21, 2489-2498	3.6	17
126	Time-dependent electron transfer rate between geminate ions with strong Coulomb interaction and distance-dependent reactivity. *Journal of Chemical Physics*, **2019**, 150, 214104	3.9	3
125	Efficient implementations of analytic energy gradient for mixed-reference spin-flip time-dependent density functional theory (MRSF-TDDFT). *Journal of Chemical Physics*, **2019**, 150, 184111	3.9	21
124	Design of singlet fission chromophores with cyclic (alkyl)(amino) carbene building blocks. *Journal of Chemical Physics*, **2019**, 150, 234306	3.9	24
123	Heartbeat detection using a Doppler radar sensor based on the scaling function of wavelet transform. *Microwave and Optical Technology Letters*, **2019**, 61, 1792-1796	1.2	9
122	Design and photoisomerization dynamics of a new family of synthetic 2-stroke light driven molecular rotary motors. *Chemical Communications*, **2019**, 55, 5247-5250	5.8	19
121	Conical Intersections in Organic Molecules: Benchmarking Mixed-Reference Spin-Flip Time-Dependent DFT (MRSF-TD-DFT) vs Spin-Flip TD-DFT. *Journal of Physical Chemistry A*, **2019**, 123, 6455-6462	2.8	20
120	Theoretical Study of the thermal decomposition of primary thiols on the Si(100)-2X1 surface **2019**, 91-93		
119	Oxidative denitrogenation with TiO2@porous carbon catalyst for purification of fuel: Chemical aspects. *Applied Catalysis B: Environmental*, **2019**, 240, 215-224	21.8	30
118	Fast Overlap Evaluations for Nonadiabatic Molecular Dynamics Simulations: Applications to SF-TDDFT and TDDFT. *Journal of Chemical Theory and Computation*, **2019**, 15, 882-891	6.4	13
117	One-Dimensional Projection of Collective Variables for Effective Sampling of Complex Chemical Reaction Coordinates. *Journal of Chemical Theory and Computation*, **2018**, 14, 2312-2321	6.4	2

116	Conformers of Zwitterionic Glycine in Aqueous Phase. *Bulletin of the Korean Chemical Society*, **2018**, 39, 227-230	1.2	1
115	Resummation of the Brillouin-Wigner Perturbation Series. *Bulletin of the Korean Chemical Society*, **2018**, 39, 347-355	1.2	
114	Na+, F□Br□and Cl□Adsorptions and Penetrations on an Ice Surface. *ACS Earth and Space Chemistry* , **2018**, 2, 56-63	3.2	2
113	Heat of formation prediction by G4MP2-SFM schemes: An application to various nitroazole derivatives. *Computational and Theoretical Chemistry*, **2018**, 1130, 148-159	2	2
112	Ligand-Specific Dissolution of Iron Oxides in Frozen Solutions. *Environmental Science & Technology*, **2018**, 52, 13766-13773	10.3	15
111	Eliminating spin-contamination of spin-flip time dependent density functional theory within linear response formalism by the use of zeroth-order mixed-reference (MR) reduced density matrix. *Journal of Chemical Physics*, **2018**, 149, 104101	3.9	39
110	Highly selective imidazole-appended 9,10-N,N?-diaminomethylanthracene fluorescent probe for switch-on Zn2+ detection and switch-off H2PO4□and CN□detection in 80% aqueous DMSO, and applications to sequential logic gate operations. *Sensors and Actuators B: Chemical*, **2017**, 247, 840-849	8.5	34
109	Correlation between experimental data of protonation of aromatic compounds at (+) atmospheric pressure photoionization and theoretically calculated enthalpies. *Rapid Communications in Mass Spectrometry*, **2017**, 31, 1023-1030	2.2	3
108	Adsorptive Denitrogenation of Model Fuel with CuCl-Loaded Adsorbents: Contribution of □Complexation and Direct Interaction between Adsorbates and Cuprous Ions. *Journal of Physical Chemistry C*, **2017**, 121, 11601-11608	3.8	17
107	Coherent intermolecular proton transfer in the acid-base reaction of excited state pyranine. *Physical Chemistry Chemical Physics*, **2017**, 19, 18243-18251	3.6	16
106	What Authentication Technology Should Be Chosen for Construction Manpower Management?. *Procedia Engineering*, **2017**, 196, 309-314		2
105	Effects of external electric field and anisotropic long-range reactivity on charge separation probability. *Journal of Chemical Physics*, **2017**, 147, 144111	3.9	4
104	Efficient Thermal Reactions of Sulfur Dioxide on Ice Surfaces at Low Temperature: A Combined Experimental and Theoretical Study. *ACS Earth and Space Chemistry*, **2017**, 1, 503-510	3.2	5
103	Measurement of Construction BIM Value Based on a Case Study of a Large-Scale Building Project. *Journal of Management in Engineering - ASCE*, **2017**, 33, 05017005	5.3	27
102	Origin of Acid-Base Catalytic Effects on Formaldehyde Hydration. *Journal of Physical Chemistry A*, **2016**, 120, 9598-9606	2.8	2
101	A priori predictions of molecular density by EFP2-MD. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	2
100	Conformational free energy surfaces of non-ionized glycine in aqueous solution. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	4
99	Selective fluorescence sensing of salicylic acids using a simple pyrenesulfonamide receptor. *RSC Advances*, **2015**, 5, 23613-23621	3.7	18

98	Gauche effects of glucopyranose by QM/MM-MD simulations. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	9
97	Heat of formation predictions of various nitro-substituted azoles by G4MP2-SFM scheme. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	7
96	Like-charge ion pairs of hydronium and hydroxide in aqueous solution?. *Physical Chemistry Chemical Physics*, **2015**, 17, 16233-7	3.6	4
95	Translation symmetry breakdown in low-dimensional lattices of pentagonal rings. *Journal of Physical Chemistry Letters*, **2015**, 6, 4525-31	6.4	26
94	Mechanistic study on lowering the sensitivity of positive atmospheric pressure photoionization mass spectrometric analyses: size-dependent reactivity of solvent clusters. *Rapid Communications in Mass Spectrometry*, **2015**, 29, 2095-101	2.2	15
93	A Development of Framework for Selecting Labor Attendance Management System Considering Condition of Construction Site. *Korean Journal of Construction Engineering and Management*, **2015**, 16, 60-69		1
92	Synthesis and characterization of a novel laser ablation sensitive triazene incorporated epoxy resin. *Electronic Materials Letters*, **2014**, 10, 173-182	2.9	2
91	Asymmetric Transport Mechanisms of Hydronium and Hydroxide Ions in Amorphous Solid Water: Hydroxide Goes Brownian while Hydronium Hops. *Journal of Physical Chemistry Letters*, **2014**, 5, 2568-72	6.4	14
90	Elucidating molecular structures of nonalkylated and short-chain alkyl (n Analytical Chemistry, **2014** , 86, 3300-7	7.8	44
89	A priori prediction of heats of vaporization and sublimation by EFP2-MD. *Journal of Physical Chemistry B*, **2014**, 118, 4876-82	3.4	7
88	Fast and accurate predictions of heat of formation by G4MP2-SFM parameterization scheme: An application to imidazole derivatives. *Chemical Physics Letters*, **2014**, 599, 57-62	2.5	3
87	Dual function of a living polymerization initiator through the formation of a chain-end-protecting cluster: density functional theory calculation. *Physical Chemistry Chemical Physics*, **2014**, 16, 24929-35	3.6	9
86	Comparative proton transfer efficiencies of hydronium and hydroxide in aqueous solution: proton transfer vs Brownian motion. *Journal of Physical Chemistry B*, **2014**, 118, 13671-8	3.4	12
85	Which hydrogen atom of toluene protonates PAH molecules in (+)-mode APPI MS analysis?. *Journal of the American Society for Mass Spectrometry*, **2013**, 24, 316-9	3.5	11
84	New regioisomeric naphtholthiazole based turn-on fluorescent chemosensor for Al3+. *Tetrahedron*, **2013**, 69, 9600-9608	2.4	27
83	Microscopic nature of mobile fluoride anions on sp2 carbon surfaces. *Chemical Physics Letters*, **2013** , 570, 85-89	2.5	4
82	Direct absolute pKa predictions and proton transfer mechanisms of small molecules in aqueous solution by QM/MM-MD. *Journal of Physical Chemistry B*, **2013**, 117, 6269-75	3.4	44
81	Efficient parallel implementations of QM/MM-REMD (quantum mechanical/molecular mechanics-replica-exchange MD) and umbrella sampling: isomerization of H2O2 in aqueous solution. *Journal of Physical Chemistry B*, **2013**, 117, 7996-8002	3.4	21

80	Interionic hydration structures of NaCl in aqueous solution: a combined study of quantum mechanical cluster calculations and QM/EFP-MD simulations. *Journal of Physical Chemistry B*, **2013**, 117, 289-95	3.4	37
79	Solvent electronic polarization effects on Na(+)-Na(+) and Cl(-)-Cl(-) pair associations in aqueous solution. *Journal of Physical Chemistry B*, **2013**, 117, 9273-9	3.4	19
78	Adsorptions of Formic and Acetic Acids on Ice Surface: Surface Binding Configurations and a Possibility of Interfacial Proton Transfer. *Journal of Physical Chemistry C*, **2013**, 117, 4181-4188	3.8	11
77	A Variant of the Brillouin-Wigner Perturbation Theory with Epstein-Nesbet Partitioning. *Bulletin of the Korean Chemical Society*, **2013**, 34, 3279-3283	1.2	1
76	Mean Gradient Charge: A new definition of atomic charge using induced atomic gradient. *Chemical Physics Letters*, **2012**, 524, 107-111	2.5	3
75	New regioisomeric naphthol-substituted thiazole based ratiometric fluorescence sensor for Zn2+ with a remarkable red shift in emission spectra. *Tetrahedron*, **2012**, 68, 647-653	2.4	50
74	Direct simulations of anharmonic infrared spectra using quantum mechanical/effective fragment potential molecular dynamics (QM/EFP-MD): methanol in water. *Journal of Physical Chemistry A*, **2012**, 116, 8965-71	2.8	17
73	Mechanisms behind the generation of protonated ions for polyaromatic hydrocarbons by atmospheric pressure photoionization. *Analytical Chemistry*, **2012**, 84, 1146-51	7.8	26
72	Adsorptions of HOCl on Ice Surface: Effects of Long-Range Electrostatics, Surface Heterogeneity, and Hydrogen Disorders of Ice Crystal. *Journal of Physical Chemistry C*, **2012**, 116, 3694-3701	3.8	12
71	Quantum mechanical/effective fragment potential molecular dynamics (QM/EFP-MD) study on intra-molecular proton transfer of glycine in water. *Chemical Physics Letters*, **2012**, 539-540, 218-221	2.5	23
70	Reducing the scaling of the fragment molecular orbital method using the multipole method. *Chemical Physics Letters*, **2012**, 543, 159-165	2.5	11
69	Hydrophobic and hydrophilic associations of a methanol pair in aqueous solution. *Journal of Physical Chemistry B*, **2012**, 116, 14254-60	3.4	25
68	Relativistic potential energy surfaces of initial oxidations of Si(100) by atomic oxygen: the importance of surface dimer triplet state. *Journal of Chemical Physics*, **2012**, 136, 214704	3.9	2
67	Adsorption Mechanisms of NH3 on Chlorinated Si(100)-2□ Surface. *Bulletin of the Korean Chemical Society*, **2012**, 33, 775-778	1.2	4
66	Electronic Structure of [NiS4]-Investigated by Single-Crystal EPR and Density Functional Theory. *Journal of the Korean Magnetic Resonance Society*, **2012**, 16, 78-90		
65	Ab initio study of Kubas-type dihydrogen fixation onto d-orbital states of Ca adatoms. *Chemical Physics Letters*, **2011**, 513, 256-260	2.5	8
64	The concerted and stepwise chemisorption mechanisms of isothiazole and thiazole on Si(100)2 □1 surface. *Theoretical Chemistry Accounts*, **2011**, 130, 507-513	1.9	1
63	Chromogenic and fluorogenic sensing of Cu2+ based on coumarin. *Tetrahedron*, **2011**, 67, 2794-2802	2.4	116

62	Adsorption mechanisms of isoxazole and oxazole on Si(100)-2 □1 surface: Si-N dative bond addition vs. [4+2] cycloaddition. *Journal of Chemical Physics*, **2011**, 135, 244707	3.9	2
61	Thermal decomposition mechanisms of methylamine, ethylamine, and 1-propylamine on Si(100)-2 □ 1 surface. *Journal of Chemical Physics*, **2011**, 134, 194701	3.9	11
60	Structural Isomers and Excited States of HN3. *Bulletin of the Korean Chemical Society*, **2011**, 32, 3641-3643	1.2	2
59	Cha, Choi, and Park Reply:. *Physical Review Letters*, **2010**, 104,	7.4	4
58	Theoretical Study of Initial Adsorptions and Subsequent Surface Rearrangements of HC□?CCOH on Si(100)-2 □1 Surface. *Journal of Physical Chemistry C*, **2010**, 114, 14187-14192	3.8	4
57	Theoretical Study of Cycloaddition Reactions of C60on the Si(100)-2□1 Surface. *Bulletin of the Korean Chemical Society*, **2010**, 31, 1681-1688	1.2	1
56	Theoretical Studies on MXO4(M=Li, Na, K and X=F, Cl, Br, I) Salt Ion Pairs. *Bulletin of the Korean Chemical Society*, **2010**, 31, 2215-2218	1.2	
55	Visible laser□nduced photoreduction of silver 4-nitrobenzenethiolate revealed by Raman scattering spectroscopy. *Journal of Raman Spectroscopy*, **2009**, 41, n/a-n/a	2.3	3
54	Inaccuracy of density functional theory calculations for dihydrogen binding energetics onto Ca cation centers. *Physical Review Letters*, **2009**, 103, 216102	7.4	32
53	New deep cavitand with imidazoquinoxaline flaps: formation of static helical alkane inclusion complexes by enhanced CH/pi interactions. *Chemical Communications*, **2009**, 4971-3	5.8	13
52	Adsorption Reactions of Trimethylgallium and Arsine on H/Si(100)-2x1 Surface. *Bulletin of the Korean Chemical Society*, **2009**, 30, 1805-1810	1.2	4
51	Pristine Multiwalled Carbon Nanotube/Polyethylene Nanocomposites by Immobilized Catalysts. *Chemistry of Materials*, **2008**, 20, 4588-4594	9.6	43
50	Surface Reaction of 1,2,-Dichloroethylene on Si(100)-2 □1: Importance of Surface Isomerization Channel. *Journal of Physical Chemistry C*, **2008**, 112, 9327-9335	3.8	7
49	Thermal Decomposition Mechanisms of Methanol, Ethanol, and 1-Propanol on the Si(100)-2 □1 Surface. *Journal of Physical Chemistry C*, **2008**, 112, 6907-6913	3.8	11
48	Cluster study of surface radicals of Si(111)-7 □7 reconstructed surface. *Theoretical Chemistry Accounts*, **2008**, 120, 79-83	1.9	8
47	A stair-shaped molecular silver(0) chain. *Angewandte Chemie - International Edition*, **2008**, 47, 8390-3	16.4	13
46	Initial adsorption mechanisms of TiCl4 on OH/Si(100)-2□1. *Chemical Physics Letters*, **2008**, 457, 69-73	2.5	14
45	Adsorption of TiCl4 on H/Si(1 0 0)-2 □1 Surface. *Chemical Physics Letters*, **2008**, 461, 249-253	2.5	10

44	New implementation of a combined quantum mechanical and molecular mechanical method using modified generalized hybrid orbitals. *Journal of Chemical Physics*, **2007**, 127, 204102	3.9	26
43	A theoretical study of thermal [1,3]-sigmatropic rearrangements of 3-trimethylsilyl-1-pyrazoline: concerted vs. stepwise mechanisms. *Journal of Computational Chemistry*, **2006**, 27, 228-37	3.5	6
42	Adsorption reactions of dimethylaluminum isopropoxide and water on the H/Si(100)-2 x 1 surface: initial reactions for atomic layer deposition of Al2O3. *Journal of Physical Chemistry B*, **2006**, 110, 11277-83	3.4	15
41	The initial mechanisms of Al2O3 atomic layer deposition on OH/Si(1 0 0)-2 □1 surface by tri-methylaluminum and water. *Chemical Physics Letters*, **2006**, 426, 365-369	2.5	23
40	Surface S(N)2 reaction by H2O on chlorinated Si(100)-2 x 1 surface. *Journal of Physical Chemistry B*, **2005**, 109, 10909-14	3.4	7
39	Comparative study of surface cycloadditions of ethylene and 2-butene on the Si(100)-2 x 1 surface. *Journal of Physical Chemistry B*, **2005**, 109, 5067-72	3.4	23
38	Cycloaddition isomerizations of adsorbed 1,3-cyclohexadiene on Si(100)-2x1 surface: first neighbor interactions. *Journal of the American Chemical Society*, **2005**, 127, 8485-91	16.4	17
37	Surface-stabilized amorphous germanium nanoparticles for lithium-storage material. *Journal of Physical Chemistry B*, **2005**, 109, 20719-23	3.4	104
36	Conjugated polymers and aromaticity. *Chemical Reviews*, **2005**, 105, 3448-81	68.1	396
35	Ground and excited states of Al2O2 and its anion. *Chemical Physics Letters*, **2005**, 411, 297-301	2.5	9
34	Direct determination of multipole moments of Cartesian Gaussian functions in spherical polar coordinates. *Journal of Chemical Physics*, **2004**, 120, 3535-43	3.9	9
33	Cycloaddition reactions of cyanogen (C2N2) on the Si(100)-2x1 surface. *Journal of Chemical Physics*, **2004**, 121, 5445-50	3.9	1
32	Surface reaction mechanisms of hydrazine on Si(100)-2 x 1 surface: NH3 desorption pathways. *Journal of Chemical Physics*, **2004**, 120, 979-87	3.9	9
31	Atomistic modeling of morphological evolution during simultaneous etching and oxidation of Si(100). *Surface Science*, **2004**, 555, 51-67	1.8	13
30	Cycloaddition Reactions of Dienes on the SI(100)-2 □1 Surface. *International Journal of Modern Physics B*, **2003**, 17, 1205-1210	1.1	2
29	Vibrational properties of [33](1,3,5)-cyclophane and bridged-hexaprismane. *Journal of Molecular Structure*, **2003**, 655, 351-359	3.4	4
28	Cycloaddition Reactions of 1-Pyrazoline on the Si(100) 2 □1 Surface: A Possible Route to an SiN Interfacial Double Bond. *Journal of Physical Chemistry B*, **2003**, 107, 6853-6858	3.4	3
27	Unusual flexibility of 2,5-bis(4-pyridylethynyl)thiophene self-assembled with Co(NCS)2 in a novel coordination polymer. *Chemical Communications*, **2003**, 2528-9	5.8	22

26	Theoretical study of C20 fullerene dimerization: a facile [2+2] cycloaddition. *Chemical Physics Letters*, **2002**, 359, 446-452	2.5	21
25	Cycloaddition reactions of acrylonitrile on the Si(100)-2 x 1 surface. *Journal of the American Chemical Society*, **2002**, 124, 6162-7	16.4	43
24	Passive and active oxidation of Si(100) by atomic oxygen: a theoretical study of possible reaction mechanisms. *Journal of the American Chemical Society*, **2002**, 124, 8730-40	16.4	43
23	New parallel optimal-parameter fast multipole method (OPFMM). *Journal of Computational Chemistry*, **2001**, 22, 1484-1501	3.5	44
22	Ab initio electronic structure studies of Na2OH and its anion. *Chemical Physics Letters*, **2001**, 349, 530-536	2.5	2
21	Adsorption of Water on the Si(100) Surface: An Ab Initio and QM/MM Cluster Study. *Journal of Physical Chemistry B*, **2001**, 105, 4039-4044	3.4	38
20	Modeling of the Transition From Active to Passive Oxidation of Si(100). *Materials Research Society Symposia Proceedings*, **2000**, 619, 173		2
19	Vibrational Assignment of All 46 Fundamentals of C60 and C606-: Scaled Quantum Mechanical Results Performed in Redundant Internal Coordinates and Compared to Experiments. *Journal of Physical Chemistry A*, **2000**, 104, 102-112	2.8	78
18	Rapid and stable determination of rotation matrices between spherical harmonics by direct recursion. *Journal of Chemical Physics*, **1999**, 111, 8825-8831	3.9	121
17	Argon-matrix-isolation Raman spectra and density functional study of 1,3-butadiene conformers. *Theoretical Chemistry Accounts*, **1999**, 102, 196-206	1.9	25
16	Cycloaddition Reactions of 1,3-Cyclohexadiene on the Silicon(001) Surface. *Journal of the American Chemical Society*, **1999**, 121, 11311-11317	16.4	108
15	Conformational Fingerprints in the IR and Raman Spectra of Oligoanilines: A Combined Theoretical and Experimental Study. *Chemistry of Materials*, **1999**, 11, 855-857	9.6	13
14	Is a 1.90 □C□ bond length in polymeric fullerides possible?. *Chemical Physics Letters*, **1998**, 282, 318-324	2.5	17
13	New Interpretation of the Valence Tautomerism of 1,6-Methano[10]annulenes and Its Application to Fullerene Derivatives. *Journal of Physical Chemistry A*, **1998**, 102, 3429-3437	2.8	20
12	Bond length alternation and aromaticity in large annulenes. *Journal of Chemical Physics*, **1998**, 108, 6681-6688	3.9	77
11	The effects of electron correlation on the degree of bond alternation and electronic structure of oligomers of polyacetylene. *Journal of Chemical Physics*, **1997**, 107, 6712-6721	3.9	136
10	Consistencies between experiments and quantum calculations of strained C□ single bond lengths. *Chemical Communications*, **1997**, 2199-2200	5.8	20
9	Conformational Studies of Vibrational Properties and Electronic States of Leucoemeraldine Base and Its Oligomers. *Macromolecules*, **1997**, 30, 620-630	5.5	33

8	Do Localized Structures of [14]- and [18]Annulenes Exist?. *Journal of the American Chemical Society*, **1997**, 119, 11994-11995	16.4	33
7	Conformational Information from Vibrational Spectra of Styrene, trans-Stilbene, and cis-Stilbene. *Journal of Physical Chemistry A*, **1997**, 101, 3823-3831	2.8	261
6	Single-Bond Torsional Potentials in Conjugated Systems: A Comparison of abInitio and Density Functional Results. *Journal of Physical Chemistry A*, **1997**, 101, 7426-7433	2.8	247
5	Conformational information from vibrational spectra of polyaniline. *Synthetic Metals*, **1997**, 85, 1073-1076	1.66	13
4	Limitations of current density functional theories for the description of partial Ebond breaking. *Chemical Physics Letters*, **1997**, 276, 266-268	2.5	48
3	Density Functional Studies of Vibrational Properties of HCN, H2O, CH2O, CH4, and C2H4. *The Journal of Physical Chemistry*, **1996**, 100, 16530-16537		21
2	A new partition of the atomic polar tensor: the benzene molecule. *Chemical Physics Letters*, **1996**, 263, 697-702	2.5	5
1	Chemistry on Silicon Surfaces821-851		10