Jacob Kongsted

List of Publications by Year in descending order

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246 papers	9,973 citations	34076 52 h-index	51562 86 g-index
251 all docs	251 docs citations	251 times ranked	6933 citing authors

#	Article	IF	Citations
1	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	6.2	1,166
2	Excited States in Solution through Polarizable Embedding. Journal of Chemical Theory and Computation, 2010, 6, 3721-3734.	2.3	293
3	Electronic Energy Transfer in Condensed Phase Studied by a Polarizable QM/MM Model. Journal of Chemical Theory and Computation, 2009, 5, 1838-1848.	2.3	259
4	Polarizability of molecular clusters as calculated by a dipole interaction model. Journal of Chemical Physics, 2002, 116, 4001-4010.	1.2	180
5	Benchmarking two-photon absorption cross sections: performance of CC2 and CAM-B3LYP. Physical Chemistry Chemical Physics, 2015, 17, 19306-19314.	1.3	160
6	Molecular Properties through Polarizable Embedding. Advances in Quantum Chemistry, 2011, 61, 107-143.	0.4	145
7	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
8	The Journey of HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitors (NNRTIs) from Lab to Clinic. Journal of Medicinal Chemistry, 2019, 62, 4851-4883.	2.9	124
9	Photosynthetic Light-Harvesting Is Tuned by the Heterogeneous Polarizable Environment of the Protein. Journal of the American Chemical Society, 2011, 133, 3078-3084.	6.6	123
10	Benchmarking Time-Dependent Density Functional Theory for Excited State Geometries of Organic Molecules in Gas-Phase and in Solution. Journal of Chemical Theory and Computation, 2013, 9, 2209-2220.	2.3	123
11	The QM/MM approach for wavefunctions, energies and response functions within self-consistent field and coupled cluster theories. Molecular Physics, 2002, 100, 1813-1828.	0.8	122
12	An improved method to predict the entropy term with the MM/PBSA approach. Journal of Computer-Aided Molecular Design, 2009, 23, 63-71.	1.3	122
13	Excitation Energies in Solution: The Fully Polarizable QM/MM/PCM Method. Journal of Physical Chemistry B, 2011, 115, 3027-3037.	1.2	118
14	Linear response functions for coupled cluster/molecular mechanics including polarization interactions. Journal of Chemical Physics, 2003, 118, 1620-1633.	1.2	117
15	The polarizable embedding coupled cluster method. Journal of Chemical Physics, 2011, 134, 104108.	1.2	117
16	Overview of Recent Strategic Advances in Medicinal Chemistry. Journal of Medicinal Chemistry, 2019, 62, 9375-9414.	2.9	108
17	Coupled Cluster Calculation of the n â†' Ï€* Electronic Transition of Acetone in Aqueous Solution. Journal of Physical Chemistry A, 2005, 109, 8001-8010.	1.1	107
18	Coupled cluster calculations of the optical rotation of S-propylene oxide in gas phase and solution. Chemical Physics Letters, 2005, 401, 385-392.	1.2	94

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19	Scrutinizing the effects of polarization in QM/MM excited state calculations. Physical Chemistry Chemical Physics, 2011, 13, 18551.	1.3	94
20	Breakdown of the first hyperpolarizability/bond-length alternation parameter relationship. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 16453-16458.	3.3	84
21	Ligand Affinities Estimated by Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2010, 6, 1726-1737.	2.3	81
22	Failures of TDDFT in describing the lowest intramolecular charge-transfer excitation in para-nitroaniline. Molecular Physics, 2013, 111, 1235-1248.	0.8	79
23	Optimized Basis Sets for Calculation of Electron Paramagnetic Resonance Hyperfine Coupling Constants: aug-cc-pVTZ-J for the 3d Atoms Scâ€“Zn. Journal of Chemical Theory and Computation, 2011, 7, 4077-4087.	2.3	78
24	Polarizable Density Embedding: A New QM/QM/MM-Based Computational Strategy. Journal of Physical Chemistry A, 2015, 119, 5344-5355.	1.1	78
25	Excited states in large molecular systems through polarizable embedding. Physical Chemistry Chemical Physics, 2016, 18, 20234-20250.	1.3	78
26	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
27	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
28	A combined quantum mechanics/molecular mechanics study of the one- and two-photon absorption in the green fluorescent protein. Physical Chemistry Chemical Physics, 2012, 14, 5440.	1.3	76
29	Solvent effects on the nâ†'Ï€[sup â^—] electronic transition in formaldehyde: A combined coupled cluster/molecular dynamics study. Journal of Chemical Physics, 2004, 121, 8435.	1.2	75
30	Solvation Effects on Electronic Transitions: Exploring the Performance of Advanced Solvent Potentials in Polarizable Embedding Calculations. Journal of Chemical Theory and Computation, 2011, 7, 2209-2217.	2.3	75
31	PERIâ€“CC2: A Polarizable Embedded RI-CC2 Method. Journal of Chemical Theory and Computation, 2012, 8, 3274-3283.	2.3	75
32	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
33	Automatic generation of force fields and property surfaces for use in variational vibrational calculations of anharmonic vibrational energies and zero-point vibrational averaged properties. Journal of Chemical Physics, 2006, 125, 124108.	1.2	72
34	Benchmarking NMR indirect nuclear spin-spin coupling constants: SOPPA, SOPPA(CC2), and SOPPA(CCSD) versus CCSD. Journal of Chemical Physics, 2010, 133, 144106.	1.2	72
35	Coupled Cluster/Molecular Mechanics Method:â€‰ Implementation and Application to Liquid Water. Journal of Physical Chemistry A, 2003, 107, 2578-2588.	1.1	70
36	Recent developments in the medicinal chemistry of single boron atom-containing compounds. Acta Pharmaceutica Sinica B, 2021, 11, 3035-3059.	5.7	70

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37	How accurate are continuum solvation models for drug-like molecules?. Journal of Computer-Aided Molecular Design, 2009, 23, 395-409.	1.3	68
38	Second harmonic generation second hyperpolarizability of water calculated using the combined coupled cluster dielectric continuum or different molecular mechanics methods. Journal of Chemical Physics, 2004, 120, 3787-3798.	1.2	67
39	The combined multiconfigurational self-consistent-field/molecular mechanics wave function approach. Journal of Chemical Physics, 2001, 115, 2393-2400.	1.2	66
40	Solvatochromic Shifts in Uracil: A Combined MD-QM/MM Study. Journal of Chemical Theory and Computation, 2010, 6, 249-256.	2.3	66
41	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
42	How to Model Solvent Effects on Molecular Properties Using Quantum Chemistry? Insights from Polarizable Discrete or Continuum Solvation Models. Journal of Physical Chemistry A, 2007, 111, 9890-9900.	1.1	62
43	Basis Set Convergence of Indirect Spinâ€“Spin Coupling Constants in the Kohnâ€“Sham Limit for Several Small Molecules. Journal of Physical Chemistry A, 2012, 116, 3728-3738.	1.1	61
44	Local electric fields and molecular properties in heterogeneous environments through polarizable embedding. Physical Chemistry Chemical Physics, 2016, 18, 10070-10080.	1.3	60
45	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
46	Interpretation of the Ultrafast Photoinduced Processes in Pentacene Thin Films. Journal of the American Chemical Society, 2010, 132, 3431-3439.	6.6	59
47	Accurate Predictions of Nonpolar Solvation Free Energies Require Explicit Consideration of Binding-Site Hydration. Journal of the American Chemical Society, 2011, 133, 13081-13092.	6.6	56
48	Nonlinear optical response properties of molecules in condensed phases using the coupled cluster/dielectric continuum or molecular mechanics methods. Journal of Chemical Physics, 2003, 119, 10519-10535.	1.2	55
49	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
50	Demystifying the solvatochromic reversal in Brookerâ€™s merocyanine dye. Physical Chemistry Chemical Physics, 2011, 13, 1290-1292.	1.3	55
51	Automatic generation of potential energy and property surfaces of polyatomic molecules in normal coordinates. Journal of Chemical Physics, 2007, 127, 204106.	1.2	54
52	Molecular-Level Insight into the Spectral Tuning Mechanism of the DsRed Chromophore. Journal of Physical Chemistry Letters, 2012, 3, 3513-3521.	2.1	54
53	Polarizable Density Embedding: A Solution to the Electron Spill-Out Problem in Multiscale Modeling. Journal of Physical Chemistry Letters, 2017, 8, 5949-5958.	2.1	53
54	Linear Response Properties of Liquid Water Calculated Using CC2 and CCSD within Different Molecular Mechanics Methodsâ€. Journal of Physical Chemistry A, 2004, 108, 8646-8658.	1.1	52

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55	Modeling the Structure and Absorption Spectra of Stilbazolium Merocyanine in Polar and Nonpolar Solvents Using Hybrid QM/MM Techniques. Journal of Physical Chemistry B, 2010, 114, 13349-13357.	1.2	52
56	Toward Reliable Prediction of the Energy Ladder in Multichromophoric Systems: A Benchmark Study on the FMO Light-Harvesting Complex. Journal of Chemical Theory and Computation, 2013, 9, 4928-4938.	2.3	52
57	Theoretical Study of the Electronic Gas-Phase Spectrum of Glycine, Alanine, and Related Amines and Carboxylic Acids. Journal of Physical Chemistry A, 2005, 109, 1430-1440.	1.1	51
58	Linear response functions for a vibrational configuration interaction state. Journal of Chemical Physics, 2006, 125, 214309.	1.2	51
59	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
60	Performance of popular XCâ€functionals for the description of excitation energies in GFPâ€like chromophore models. International Journal of Quantum Chemistry, 2012, 112, 789-800.	1.0	51
61	Solvent effects on zero-point vibrational corrections to optical rotations and nuclear magnetic resonance shielding constants. Chemical Physics Letters, 2008, 451, 226-232.	1.2	50
62	Accuracy of Protein Embedding Potentials: An Analysis in Terms of Electrostatic Potentials. Journal of Chemical Theory and Computation, 2015, 11, 1832-1842.	2.3	50
63	Energy Flow in the Cryptophyte PE545 Antenna Is Directed by Bilin Pigment Conformation. Journal of Physical Chemistry B, 2013, 117, 4263-4273.	1.2	49
64	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
65	On the Photophysics of Carotenoids: A Multireference DFT Study of Peridinin. Journal of Physical Chemistry B, 2013, 117, 13808-13815.	1.2	48
66	Damped Response Theory in Combination with Polarizable Environments: The Polarizable Embedding Complex Polarization Propagator Method. Journal of Chemical Theory and Computation, 2014, 10, 1164-1171.	2.3	48
67	Dipole and quadrupole moments of liquid water calculated within the coupled cluster/molecular mechanics method. Chemical Physics Letters, 2002, 364, 379-386.	1.2	47
68	Analysis of computational models for an accurate study of electronic excitations in GFP. Physical Chemistry Chemical Physics, 2015, 17, 2582-2588.	1.3	47
69	The multi-configuration self-consistent field method within a polarizable embedded framework. Journal of Chemical Physics, 2013, 139, 044101.	1.2	46
70	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. Journal of Chemical Physics, 2020, 152, 214115.	1.2	45
71	Thenâ†' Ï€* Electronic Transition in Microsolvated Formaldehyde. A Coupled Cluster and Combined Coupled Cluster/Molecular Mechanics Studyâ€. Journal of Physical Chemistry A, 2004, 108, 8624-8632.	1.1	44
72	Inclusion of Terpenoid Plant Extracts in Lipid Bilayers Investigated by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 15825-15831.	1.2	44

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73	A polarizable embedding DFT study of one-photon absorption in fluorescent proteins. Physical Chemistry Chemical Physics, 2013, 15, 4735.	1.3	44
74	Carotenoids and Light-Harvesting: From DFT/MRCI to the Tammâ€“Dancoff Approximation. Journal of Chemical Theory and Computation, 2015, 11, 655-666.	2.3	44
75	Calculation of Vibrational Infrared Intensities and Raman Activities Using Explicit Anharmonic Wave Functions. Journal of Physical Chemistry A, 2007, 111, 11205-11213.	1.1	43
76	On the importance of vibrational contributions to small-angle optical rotation: Fluoro-oxirane in gas phase and solution. Journal of Chemical Physics, 2009, 130, 034310.	1.2	43
77	Frequency-Dependent Polarizability of Boron Nitride Nanotubes:Â A Theoretical Study. Journal of Physical Chemistry B, 2001, 105, 10243-10248.	1.2	42
78	Solvent Effects on Rotatory Strength Tensors. 1. Theory and Application of the Combined Coupled Cluster/Dielectric Continuum Model. Journal of Physical Chemistry A, 2004, 108, 3632-3641.	1.1	42
79	Averaged Solvent Embedding Potential Parameters for Multiscale Modeling of Molecular Properties. Journal of Chemical Theory and Computation, 2016, 12, 1684-1695.	2.3	42
80	Color modeling of protein optical probes. Physical Chemistry Chemical Physics, 2012, 14, 1107-1112.	1.3	40
81	The Role of Molecular Conformation and Polarizable Embedding for One- and Two-Photon Absorption of Disperse Orange 3 in Solution. Journal of Physical Chemistry B, 2012, 116, 8169-8181.	1.2	40
82	Unraveling the similarity of the photoabsorption of deprotonated p-coumaric acid in the gas phase and within the photoactive yellow protein. Physical Chemistry Chemical Physics, 2011, 13, 1585-1589.	1.3	39
83	Relation between Nonlinear Optical Properties of Pushâ€“Pull Molecules and Metric of Charge Transfer Excitations. Journal of Chemical Theory and Computation, 2015, 11, 4182-4188.	2.3	39
84	Charge transfer excitation energies in pyridineâ€“silver complexes studied by a QM/MM method. Chemical Physics Letters, 2009, 470, 285-288.	1.2	38
85	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
86	Mutations in the Bacterial Ribosomal Protein L3 and Their Association with Antibiotic Resistance. Antimicrobial Agents and Chemotherapy, 2015, 59, 3518-3528.	1.4	38
87	A CC2 dielectric continuum model and a CC2 molecular mechanics model. Molecular Physics, 2003, 101, 2055-2071.	0.8	37
88	Gas phase optical rotation calculated from coupled cluster theory with zeroâ€point vibrational corrections from density functional theory. Chirality, 2009, 21, E68-75.	1.3	37
89	Nuclear Magnetic Shielding Constants from Quantum Mechanical/Molecular Mechanical Calculations Using Polarizable Embedding: Role of the Embedding Potential. Journal of Chemical Theory and Computation, 2014, 10, 981-988.	2.3	37
90	Response properties of embedded molecules through the polarizable embedding model. International Journal of Quantum Chemistry, 2019, 119, e25717.	1.0	37

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91	Convergence of environment polarization effects in multiscale modeling of excitation energies. Computational and Theoretical Chemistry, 2014, 1040-1041, 304-311.	1.1	36
92	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
93	Twoâ€Photon Solvatochromism II: Experimental and Theoretical Study of Solvent Effects on the Twoâ€Photon Absorption Spectrum of Reichardtâ€™s Dye. ChemPhysChem, 2013, 14, 3731-3739.	1.0	32
94	The Quality of the Embedding Potential Is Decisive for Minimal Quantum Region Size in Embedding Calculations: The Case of the Green Fluorescent Protein. Journal of Chemical Theory and Computation, 2017, 13, 6230-6236.	2.3	32
95	Benchmarking SOPPA(CC2) for the calculation of indirect nuclear spinâ€“spin coupling constants: Carbocycles. Chemical Physics, 2011, 381, 35-43.	0.9	31
96	Quantification of the Ï€â€“Ï€ Interactions that Govern Tertiary Structure in Donorâ€“Acceptor [2]Pseudorotaxanes. Journal of the American Chemical Society, 2012, 134, 3857-3863.	6.6	31
97	Improving the calculation of electron paramagnetic resonance hyperfine coupling tensors for d-block metals. Physical Chemistry Chemical Physics, 2012, 14, 10669.	1.3	31
98	Computational screening of one- and two-photon spectrally tuned channelrhodopsin mutants. Physical Chemistry Chemical Physics, 2013, 15, 7567.	1.3	31
99	Dehydroergosterol as an Analogue for Cholesterol: Why It Mimics Cholesterol So Wellâ€”or Does It?. Journal of Physical Chemistry B, 2014, 118, 7345-7357.	1.2	31
100	A Click Chemistry Approach to Pleuromutilin Derivatives, Part 2: Conjugates with Acyclic Nucleosides and Their Ribosomal Binding and Antibacterial Activity. Journal of Medicinal Chemistry, 2012, 55, 2067-2077.	2.9	30
101	Validating and Analyzing EPR Hyperfine Coupling Constants with Density Functional Theory. Journal of Chemical Theory and Computation, 2013, 9, 2380-2388.	2.3	29
102	Amyloid Fibril-Induced Structural and Spectral Modifications in the Thioflavin-T Optical Probe. Journal of Physical Chemistry Letters, 2013, 4, 70-77.	2.1	29
103	Polarizable embedding with a multiconfiguration short-range density functional theory linear response method. Journal of Chemical Physics, 2015, 142, 114113.	1.2	29
104	Avoiding Electron Spill-Out in QM/MM Calculations on Excited States with Simple Pseudopotentials. Journal of Chemical Theory and Computation, 2020, 16, 1373-1381.	2.3	29
105	A Theoretical Study of the Reaction between CH3S(OH)CH3and O2â€. Journal of Physical Chemistry A, 2004, 108, 8659-8671.	1.1	28
106	Molecular design opportunities presented by solventâ€exposed regions of target proteins. Medicinal Research Reviews, 2019, 39, 2194-2238.	5.0	28
107	Virtual Screening Models for Prediction of HIV-1 RT Associated RNase H Inhibition. PLoS ONE, 2013, 8, e73478.	1.1	28
108	Association Dynamics and Linear and Nonlinear Optical Properties of an N-Acetylaladanamide Probe in a POPC Membrane. Journal of the American Chemical Society, 2013, 135, 13590-13597.	6.6	27

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109	Transition-State Docking of Flunitrazepam and Progesterone in Cytochrome P450. Journal of Chemical Theory and Computation, 2008, 4, 673-681.	2.3	26
110	Nonpolar Solvation Free Energies of Proteinâ^'Ligand Complexes. Journal of Chemical Theory and Computation, 2010, 6, 3558-3568.	2.3	26
111	Basis Set Recommendations for DFT Calculations of Gas-Phase Optical Rotation at Different Wavelengths. Journal of Chemical Theory and Computation, 2012, 8, 4425-4433.	2.3	26
112	Computational Approach for Studying Optical Properties of DNA Systems in Solution. Journal of Chemical Theory and Computation, 2016, 12, 5050-5057.	2.3	26
113	Importance of Accurate Structures for Quantum Chemistry Embedding Methods: Which Strategy Is Better?. Journal of Chemical Theory and Computation, 2018, 14, 4309-4319.	2.3	26
114	Polarizable Embedding Combined with the Algebraic Diagrammatic Construction: Tackling Excited States in Biomolecular Systems. Journal of Chemical Theory and Computation, 2018, 14, 4870-4883.	2.3	26
115	Frontiers in Multiscale Modeling of Photoreceptor Proteins. Photochemistry and Photobiology, 2021, 97, 243-269.	1.3	26
116	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
117	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
118	Promising two-photon probes for in vivo detection of Î² amyloid deposits. Chemical Communications, 2014, 50, 11694-11697.	2.2	25
119	Prediction and Rationalization of the pH Dependence of the Activity and Stability of Family 11 Xylanases. Biochemistry, 2007, 46, 13581-13592.	1.2	24
120	Density-Dependent Formulation of Dispersionâ€“Repulsion Interactions in Hybrid Multiscale Quantum/Molecular Mechanics (QM/MM) Models. Journal of Chemical Theory and Computation, 2018, 14, 1671-1681.	2.3	24
121	Discovery of piperidine-substituted thiazolo[5,4-d]pyrimidine derivatives as potent and orally bioavailable HIV-1 non-nucleoside reverse transcriptase inhibitors. Communications Chemistry, 2019, 2, .	2.0	24
122	Effect of chromophore encapsulation on linear and nonlinear optical properties: the case of â€œminiSOGâ€, a protein-encased flavin. Physical Chemistry Chemical Physics, 2014, 16, 9950.	1.3	23
123	One- and Two-Photon Absorption of a Spiropyranâ€“Merocyanine System: Experimental and Theoretical Studies. Journal of Physical Chemistry B, 2015, 119, 1515-1522.	1.2	23
124	Open-ended response theory with polarizable embedding: multiphoton absorption in biomolecular systems. Physical Chemistry Chemical Physics, 2016, 18, 28339-28352.	1.3	23
125	Solvent effects on the electronic absorption spectrum of camphor using continuum, discrete or explicit approaches. Chemical Physics Letters, 2010, 484, 185-191.	1.2	22
126	Revealing Spectral Features in Two-Photon Absorption Spectrum of Hoechst 33342: A Combined Experimental and Quantum-Chemical Study. Journal of Physical Chemistry B, 2013, 117, 12013-12019.	1.2	22

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127	Low-voltage organic phototransistors based on naphthyl end-capped oligothiophene nanofibers. Organic Electronics, 2014, 15, 1273-1281.	1.4	22
128	Multiscale Modeling of the Active Site of [Fe] Hydrogenase: The H₂ Binding Site in Open and Closed Protein Conformations. Angewandte Chemie - International Edition, 2015, 54, 6246-6250.	7.2	22
129	A virtual vibrational self-consistent-field method for efficient calculation of molecular vibrational partition functions and thermal effects on molecular properties. Journal of Chemical Physics, 2008, 128, 174106.	1.2	21
130	Estimates of ligand-binding affinities supported by quantum mechanical methods. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 21-37.	2.2	21
131	Approximate Inclusion of Triple Excitations in Combined Coupled Cluster/Molecular Mechanics: Calculations of Electronic Excitation Energies in Solution for Acrolein, Water, Formamide, and N-Methylacetamide. Journal of Chemical Theory and Computation, 2010, 6, 839-850.	2.3	21
132	Theoretical ⁵⁷Fe MÃ¶ssbauer spectroscopy: isomer shifts of [Fe]-hydrogenase intermediates. Physical Chemistry Chemical Physics, 2014, 16, 4853-4863.	1.3	21
133	The Effect of Solvation on the Mean Excitation Energy of Glycine. Journal of Physical Chemistry Letters, 2010, 1, 242-245.	2.1	20
134	Density Functional Theory/Molecular Mechanics Approach for Electronic g-Tensors of Solvated Molecules. Journal of Physical Chemistry B, 2011, 115, 4350-4358.	1.2	20
135	Experimental and computational study of solvent effects on one- and two-photon absorption spectra of chlorinated harmines. Physical Chemistry Chemical Physics, 2015, 17, 12090-12099.	1.3	20
136	Polarizable Density Embedding Coupled Cluster Method. Journal of Chemical Theory and Computation, 2018, 14, 1351-1360.	2.3	20
137	The Reaction of Oxy Hemoglobin with Nitrite: Mechanism, Antioxidant-Modulated Effect, and Implications for Blood Substitute Evaluation. Molecules, 2018, 23, 350.	1.7	20
138	CPPE: An Open-Source C++ and Python Library for Polarizable Embedding. Journal of Chemical Theory and Computation, 2019, 15, 6154-6163.	2.3	20
139	Discovery of a Potent Adenineâ€“Benzyltriazoloâ€“Pleuromutilin Conjugate with Pronounced Antibacterial Activity against MRSA. Journal of Medicinal Chemistry, 2020, 63, 15693-15708.	2.9	20
140	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
141	Encapsulation Influence on EPR Parameters of Spin-Labels: 2,2,6,6-Tetramethyl-4-methoxypiperidine-1-oxyl in Cucurbit[8]uril. Journal of Chemical Theory and Computation, 2012, 8, 257-263.	2.3	19
142	Lanczos-driven coupledâ€“cluster damped linear response theory for molecules in polarizable environments. Journal of Chemical Physics, 2014, 141, 244107.	1.2	19
143	Self-Aggregation and Optical Absorption of Stilbazolium Merocyanine in Chloroform. Journal of Physical Chemistry B, 2014, 118, 1715-1725.	1.2	19
144	Revealing Nucleic Acid Mutations Using FÃ¶rster Resonance Energy Transfer-Based Probes. Sensors, 2016, 16, 1173.	2.1	19

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145	Embedding beyond electrostaticsâ€"The role of wave function confinement. Journal of Chemical Physics, 2016, 145, 104102.	1.2	19
146	Substituted 9-Diethylaminobenzo[a]phenoxazin-5-ones (Nile Red Analogues): Synthesis and Photophysical Properties. Journal of Organic Chemistry, 2021, 86, 1471-1488.	1.7	19
147	A coupled cluster study of the oriented circular dichroism of the nâ†'Ï€â^— electronic transition in cyclopropanone and natural optical active related structures. Chemical Physics Letters, 2004, 391, 259-266.	1.2	18
148	Uptake of Phenol on Aerosol Particlesâ€. Journal of Physical Chemistry A, 2006, 110, 660-670.	1.1	18
149	Vibrational and thermal effects on the dipole polarizability of methane and carbon tetrachloride from vibrational structure calculations. Journal of Chemical Physics, 2007, 127, 154315.	1.2	18
150	Density Functional Restrictedâ€"Unrestricted/Molecular Mechanics Theory for Hyperfine Coupling Constants of Molecules in Solution. Journal of Chemical Theory and Computation, 2011, 7, 3261-3271.	2.3	18
151	Photoabsorption of Acridine Yellow and Proflavin Bound to Human Serum Albumin Studied by Means of Quantum Mechanics/Molecular Dynamics. Journal of Physical Chemistry B, 2013, 117, 2069-2080.	1.2	18
152	Automated Fragmentation Polarizable Embedding Density Functional Theory (PE-DFT) Calculations of Nuclear Magnetic Resonance (NMR) Shielding Constants of Proteins with Application to Chemical Shift Predictions. Journal of Chemical Theory and Computation, 2017, 13, 525-536.	2.3	18
153	Structure-guided approach identifies a novel class of HIV-1 ribonuclease H inhibitors: binding mode insights through magnesium complexation and site-directed mutagenesis studies. MedChemComm, 2018, 9, 562-575.	3.5	18
154	Vibrational Contributions to Indirect Spinâ^'Spin Coupling Constants Calculated via Variational Anharmonic Approaches. Journal of Physical Chemistry A, 2008, 112, 8436-8445.	1.1	17
155	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
156	Binding free energy based structural dynamics analysis of HIV-1 RT RNase Hâ€"inhibitor complexes. Integrative Biology (United Kingdom), 2014, 6, 1010-1022.	0.6	17
157	Design of new fluorescent cholesterol and ergosterol analogs: Insights from theory. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 2188-2199.	1.4	17
158	Molecular quantum mechanical gradients within the polarizable embedding approachâ€"Application to the internal vibrational Stark shift of acetophenone. Journal of Chemical Physics, 2015, 142, 034119.	1.2	17
159	Electronic Energy Transfer in Polarizable Heterogeneous Environments: A Systematic Investigation of Different Quantum Chemical Approaches. Journal of Chemical Theory and Computation, 2015, 11, 4283-4293.	2.3	17
160	Computational Analysis of Sterol Ligand Specificity of the Niemann Pick C2 Protein. Biochemistry, 2016, 55, 5165-5179.	1.2	17
161	Inhibitor Ranking through QM Based Chelation Calculations for Virtual Screening of HIV-1 RNase H Inhibition. PLoS ONE, 2014, 9, e98659.	1.1	17
162	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

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