K V Mikkelsen

List of Publications by Year
in descending order

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314	11,830	30551	46524
papers	citations	56	93
		h-index	g-index

328	328	328	8267
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantum computing for chemical and biomolecular product design. Current Opinion in Chemical Engineering, 2022, 36, 100754.	3.8	26
2	Synthesis, characterization and computational evaluation of bicyclooctadienes towards molecular solar thermal energy storage. Chemical Science, 2022, 13, 834-841.	3.7	14
3	Subphthalocyanineâ€“triangulene dyads: Property tuning for lightâ€harvesting device applications. Energy Science and Engineering, 2022, 10, 1752-1762.	1.9	3
4	A benchmark study of aromaticity indexes for benzene, pyridine and the diazines â€“ I. Ground state aromaticity. RSC Advances, 2022, 12, 2830-2842.	1.7	19
5	Optimization of the thermochemical properties of the norbornadiene/quadricyclane photochromic couple for solar energy storage using nanoparticles. Physical Chemistry Chemical Physics, 2022, 24, 5506-5521.	1.3	5
6	The effects of solvation on the back reaction and storage capabilities of solar thermal energy storage systems. Physical Chemistry Chemical Physics, 2022, 24, 5564-5577.	1.3	6
7	Density Functional Theory Study of Carbamoyl-Substituted Dihydroazulene/Vinylheptafulvene Derivatives and Solvent Effects. Journal of Physical Chemistry C, 2022, 126, 4815-4825.	1.5	1
8	A Neural Network Approach for Property Determination of Molecular Solar Cell Candidates. Journal of Physical Chemistry A, 2022, 126, 1681-1688.	1.1	4
9	Perturbation of the UV transitions of formaldehyde by TiO2 photocatalysts and Aun nanoclusters. Physical Chemistry Chemical Physics, 2022, , .	1.3	0
10	Prospects of Improving Molecular Solar Energy Storage of the Norbornadiene/Quadricyclane System through Bridgehead Modifications. Journal of Physical Chemistry A, 2022, 126, 2670-2676.	1.1	13
11	Electric Properties of Photochromic Molecules Physisorbed on Silver and Copper Nanoparticles. Journal of Physical Chemistry A, 2022, 126, 3145-3156.	1.1	1
12	Bypassing the multireference character of singlet molecular oxygen, part 1:1,4â€cycloâ€addition. International Journal of Quantum Chemistry, 2021, 121, e26523.	1.0	2
13	Simulating fullerene polyhedral formation from planar precursors. Physical Chemistry Chemical Physics, 2021, 23, 6561-6573.	1.3	0
14	A QM/MM study of the conformation stability and electronic structure of the photochromic switches derivatives of DHA/VHF in acetonitrile solution. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 251, 119434.	2.0	10
15	Fulvaleneâ€Based Polycyclic Aromatic Hydrocarbon Ladderâ€Type Structures: Synthesis and Properties. Chemistry - A European Journal, 2021, 27, 8315-8324.	1.7	13
16	Dihydroazuleneâ€Azobenzeneâ€Dihydroazulene Triad Photoswitches. Chemistry - A European Journal, 2021, 27, 12437-12446.	1.7	8
17	Benchmark study on the optical and thermochemical properties of the norbornadiene-quadricyclane photoswitch. Chemical Physics Letters, 2021, 779, 138665.	1.2	8
18	Promoting the thermal back reaction of vinylheptafulvene to dihydroazulene by physisorbtion on nanoparticles. Physical Chemistry Chemical Physics, 2021, 23, 12889-12899.	1.3	4

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19	Dynamics of nuclear recoil: QM-BOMD simulations of model systems following Î²-decay. Physical Chemistry Chemical Physics, 2021, 23, 25689-25698.	1.3	3
20	Virtual screening of norbornadiene-based molecular solar thermal energy storage systems using a genetic algorithm. Journal of Chemical Physics, 2021, 155, 184105.	1.2	7
21	Investigation of the Structural and Thermochemical Properties of [2.2.2]-Bicyclooctadiene Photoswitches. Journal of Physical Chemistry A, 2021, 125, 10330-10339.	1.1	8
22	User-friendly interface for fast and easy construction of Dalton input files. Journal of Molecular Modeling, 2020, 26, 274.	0.8	0
23	Tuning the dihydroazulene â€“ vinylheptafulvene couple for storage of solar energy. Russian Chemical Reviews, 2020, 89, 573-586.	2.5	43
24	Hydration of Atmospheric Molecular Clusters III: Procedure for Efficient Free Energy Surface Exploration of Large Hydrated Clusters. Journal of Physical Chemistry A, 2020, 124, 5253-5261.	1.1	16
25	Interfacial tension in water/n-decane/naphthenic acid systems predicted by a combined COSMO-RS theory and pendant drop experimental study. Molecular Physics, 2020, 118, e1764645.	0.8	3
26	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. Journal of Chemical Physics, 2020, 152, 214115.	1.2	45
27	Photo- and Collision-Induced Isomerization of a Charge-Tagged Norbornadieneâ€“Quadricyclane System. Journal of Physical Chemistry Letters, 2020, 11, 6045-6050.	2.1	15
28	The unexpected effect of aqueous ion pairs on the forbidden n â†' Ï€* transition in nitrate. Physical Chemistry Chemical Physics, 2020, 22, 11678-11685.	1.3	2
29	The influence of gold nanoparticles on the two photon absorption of photochromic molecular systems. Physical Chemistry Chemical Physics, 2019, 21, 18577-18588.	1.3	5
30	Synthesis of radiaannulene oligomers to model the elusive carbon allotrope 6,6,12-graphyne. Nature Communications, 2019, 10, 3714.	5.8	33
31	Norbornadieneâ€“dihydroazulene conjugates. Organic and Biomolecular Chemistry, 2019, 17, 7735-7746.	1.5	25
32	Benchmarking sampling methodology for calculations of Rayleigh light scattering properties of atmospheric molecular clusters. Physical Chemistry Chemical Physics, 2019, 21, 17274-17287.	1.3	4
33	Computational construction of the electronic Hamiltonian for photoinduced electron transfer and Redfield propagation. Physical Chemistry Chemical Physics, 2019, 21, 17366-17377.	1.3	3
34	Theoretical Investigation on the Control of Macrocyclic Dihydroazulene/Azobenzene Photoswitches. Journal of Physical Chemistry C, 2019, 123, 25579-25584.	1.5	7
35	Molecular solar thermal energy storage properties of photochromic molecules physisorbed onto nanoparticles. Chemical Physics Letters, 2019, 733, 136661.	1.2	7
36	The riddle of the forbidden UV absorption of aqueous nitrate: the oscillator strength of the n â†' Ï€* transition in NO₃^{â^'} including second order vibronic coupling. Physical Chemistry Chemical Physics, 2019, 21, 23466-23472.	1.3	2

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37	Mechanism of Photoinduced Dihydroazulene Ring-Opening Reaction. Journal of Physical Chemistry Letters, 2019, 10, 3944-3949.	2.1	19
38	Excitedâ€State Topology Modifications of the Dihydroazulene Photoswitch Through Aromaticity. ChemPhotoChem, 2019, 3, 619-629.	1.5	10
39	Electronic Predissociation in the Dichloromethane Cation CH₂Cl₂⁺ Electronic State ²A₁. Journal of Physical Chemistry A, 2019, 123, 4048-4056.	1.1	2
40	The influence of nanoparticles on the excitation energies of the photochromic dihydroazulene/vinylheptafulvene system. Physical Chemistry Chemical Physics, 2019, 21, 6689-6698.	1.3	12
41	Graphical user interface for an easy and reliable construction of input files to CP2K. Journal of Molecular Modeling, 2019, 25, 115.	0.8	1
42	Luminescence Spectroscopy of Rhodamine Homodimer Dications in Vacuo Reveals Strong Dyeâ€Dye Interactions. ChemPhysChem, 2019, 20, 533-537.	1.0	11
43	Simulation framework for screening of molecular solar thermal systems in the context of a hybrid device. Chemical Physics, 2019, 519, 92-100.	0.9	10
44	Molecular Solar Thermal Energy Storage Systems with Long Discharge Times Based on the Dihydroazulene/Vinylheptafulvene Couple. European Journal of Organic Chemistry, 2019, 2019, 1986-1993.	1.2	28
45	Theoretical study of the NMR chemical shift of Xe in supercritical condition. Journal of Molecular Modeling, 2018, 24, 62.	0.8	3
46	The quest for determining one-electron redox potentials of azulene-1-carbonitriles by calculation. Physical Chemistry Chemical Physics, 2018, 20, 7438-7446.	1.3	12
47	Multistate Photoswitches: Macrocyclic Dihydroazulene/Azobenzene Conjugates. Angewandte Chemie - International Edition, 2018, 57, 6069-6072.	7.2	32
48	Multistate Photoswitches: Macrocyclic Dihydroazulene/Azobenzene Conjugates. Angewandte Chemie, 2018, 130, 6177-6180.	1.6	15
49	Benchmarking tripletâ€“triplet annihilation photon upconversion schemes. Physical Chemistry Chemical Physics, 2018, 20, 12182-12192.	1.3	19
50	Subphthalocyanine-radiaannulene scaffold â€“ a multi-electron acceptor and strong chromophore. Chemical Communications, 2018, 54, 2763-2766.	2.2	6
51	Molecular solar thermal systems â€“ control of light harvesting and energy storage by protonation/deprotonation. RSC Advances, 2018, 8, 6356-6364.	1.7	21
52	Elucidation of the intrinsic optical properties of hydrogen-bonded and protonated flavin chromophores by photodissociation action spectroscopy. Physical Chemistry Chemical Physics, 2018, 20, 28678-28684.	1.3	9
53	Hydration of Atmospheric Molecular Clusters II: Organic Acidâ€“Water Clusters. Journal of Physical Chemistry A, 2018, 122, 8549-8556.	1.1	36
54	Complexation of Fullerenes by Subphthalocyanine Dimers. Organic Letters, 2018, 20, 5821-5825.	2.4	20

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55	Density Functional Theory Investigation on Boron Subphthalocyanineâ€“Ferrocene Dyads. Journal of Physical Chemistry A, 2018, 122, 7620-7627.	1.1	3
56	Donorâ^'Acceptorâ€Functionalized Subphthalocyanines for Dyeâ€Sensitized Solar Cells. ChemPhotoChem, 2018, 2, 976-985.	1.5	31
57	Hydration of Atmospheric Molecular Clusters: A New Method for Systematic Configurational Sampling. Journal of Physical Chemistry A, 2018, 122, 5026-5036.	1.1	53
58	The influence of nanoparticles on the polarizabilities and hyperpolarizabilities of photochromic molecules. Physical Chemistry Chemical Physics, 2018, 20, 23320-23327.	1.3	9
59	Heterogeneous nucleation of polymorphs on polymer surfaces: polymerâ€“molecule interactions using a heterogeneous dielectric solvation model. Journal of Molecular Modeling, 2018, 24, 156.	0.8	2
60	Heterogeneous nucleation of polymorphs on polymer surfaces: polymerâ€“molecule interactions using a Coulomb and van der Waals model. Journal of Molecular Modeling, 2018, 24, 155.	0.8	5
61	A DFT Study of Multimode Switching in a Combined DHA/VHF-DTE/DHB System for Use in Solar Heat Batteries. Journal of Physical Chemistry C, 2017, 121, 195-201.	1.5	17
62	Dialkylated Dihydroazulene and Vinylheptafulvene Derivatives â€“ Synthesis and Switching Properties. European Journal of Organic Chemistry, 2017, 2017, 2932-2939.	1.2	15
63	Predicting transport regime and local electrostatic environment from Coulomb blockade diamond sizes. Journal of Chemical Physics, 2017, 146, 104306.	1.2	2
64	A Study of Electrocyclic Reactions in a Molecular Junction: Mechanistic and Energetic Requirements for Switching in the Coulomb Blockade Regime. ChemPhysChem, 2017, 18, 1492-1492.	1.0	0
65	Single-molecule detection of dihydroazulene photo-thermal reaction using break junction technique. Nature Communications, 2017, 8, 15436.	5.8	106
66	Benchmark Study of the Structural and Thermochemical Properties of a Dihydroazulene/Vinylheptafulvene Photoswitch. Journal of Physical Chemistry A, 2017, 121, 3148-3154.	1.1	23
67	A Study of Electrocyclic Reactions in a Molecular Junction: Mechanistic and Energetic Requirements for Switching in the Coulomb Blockade Regime. ChemPhysChem, 2017, 18, 1517-1525.	1.0	2
68	Stepwise â€œDark Photoswitchingâ€•of Photochromic Dimers in a Junction. Journal of Physical Chemistry C, 2017, 121, 3163-3170.	1.5	3
69	Towards Storage of Solar Energy in Photochromic Molecules: Benzannulation of the Dihydroazulene/Vinylheptafulvene Couple. ChemPhotoChem, 2017, 1, 206-212.	1.5	29
70	Expanding the Hammett Correlations for the Vinylheptafulvene Ringâ€Closure Reaction. European Journal of Organic Chemistry, 2017, 2017, 1052-1062.	1.2	8
71	Thienoâ€Fused Subporphyrazines: A New Class of Light Harvesters. Chemistry - A European Journal, 2017, 23, 16194-16198.	1.7	21
72	Photoswitchable Dihydroazulene Macrocycles for Solar Energy Storage: The Effects of Ring Strain. Journal of Organic Chemistry, 2017, 82, 10398-10407.	1.7	33

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73	Molecular Properties of Sandwiched Molecules Between Electrodes and Nanoparticles. Advances in Quantum Chemistry, 2017, 75, 53-102.	0.4	7
74	Density Functional Theory Study of the Solvent Effects on Systematically Substituted Dihydroazulene/Vinylheptafulvene Systems: Improving the Capability of Molecular Energy Storage. Journal of Physical Chemistry A, 2017, 121, 8856-8865.	1.1	18
75	Solar Thermal Energy Storage in a Photochromic Macrocycle. Chemistry - A European Journal, 2016, 22, 10796-10800.	1.7	36
76	Fine-tuning the lifetimes and energy storage capacities of meta-stable vinylheptafulvenes via substitution at the vinyl position. RSC Advances, 2016, 6, 49003-49010.	1.7	23
77	Boron Subphthalocyanine Based Molecular Triad Systems for the Capture of Solar Energy. Journal of Physical Chemistry A, 2016, 120, 7694-7703.	1.1	10
78	Aromaticityâ€Controlled Energy Storage Capacity of the Dihydroazuleneâ€Vinylheptafulvene Photochromic System. Chemistry - A European Journal, 2016, 22, 14567-14575.	1.7	55
79	First hyperpolarizability of para-aminoaniline induced by a variety of gold nano particles. Physical Chemistry Chemical Physics, 2016, 18, 24343-24349.	1.3	3
80	Theoretical Investigation of Substituent Effects on the Dihydroazulene/Vinylheptafulvene Photoswitch: Increasing the Energy Storage Capacity. Journal of Physical Chemistry A, 2016, 120, 9782-9793.	1.1	39
81	Characterisation of dihydroazulene and vinylheptafulvene derivatives using Raman spectroscopy: The CN-stretching region. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 161, 70-76.	2.0	3
82	Azulenium chemistry: towards new derivatives of photochromic dihydroazulenes. Organic and Biomolecular Chemistry, 2016, 14, 2403-2412.	1.5	14
83	Gas-Phase Spectroscopy of a Vinylheptafulvene Chromophore. European Journal of Mass Spectrometry, 2015, 21, 569-577.	0.5	3
84	Controlling Twoâ€Step Multimode Switching of Dihydroazulene Photoswitches. Chemistry - A European Journal, 2015, 21, 3968-3977.	1.7	36
85	Towards Solar Energy Storage in the Photochromic Dihydroazuleneâ€“Vinylheptafulvene System. Chemistry - A European Journal, 2015, 21, 7454-7461.	1.7	79
86	Tracking molecular resonance forms of donorâ€“acceptor pushâ€“pull molecules by single-molecule conductance experiments. Nature Communications, 2015, 6, 10233.	5.8	36
87	Computational Study of the Effect of Glyoxalâ€“Sulfate Clustering on the Henryâ€™s Law Coefficient of Glyoxal. Journal of Physical Chemistry A, 2015, 119, 4509-4514.	1.1	35
88	Computational Methodology Study of the Optical and Thermochemical Properties of a Molecular Photoswitch. Journal of Physical Chemistry A, 2015, 119, 896-904.	1.1	57
89	Dark Photoswitching Induces Coulomb Blockade Diamond Collapse. Journal of Physical Chemistry C, 2015, 119, 14829-14833.	1.5	6
90	Rayleigh light scattering properties of atmospheric molecular clusters consisting of sulfuric acid and bases. Physical Chemistry Chemical Physics, 2015, 17, 15701-15709.	1.3	14

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91	Optical properties of pyridine and methyl-pyridinium in water using DFT/MM. Molecular Physics, 2015, 113, 3253-3263.	0.8	2
92	Glyoxal and Methylglyoxal Setschenow Salting Constants in Sulfate, Nitrate, and Chloride Solutions: Measurements and Gibbs Energies. Environmental Science & Technology, 2015, 49, 11500-11508.	4.6	64
93	The chemistry of Coulomb blockade diamonds for 1,4-diamino-benzene. Chemical Physics, 2015, 459, 40-44.	0.9	3
94	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	6.2	1,166
95	Computational assignment of redox states to Coulomb blockade diamonds. Physical Chemistry Chemical Physics, 2014, 16, 17473-17478.	1.3	11
96	Computational approaches for efficiently modelling of small atmospheric clusters. Chemical Physics Letters, 2014, 615, 26-29.	1.2	75
97	Computational study of the Rayleigh light scattering properties of atmospheric pre-nucleation clusters. Physical Chemistry Chemical Physics, 2014, 16, 10883-10890.	1.3	37
98	A Hybrid Density Functional Theory/Molecular Mechanics Approach for Linear Response Properties in Heterogeneous Environments. Journal of Chemical Theory and Computation, 2014, 10, 989-1003.	2.3	39
99	QM/MM-MD Simulations of Conjugated Polyelectrolytes: A Study of Luminescent Conjugated Oligothiophenes for Use as Biophysical Probes. Journal of Physical Chemistry A, 2014, 118, 3419-3428.	1.1	26
100	Molecular Interaction of Pinic Acid with Sulfuric Acid: Exploring the Thermodynamic Landscape of Cluster Growth. Journal of Physical Chemistry A, 2014, 118, 7892-7900.	1.1	64
101	Failures of TDDFT in describing the lowest intramolecular charge-transfer excitation in para-nitroaniline. Molecular Physics, 2013, 111, 1235-1248.	0.8	79
102	Assessment of binding energies of atmospherically relevant clusters. Physical Chemistry Chemical Physics, 2013, 15, 16442.	1.3	130
103	Ambient reaction kinetics of atmospheric oxygenated organics with the OH radical: a computational methodology study. Physical Chemistry Chemical Physics, 2013, 15, 9636.	1.3	36
104	Interaction of Glycine with Common Atmospheric Nucleation Precursors. Journal of Physical Chemistry A, 2013, 117, 12990-12997.	1.1	55
105	Influence of Nucleation Precursors on the Reaction Kinetics of Methanol with the OH Radical. Journal of Physical Chemistry A, 2013, 117, 6695-6701.	1.1	51
106	Structures and reaction rates of the gaseous oxidation of SO₂ by an O₃^{â^'}(H<sub>2</sub&amp cluster â€“ a density functional theory investigation. Atmospheric Chemistry and Physics, 2012, 12, 3639-3652.	1.2	24
107	Assessment of Density Functional Theory in Predicting Structures and Free Energies of Reaction of Atmospheric Prenucleation Clusters. Journal of Chemical Theory and Computation, 2012, 8, 2071-2077.	2.3	168
108	Obtaining Enhanced Circular Dichroism in [4]Heterohelicenium Analogues. Journal of Physical Chemistry A, 2012, 116, 8744-8752.	1.1	14

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109	On the importance of excited state dynamic response electron correlation in polarizable embedding methods. Journal of Computational Chemistry, 2012, 33, 2012-2022.	1.5	38
110	Hybrid density functional theory/molecular mechanics calculations of two-photon absorption of dimethylamino nitro stilbene in solution. Physical Chemistry Chemical Physics, 2011, 13, 12506.	1.3	64
111	Racemization Mechanisms and Electronic Circular Dichroism of [4]Heterohelicenium Dyes: A Theoretical Study. Journal of Physical Chemistry A, 2011, 115, 12025-12033.	1.1	18
112	Ab initio studies of O₂^{â^'}(H<sub>2</sub&amp and O₃^{â^'}(H<sub>2</sub&amp anionic molecular clusters, <i>n</i>â‰12. Atmospheric Chemistry and Physics, 2011, 11, 7133-7142.	1.9	43
113	Direct probing of ion pair formation using a symmetric triangulenium dye. Photochemical and Photobiological Sciences, 2011, 10, 1963-1973.	1.6	26
114	A theoretical approach to molecular single-electron transistors. Theoretical Chemistry Accounts, 2011, 130, 839-850.	0.5	9
115	Fluorescence and phosphorescence of acetone in neat liquid and aqueous solution studied by QM/MM and PCM approaches. International Journal of Quantum Chemistry, 2011, 111, 1511-1520.	1.0	17
116	Determining moleculeâ€"particle reaction parameters. International Journal of Quantum Chemistry, 2011, 111, 1740-1747.	1.0	3
117	The iterative selfâ€consistent reactionâ€field method: The refractive index of pure water. International Journal of Quantum Chemistry, 2011, 111, 904-913.	1.0	5
118	Computational protocols for prediction of solute NMR relative chemical shifts. A case study of <scp>L</scp>â€tryptophan in aqueous solution. Journal of Computational Chemistry, 2011, 32, 2853-2864.	1.5	25
119	Outcome in high risk patients with unprotected left main coronary artery stenosis treated with percutaneous coronary intervention. Catheterization and Cardiovascular Interventions, 2010, 75, 101-108.	0.7	23
120	Calculated two-photon electronic transitions in sulfuric acid and its atmospheric relevance. Chemical Physics Letters, 2010, 498, 18-21.	1.2	1
121	Nonlinear optical properties of solvated molecules. Journal of Computational Methods in Sciences and Engineering, 2010, 10, 489-499.	0.1	0
122	Nonlinear Optical Effects Induced by Nanoparticles in Symmetric Molecules. Journal of Physical Chemistry C, 2010, 114, 20870-20876.	1.5	15
123	Solvatochromic Shifts in Uracil: A Combined MD-QM/MM Study. Journal of Chemical Theory and Computation, 2010, 6, 249-256.	2.3	66
124	The Effect of Solvation on the Mean Excitation Energy of Glycine. Journal of Physical Chemistry Letters, 2010, 1, 242-245.	2.1	20
125	Tribute to Mark A. Ratner. Journal of Physical Chemistry C, 2010, 114, 20293-20294.	1.5	0
126	On the existence of the H3 tautomer of adenine in aqueous solution. Rationalizations based on hybrid quantum mechanics/molecular mechanics predictions. Physical Chemistry Chemical Physics, 2010, 12, 761-768.	1.3	25

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127	Interpretation of the Ultrafast Photoinduced Processes in Pentacene Thin Films. Journal of the American Chemical Society, 2010, 132, 3431-3439.	6.6	59
128	Are there long-term benefits in following stable heart failure patients in a heart failure clinic?. Scandinavian Cardiovascular Journal, 2009, 43, 158-162.	0.4	6
129	Charge transfer excitation energies in pyridineâ€“silver complexes studied by a QM/MM method. Chemical Physics Letters, 2009, 470, 285-288.	1.2	38
130	Charge-resonance excitations in symmetric molecules â€“ Comparison of linear response DFT with CC3 for the excited states of a model dimer. Chemical Physics Letters, 2009, 478, 127-131.	1.2	11
131	Molecular Mechanics Interaction Models for Optical Electronic Properties. Journal of Computational and Theoretical Nanoscience, 2009, 6, 270-291.	0.4	7
132	On the accurate calculation of polarizabilities and second hyperpolarizabilities of polyacetylene oligomer chains using the CAM-B3LYP density functional. Journal of Chemical Physics, 2009, 130, 194114.	1.2	256
133	Prediction of spin-spin coupling constants in solution based on combined density functional theory/molecular mechanics. Journal of Chemical Physics, 2009, 130, 134508.	1.2	48
134	Solvent effects on the nitrogen NMR shielding and nuclear quadrupole coupling constants in 1-methyltriazoles. Chemical Physics Letters, 2008, 460, 129-136.	1.2	16
135	Determination of rate constants for the uptake process involving SO2 and an aerosol particle. A quantum mechanics/molecular mechanics and quantum statistical investigation. Chemical Physics, 2008, 348, 21-30.	0.9	7
136	On the Accuracy of Density Functional Theory to Predict Shifts in Nuclear Magnetic Resonance Shielding Constants due to Hydrogen Bonding. Journal of Chemical Theory and Computation, 2008, 4, 267-277.	2.3	51
137	From Molecules to Droplets. Advances in Quantum Chemistry, 2008, 55, 355-385.	0.4	4
138	Computational Quantum Chemistry: A New Approach to Atmospheric Nucleation. Advances in Quantum Chemistry, 2008, , 449-478.	0.4	39
139	On the performance of quantum chemical methods to predict solvatochromic effects: The case of acrolein in aqueous solution. Journal of Chemical Physics, 2008, 128, 194503.	1.2	76
140	Modelling spectroscopic properties of large molecular systems. The combined Density Functional Theory/Molecular Mechanics approach. Journal of Computational Methods in Sciences and Engineering, 2008, 7, 135-158.	0.1	4
141	Linear Response Theory in Connection to Density Functional Theory/Molecular Dynamics and Coupled Cluster/Molecular Dynamics Methods. Challenges and Advances in Computational Chemistry and Physics, 2008, , 349-380.	0.6	2
142	Density functional self-consistent quantum mechanics/molecular mechanics theory for linear and nonlinear molecular properties: Applications to solvated water and formaldehyde. Journal of Chemical Physics, 2007, 126, 154112.	1.2	144
143	NadyktoetÂal.Reply:. Physical Review Letters, 2007, 98, .	2.9	9
144	Nuclear magnetic shielding constants of liquid water: Insights from hybrid quantum mechanics/molecular mechanics models. Journal of Chemical Physics, 2007, 126, 034510.	1.2	59

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145	Solvent Effects on NMR Isotropic Shielding Constants. A Comparison between Explicit Polarizable Discrete and Continuum Approaches. Journal of Physical Chemistry A, 2007, 111, 4199-4210.	1.1	74
146	Two-Photon Cross-Sections of Photosensitizers in Vacuum, in Solution and within Proteins. AIP Conference Proceedings, 2007, , .	0.3	0
147	Theoretical Methods for Structured Environments. AIP Conference Proceedings, 2007, , .	0.3	0
148	Microscopic polarization in ropes and films of aligned carbon nanotubes. Journal of Computational Methods in Sciences and Engineering, 2007, 6, 353-364.	0.1	1
149	Gauge-origin independent magnetizabilities from hybrid quantum mechanics/molecular mechanics models: Theory and applications to liquid water. Chemical Physics Letters, 2007, 442, 322-328.	1.2	3
150	Hydrogen bonding effects on infrared and Raman spectra of drug molecules. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 66, 213-224.	2.0	48
151	Quantum Nature of the Sign Preference in Ion-Induced Nucleation. Physical Review Letters, 2006, 96, 125701.	2.9	72
152	Coupled Cluster and Density Functional Theory Studies of the Vibrational Contribution to the Optical Rotation of (S)-Propylene Oxide. Journal of the American Chemical Society, 2006, 128, 976-982.	6.6	77
153	Uptake of Phenol on Aerosol Particlesâ€. Journal of Physical Chemistry A, 2006, 110, 660-670.	1.1	18
154	2004, Volume 108A Sulfuric Acid and Sulfuric Acid Hydrates in the Gas Phase:Â A DFT Investigation. Journal of Physical Chemistry A, 2006, 110, 7982-7984.	1.1	10
155	CORRELATED ELECTRONIC STRUCTURE NONLINEAR RESPONSE METHODS FOR STRUCTURED ENVIRONMENTS. Annual Review of Physical Chemistry, 2006, 57, 365-402.	4.8	11
156	Neurohormonal activation and diagnostic value of cardiac peptides in patients with suspected mild heart failure. International Journal of Cardiology, 2006, 110, 324-333.	0.8	11
157	THE (HYPER)POLARIZABILITIES OF LIQUID WATER MODELLED USING COUPLED CLUSTER/MOLECULAR MECHANICS RESPONSE THEORY METHODS. , 2006, , 215-281.		0
158	Coexistence of metastable nitric acid dihydrates: A molecular level contribution to understanding the formation of polar stratospheric clouds crystals. Chemical Physics Letters, 2006, 426, 20-25.	1.2	7
159	The electronic spectrum of the micro-solvated alanine zwitterion calculated using the combined coupled cluster/molecular mechanics method. Chemical Physics Letters, 2006, 429, 430-435.	1.2	19
160	Density functional theory calculations of hydrogen bonding energies of drug molecules. Computational and Theoretical Chemistry, 2006, 776, 61-68.	1.5	5
161	Theoretical investigation of the coexistence of Î± and Î²-nitric acid trihydrates (NAT) molecular conformations. Chemical Physics, 2006, 324, 210-215.	0.9	8
162	Tei index and neurohormonal activation in patients with incident heart failure: Serial changes and prognostic value. European Journal of Heart Failure, 2006, 8, 599-608.	2.9	32

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163	Statistical mechanically averaged molecular properties of liquid water calculated using the combined coupled cluster/molecular dynamics method. Journal of Chemical Physics, 2006, 124, 124503.	1.2	55
164	Two-photon absorption cross sections: An investigation of solvent effects. Theoretical studies on formaldehyde and water. Journal of Chemical Physics, 2006, 125, 184501.	1.2	35
165	Multiconfigurational Self-Consistent Field-Molecular Mechanics Response Methods. Challenges and Advances in Computational Chemistry and Physics, 2006, , 283-298.	0.6	0
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