

Jacob Kongsted

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245
papers

8,388
citations

50
h-index

79
g-index

251
ext. papers

9,210
ext. citations

4.5
avg, IF

6.18
L-index

#	Paper	IF	Citations
245	The Dalton quantum chemistry program system. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014 , 4, 269-284	7.9	956
244	Excited States in Solution through Polarizable Embedding. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 3721-3734	6.4	253
243	Electronic Energy Transfer in Condensed Phase Studied by a Polarizable QM/MM Model. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 1838-48	6.4	223
242	Polarizability of molecular clusters as calculated by a dipole interaction model. <i>Journal of Chemical Physics</i> , 2002 , 116, 4001-4010	3.9	158
241	Density functional self-consistent quantum mechanics/molecular mechanics theory for linear and nonlinear molecular properties: Applications to solvated water and formaldehyde. <i>Journal of Chemical Physics</i> , 2007 , 126, 154112	3.9	135
240	Molecular Properties through Polarizable Embedding. <i>Advances in Quantum Chemistry</i> , 2011 , 61, 107-143	3.4	121
239	The QM/MM approach for wavefunctions, energies and response functions within self-consistent field and coupled cluster theories. <i>Molecular Physics</i> , 2002 , 100, 1813-1828	1.7	112
238	Linear response functions for coupled cluster/molecular mechanics including polarization interactions. <i>Journal of Chemical Physics</i> , 2003 , 118, 1620-1633	3.9	111
237	Photosynthetic light-harvesting is tuned by the heterogeneous polarizable environment of the protein. <i>Journal of the American Chemical Society</i> , 2011 , 133, 3078-84	16.4	110
236	Excitation energies in solution: the fully polarizable QM/MM/PCM method. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 3027-37	3.4	108
235	The polarizable embedding coupled cluster method. <i>Journal of Chemical Physics</i> , 2011 , 134, 104108	3.9	106
234	Benchmarking two-photon absorption cross sections: performance of CC2 and CAM-B3LYP. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 19306-14	3.6	104
233	An improved method to predict the entropy term with the MM/PBSA approach. <i>Journal of Computer-Aided Molecular Design</i> , 2009 , 23, 63-71	4.2	103
232	Coupled cluster calculation of the $n \rightarrow \pi^*$ electronic transition of acetone in aqueous solution. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 8001-10	2.8	101
231	Benchmarking Time-Dependent Density Functional Theory for Excited State Geometries of Organic Molecules in Gas-Phase and in Solution. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 2209-20	6.4	95
230	Coupled cluster calculations of the optical rotation of S-propylene oxide in gas phase and solution. <i>Chemical Physics Letters</i> , 2005 , 401, 385-392	2.5	92
229	Scrutinizing the effects of polarization in QM/MM excited state calculations. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 18551-60	3.6	84

228	Coupled cluster and density functional theory studies of the vibrational contribution to the optical rotation of (S)-propylene oxide. <i>Journal of the American Chemical Society</i> , 2006 , 128, 976-82	16.4	75
227	Ligand Affinities Estimated by Quantum Chemical Calculations. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 1726-37	6.4	74
226	The Journey of HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitors (NNRTIs) from Lab to Clinic. <i>Journal of Medicinal Chemistry</i> , 2019 , 62, 4851-4883	8.3	74
225	Solvent effects on NMR isotropic shielding constants. a comparison between explicit polarizable discrete and continuum approaches. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 4199-210	2.8	73
224	Failures of TDDFT in describing the lowest intramolecular charge-transfer excitation in para-nitroaniline. <i>Molecular Physics</i> , 2013 , 111, 1235-1248	1.7	71
223	Solvent effects on the n \rightarrow pi* electronic transition in formaldehyde: a combined coupled cluster/molecular dynamics study. <i>Journal of Chemical Physics</i> , 2004 , 121, 8435-45	3.9	71
222	Breakdown of the first hyperpolarizability/bond-length alternation parameter relationship. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010 , 107, 16453-8	11.5	70
221	Solvation Effects on Electronic Transitions: Exploring the Performance of Advanced Solvent Potentials in Polarizable Embedding Calculations. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 2209-17	6.4	70
220	Automatic generation of force fields and property surfaces for use in variational vibrational calculations of anharmonic vibrational energies and zero-point vibrational averaged properties. <i>Journal of Chemical Physics</i> , 2006 , 125, 124108	3.9	69
219	Coupled Cluster/Molecular Mechanics Method: Implementation and Application to Liquid Water. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 2578-2588	2.8	69
218	On the performance of quantum chemical methods to predict solvatochromic effects: the case of acrolein in aqueous solution. <i>Journal of Chemical Physics</i> , 2008 , 128, 194503	3.9	68
217	A combined quantum mechanics/molecular mechanics study of the one- and two-photon absorption in the green fluorescent protein. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 5440-51	3.6	66
216	PERI-CC2: A Polarizable Embedded RI-CC2 Method. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 3274-83	6.4	66
215	Benchmarking NMR indirect nuclear spin-spin coupling constants: SOPPA, SOPPA(CC2), and SOPPA(CCSD) versus CCSD. <i>Journal of Chemical Physics</i> , 2010 , 133, 144106	3.9	64
214	Optimized Basis Sets for Calculation of Electron Paramagnetic Resonance Hyperfine Coupling Constants: aug-cc-pVTZ-J for the 3d Atoms Sc-Zn. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 4077-87	6.4	64
213	How accurate are continuum solvation models for drug-like molecules?. <i>Journal of Computer-Aided Molecular Design</i> , 2009 , 23, 395-409	4.2	64
212	Second harmonic generation second hyperpolarizability of water calculated using the combined coupled cluster dielectric continuum or different molecular mechanics methods. <i>Journal of Chemical Physics</i> , 2004 , 120, 3787-98	3.9	64
211	Polarizable density embedding: a new QM/QM/MM-based computational strategy. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 5344-55	2.8	63

210	How to model solvent effects on molecular properties using quantum chemistry? Insights from polarizable discrete or continuum solvation models. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 9890-900 ^{2.8}	61
209	The combined multiconfigurational self-consistent-field/molecular mechanics wave function approach. <i>Journal of Chemical Physics</i> , 2001 , 115, 2393-2400	3.9 59
208	Solvatochromic Shifts in Uracil: A Combined MD-QM/MM Study. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 249-56	6.4 58
207	Hybrid density functional theory/molecular mechanics calculations of two-photon absorption of dimethylamino nitro stilbene in solution. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 12506-16	3.6 58
206	Excited states in large molecular systems through polarizable embedding. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 20234-50	3.6 57
205	Nuclear magnetic shielding constants of liquid water: insights from hybrid quantum mechanics/molecular mechanics models. <i>Journal of Chemical Physics</i> , 2007 , 126, 034510	3.9 57
204	Basis set convergence of indirect spin-spin coupling constants in the Kohn-Sham limit for several small molecules. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 3728-38	2.8 55
203	Interpretation of the ultrafast photoinduced processes in pentacene thin films. <i>Journal of the American Chemical Society</i> , 2010 , 132, 3431-9	16.4 54
202	Nonlinear optical response properties of molecules in condensed phases using the coupled cluster/dielectric continuum or molecular mechanics methods. <i>Journal of Chemical Physics</i> , 2003 , 119, 10519-10535	3.9 54
201	Overview of Recent Strategic Advances in Medicinal Chemistry. <i>Journal of Medicinal Chemistry</i> , 2019 , 62, 9375-9414	8.3 53
200	Accurate predictions of nonpolar solvation free energies require explicit consideration of binding-site hydration. <i>Journal of the American Chemical Society</i> , 2011 , 133, 13081-92	16.4 53
199	Modeling the structure and absorption spectra of stilbazolium merocyanine in polar and nonpolar solvents using hybrid QM/MM techniques. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 13349-57	3.4 51
198	On the Accuracy of Density Functional Theory to Predict Shifts in Nuclear Magnetic Resonance Shielding Constants due to Hydrogen Bonding. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 267-77	6.4 51
197	Automatic generation of potential energy and property surfaces of polyatomic molecules in normal coordinates. <i>Journal of Chemical Physics</i> , 2007 , 127, 204106	3.9 51
196	Statistical mechanically averaged molecular properties of liquid water calculated using the combined coupled cluster/molecular dynamics method. <i>Journal of Chemical Physics</i> , 2006 , 124, 124503	3.9 50
195	Linear Response Properties of Liquid Water Calculated Using CC2 and CCSD within Different Molecular Mechanics Methods. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 8646-8658	2.8 50
194	Solvent effects on zero-point vibrational corrections to optical rotations and nuclear magnetic resonance shielding constants. <i>Chemical Physics Letters</i> , 2008 , 451, 226-232	2.5 49
193	Linear response functions for a vibrational configuration interaction state. <i>Journal of Chemical Physics</i> , 2006 , 125, 214309	3.9 49

192	Molecular-Level Insight into the Spectral Tuning Mechanism of the DsRed Chromophore. <i>Journal of Physical Chemistry Letters</i> , 2012 , 3, 3513-21	6.4	48
191	Demystifying the solvatochromic reversal in Brooker® merocyanine dye. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 1290-2	3.6	48
190	Theoretical study of the electronic gas-phase spectrum of glycine, alanine, and related amines and carboxylic acids. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 1430-40	2.8	48
189	Prediction of spin-spin coupling constants in solution based on combined density functional theory/molecular mechanics. <i>Journal of Chemical Physics</i> , 2009 , 130, 134508	3.9	46
188	On the photophysics of carotenoids: a multireference DFT study of peridinin. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 13808-15	3.4	45
187	Performance of popular XC-functionals for the description of excitation energies in GFP-like chromophore models. <i>International Journal of Quantum Chemistry</i> , 2012 , 112, 789-800	2.1	45
186	Dipole and quadrupole moments of liquid water calculated within the coupled cluster/molecular mechanics method. <i>Chemical Physics Letters</i> , 2002 , 364, 379-386	2.5	45
185	Toward Reliable Prediction of the Energy Ladder in Multichromophoric Systems: A Benchmark Study on the FMO Light-Harvesting Complex. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 4928-38	6.4	44
184	Energy flow in the cryptophyte PE545 antenna is directed by bilin pigment conformation. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 4263-73	3.4	43
183	The n → π* Electronic Transition in Microsolvated Formaldehyde. A Coupled Cluster and Combined Coupled Cluster/Molecular Mechanics Study. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 8624-8632	2.8	43
182	Local electric fields and molecular properties in heterogeneous environments through polarizable embedding. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 10070-80	3.6	42
181	Solvent Effects on Rotatory Strength Tensors. 1. Theory and Application of the Combined Coupled Cluster/Dielectric Continuum Model. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 3632-3641	2.8	41
180	Damped Response Theory in Combination with Polarizable Environments: The Polarizable Embedding Complex Polarization Propagator Method. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 1164-71	6.4	40
179	The multi-configuration self-consistent field method within a polarizable embedded framework. <i>Journal of Chemical Physics</i> , 2013 , 139, 044101	3.9	40
178	On the importance of vibrational contributions to small-angle optical rotation: Fluoro-oxirane in gas phase and solution. <i>Journal of Chemical Physics</i> , 2009 , 130, 034310	3.9	40
177	Frequency-Dependent Polarizability of Boron Nitride Nanotubes: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2001 , 105, 10243-10248	3.4	40
176	Analysis of computational models for an accurate study of electronic excitations in GFP. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 2582-8	3.6	39
175	Color modeling of protein optical probes. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 1107-12	3.6	39

174	Accuracy of Protein Embedding Potentials: An Analysis in Terms of Electrostatic Potentials. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 1832-42	6.4	38
173	A polarizable embedding DFT study of one-photon absorption in fluorescent proteins. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 4735-43	3.6	38
172	Carotenoids and light-harvesting: from DFT/MRCI to the Tamm-Dancoff approximation. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 655-66	6.4	37
171	Unraveling the similarity of the photoabsorption of deprotonated p-coumaric acid in the gas phase and within the photoactive yellow protein. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 1585-9	3.6	37
170	Inclusion of terpenoid plant extracts in lipid bilayers investigated by molecular dynamics simulations. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 15825-31	3.4	36
169	Gas phase optical rotation calculated from coupled cluster theory with zero-point vibrational corrections from density functional theory. <i>Chirality</i> , 2009 , 21 Suppl 1, E68-75	2.1	36
168	Calculation of vibrational infrared intensities and Raman activities using explicit anharmonic wave functions. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 11205-13	2.8	36
167	A CC2 dielectric continuum model and a CC2 molecular mechanics model. <i>Molecular Physics</i> , 2003 , 101, 2055-2071	1.7	36
166	Polarizable Density Embedding: A Solution to the Electron Spill-Out Problem in Multiscale Modeling. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 5949-5958	6.4	35
165	The role of molecular conformation and polarizable embedding for one- and two-photon absorption of disperse orange 3 in solution. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 8169-81	3.4	33
164	On the importance of excited state dynamic response electron correlation in polarizable embedding methods. <i>Journal of Computational Chemistry</i> , 2012 , 33, 2012-22	3.5	33
163	Charge transfer excitation energies in pyridine-silver complexes studied by a QM/MM method. <i>Chemical Physics Letters</i> , 2009 , 470, 285-288	2.5	33
162	Relation between Nonlinear Optical Properties of Push-Pull Molecules and Metric of Charge Transfer Excitations. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 4182-8	6.4	32
161	Averaged Solvent Embedding Potential Parameters for Multiscale Modeling of Molecular Properties. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 1684-95	6.4	32
160	Nuclear Magnetic Shielding Constants from Quantum Mechanical/Molecular Mechanical Calculations Using Polarizable Embedding: Role of the Embedding Potential. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 981-8	6.4	30
159	Two-photon absorption cross sections: an investigation of solvent effects. Theoretical studies on formaldehyde and water. <i>Journal of Chemical Physics</i> , 2006 , 125, 184501	3.9	30
158	Convergence of environment polarization effects in multiscale modeling of excitation energies. <i>Computational and Theoretical Chemistry</i> , 2014 , 1040-1041, 304-311	2	29
157	Quantification of the π -interactions that govern tertiary structure in donor-acceptor [2]pseudorotaxanes. <i>Journal of the American Chemical Society</i> , 2012 , 134, 3857-63	16.4	29

156	Benchmarking SOPPA(CC2) for the calculation of indirect nuclear spin-spin coupling constants: Carbocycles. <i>Chemical Physics</i> , 2011 , 381, 35-43	2.3	28
155	Recent developments in the medicinal chemistry of single boron atom-containing compounds. <i>Acta Pharmaceutica Sinica B</i> , 2021 , 11, 3035-3059	15.5	28
154	Improving the calculation of Electron Paramagnetic Resonance hyperfine coupling tensors for d-block metals. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 10669-76	3.6	27
153	Mutations in the bacterial ribosomal protein l3 and their association with antibiotic resistance. <i>Antimicrobial Agents and Chemotherapy</i> , 2015 , 59, 3518-28	5.9	26
152	Dehydroergosterol as an analogue for cholesterol: why it mimics cholesterol so well-or does it?. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 7345-57	3.4	26
151	Amyloid Fibril-Induced Structural and Spectral Modifications in the Thioflavin-T Optical Probe. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 70-7	6.4	26
150	A Theoretical Study of the Reaction between CH ₃ S(OH)CH ₃ and O ₂ . <i>Journal of Physical Chemistry A</i> , 2004 , 108, 8659-8671	2.8	26
149	Computational screening of one- and two-photon spectrally tuned channelrhodopsin mutants. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 7567-76	3.6	25
148	Polarizable embedding with a multiconfiguration short-range density functional theory linear response method. <i>Journal of Chemical Physics</i> , 2015 , 142, 114113	3.9	25
147	On the existence of the H3 tautomer of adenine in aqueous solution. Rationalizations based on hybrid quantum mechanics/molecular mechanics predictions. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 761-8	3.6	25
146	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. <i>Journal of Chemical Physics</i> , 2020 , 152, 214115	3.9	24
145	A click chemistry approach to pleuromutilin derivatives, part 2: conjugates with acyclic nucleosides and their ribosomal binding and antibacterial activity. <i>Journal of Medicinal Chemistry</i> , 2012 , 55, 2067-77	8.3	24
144	Association dynamics and linear and nonlinear optical properties of an N-acetylaladanamide probe in a POPC membrane. <i>Journal of the American Chemical Society</i> , 2013 , 135, 13590-7	16.4	24
143	Transition-State Docking of Flunitrazepam and Progesterone in Cytochrome P450. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 673-81	6.4	24
142	Two-photon solvatochromism II: experimental and theoretical study of solvent effects on the two-photon absorption spectrum of Reichardt's dye. <i>ChemPhysChem</i> , 2013 , 14, 3731-9	3.2	23
141	Validating and Analyzing EPR Hyperfine Coupling Constants with Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 2380-8	6.4	23
140	Computational protocols for prediction of solute NMR relative chemical shifts. a case study of L-tryptophan in aqueous solution. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2853-64	3.5	23
139	The Quality of the Embedding Potential Is Decisive for Minimal Quantum Region Size in Embedding Calculations: The Case of the Green Fluorescent Protein. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 6230-6236	6.4	22

138	Basis Set Recommendations for DFT Calculations of Gas-Phase Optical Rotation at Different Wavelengths. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 4425-33	6.4	22
137	Solvent effects on the electronic absorption spectrum of camphor using continuum, discrete or explicit approaches. <i>Chemical Physics Letters</i> , 2010 , 484, 185-191	2.5	22
136	Prediction and rationalization of the pH dependence of the activity and stability of family 11 xylanases. <i>Biochemistry</i> , 2007 , 46, 13581-92	3.2	22
135	Response properties of embedded molecules through the polarizable embedding model. <i>International Journal of Quantum Chemistry</i> , 2019 , 119, e25717	2.1	22
134	Promising two-photon probes for in vivo detection of β -amyloid deposits. <i>Chemical Communications</i> , 2014 , 50, 11694-7	5.8	21
133	Low-voltage organic phototransistors based on naphthyl end-capped oligothiophene nanofibers. <i>Organic Electronics</i> , 2014 , 15, 1273-1281	3.5	21
132	Nonpolar Solvation Free Energies of Protein-Ligand Complexes. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 3558-68	6.4	21
131	Density-Dependent Formulation of Dispersion-Repulsion Interactions in Hybrid Multiscale Quantum/Molecular Mechanics (QM/MM) Models. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 1671-1681	6.4	20
130	Computational Approach for Studying Optical Properties of DNA Systems in Solution. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 5050-5057	6.4	20
129	Virtual screening models for prediction of HIV-1 RT associated RNase H inhibition. <i>PLoS ONE</i> , 2013 , 8, e73478	3.7	20
128	Importance of Accurate Structures for Quantum Chemistry Embedding Methods: Which Strategy Is Better?. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 4309-4319	6.4	19
127	Effect of chromophore encapsulation on linear and nonlinear optical properties: the case of "miniSOG", a protein-encased flavin. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 9950-9	3.6	19
126	Lanczos-driven coupled-cluster damped linear response theory for molecules in polarizable environments. <i>Journal of Chemical Physics</i> , 2014 , 141, 244107	3.9	19
125	Encapsulation Influence on EPR Parameters of Spin-Labels: 2,2,6,6-Tetramethyl-4-methoxypiperidine-1-oxyl in Cucurbit[8]uril. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 257-63	6.4	19
124	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. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 839-50	6.4	19
123	Density functional theory/molecular mechanics approach for electronic g-tensors of solvated molecules. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 4350-8	3.4	19
122	Estimates of ligand-binding affinities supported by quantum mechanical methods. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , 2010 , 2, 21-37	3.5	19
121	Open-ended response theory with polarizable embedding: multiphoton absorption in biomolecular systems. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 28339-28352	3.6	19

120	Multiscale modeling of the active site of [Fe] hydrogenase: the H ₂ binding site in open and closed protein conformations. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 6246-50	16.4	18
119	Polarizable Embedding Combined with the Algebraic Diagrammatic Construction: Tackling Excited States in Biomolecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 4870-4883	6.4	18
118	Revealing spectral features in two-photon absorption spectrum of Hoechst 33342: a combined experimental and quantum-chemical study. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 12013-9	3.4	18
117	Density Functional Restricted-Unrestricted/Molecular Mechanics Theory for Hyperfine Coupling Constants of Molecules in Solution. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 3261-71	6.4	18
116	A virtual vibrational self-consistent-field method for efficient calculation of molecular vibrational partition functions and thermal effects on molecular properties. <i>Journal of Chemical Physics</i> , 2008 , 128, 174106	3.9	18
115	Uptake of phenol on aerosol particles. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 660-70	2.8	18
114	The electronic spectrum of the micro-solvated alanine zwitterion calculated using the combined coupled cluster/molecular mechanics method. <i>Chemical Physics Letters</i> , 2006 , 429, 430-435	2.5	18
113	A coupled cluster study of the oriented circular dichroism of the n→π* electronic transition in cyclopropanone and natural optical active related structures. <i>Chemical Physics Letters</i> , 2004 , 391, 259-266 ⁵	2.5	18
112	Experimental and computational study of solvent effects on one- and two-photon absorption spectra of chlorinated harmines. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 12090-9	3.6	17
111	Theoretical ⁵⁷ Fe Mössbauer spectroscopy: isomer shifts of [Fe]-hydrogenase intermediates. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 4853-63	3.6	17
110	Binding free energy based structural dynamics analysis of HIV-1 RT RNase H-inhibitor complexes. <i>Integrative Biology (United Kingdom)</i> , 2014 , 6, 1010-22	3.7	17
109	Photoabsorption of acridine yellow and proflavin bound to human serum albumin studied by means of quantum mechanics/molecular dynamics. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 2069-80	3.4	17
108	Vibrational contributions to indirect spin-spin coupling constants calculated via variational anharmonic approaches. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 8436-45	2.8	17
107	Vibrational and thermal effects on the dipole polarizability of methane and carbon tetrachloride from vibrational structure calculations. <i>Journal of Chemical Physics</i> , 2007 , 127, 154315	3.9	17
106	Embedding beyond electrostatics-The role of wave function confinement. <i>Journal of Chemical Physics</i> , 2016 , 145, 104102	3.9	17
105	Molecular design opportunities presented by solvent-exposed regions of target proteins. <i>Medicinal Research Reviews</i> , 2019 , 39, 2194-2238	14.4	16
104	Avoiding Electron Spill-Out in QM/MM Calculations on Excited States with Simple Pseudopotentials. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 1373-1381	6.4	16
103	Self-aggregation and optical absorption of stilbazolium merocyanine in chloroform. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 1715-25	3.4	16

102	Design of new fluorescent cholesterol and ergosterol analogs: Insights from theory. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2015 , 1848, 2188-99	3.8	16
101	One- and two-photon absorption of a spiropyran-merocyanine system: experimental and theoretical studies. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 1515-22	3.4	16
100	The Effect of Solvation on the Mean Excitation Energy of Glycine. <i>Journal of Physical Chemistry Letters</i> , 2010 , 1, 242-245	6.4	16
99	Revealing Nucleic Acid Mutations Using Förster Resonance Energy Transfer-Based Probes. <i>Sensors</i> , 2016 , 16,	3.8	16
98	Molecular quantum mechanical gradients within the polarizable embedding approach—application to the internal vibrational Stark shift of acetophenone. <i>Journal of Chemical Physics</i> , 2015 , 142, 034119	3.9	15
97	Electronic Energy Transfer in Polarizable Heterogeneous Environments: A Systematic Investigation of Different Quantum Chemical Approaches. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 4283-4303	6.4	15
96	Enhancement of Internal Motions of Lysozyme through Interaction with Gold Nanoclusters and its Optical Imaging. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 653-664	3.8	15
95	Polarizable Density Embedding Coupled Cluster Method. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 1351-1360	6.4	15
94	Computational Analysis of Sterol Ligand Specificity of the Niemann Pick C2 Protein. <i>Biochemistry</i> , 2016 , 55, 5165-79	3.2	15
93	Discovery of piperidine-substituted thiazolo[5,4-d]pyrimidine derivatives as potent and orally bioavailable HIV-1 non-nucleoside reverse transcriptase inhibitors. <i>Communications Chemistry</i> , 2019 , 2,	6.3	15
92	Solvent effects on the nitrogen NMR shielding and nuclear quadrupole coupling constants in 1-methyltriazoles. <i>Chemical Physics Letters</i> , 2008 , 460, 129-136	2.5	15
91	Inhibitor ranking through QM based chelation calculations for virtual screening of HIV-1 RNase H inhibition. <i>PLoS ONE</i> , 2014 , 9, e98659	3.7	15
90	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. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 525-536	6.4	14
89	NMR spin-spin coupling constants in polymethine dyes as polarity indicators. <i>Chemistry - A European Journal</i> , 2012 , 18, 11677-84	4.8	14
88	Fluorescence and phosphorescence of acetone in neat liquid and aqueous solution studied by QM/MM and PCM approaches. <i>International Journal of Quantum Chemistry</i> , 2011 , 111, 1511-1520	2.1	14
87	Molecular electric properties of liquid water calculated using the combined coupled cluster/molecular mechanics method. <i>Computational and Theoretical Chemistry</i> , 2003 , 632, 207-225		14
86	CPPE: An Open-Source C++ and Python Library for Polarizable Embedding. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 6154-6163	6.4	13
85	Nonlinear Optical Effects Induced by Nanoparticles in Symmetric Molecules. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 20870-20876	3.8	13

84	Conformational Dependence of Isotropic Polarizabilities. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 1404-14	6.4	13
83	Structure-guided approach identifies a novel class of HIV-1 ribonuclease H inhibitors: binding mode insights through magnesium complexation and site-directed mutagenesis studies. <i>MedChemComm</i> , 2018 , 9, 562-575	5	12
82	A quantum mechanics/molecular dynamics study of electric field gradient fluctuations in the liquid phase. The case of Na ⁺ in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 1621-31	3.6	12
81	How Far Does a Receptor Influence Vibrational Properties of an Odorant?. <i>PLoS ONE</i> , 2016 , 11, e0152345	5.7	12
80	A quantum-mechanical perspective on linear response theory within polarizable embedding. <i>Journal of Chemical Physics</i> , 2017 , 146, 234101	3.9	11
79	A theoretical investigation of gas phase NO ₃ initiated nitration of p-cresol. <i>Chemical Physics</i> , 2011 , 389, 39-46	2.3	11
78	Assessing frequency-dependent site polarisabilities in linear response polarisable embedding. <i>Molecular Physics</i> , 2017 , 115, 39-47	1.7	10
77	Computational Approach to Evaluation of Optical Properties of Membrane Probes. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 719-726	6.4	10
76	Absorption Spectra of FAD Embedded in Cryptochromes. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 3618-3623	6.4	10
75	Polarizable embedding based on multiconfigurational methods: Current developments and the road ahead. <i>International Journal of Quantum Chemistry</i> , 2014 , 114, 1102-1107	2.1	10
74	pH-Induced Modulation of One- and Two-Photon Absorption Properties in a Naphthalene-Based Molecular Probe. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 3660-9	6.4	10
73	A Unified Framework for the Polarizable Embedding and Continuum Methods Within Multiconfigurational Self-consistent Field Theory. <i>Advances in Quantum Chemistry</i> , 2013 , 66, 195-238	1.4	10
72	Identifying the Hamiltonian structure in linear response theory. <i>Journal of Chemical Physics</i> , 2014 , 140, 224103	3.9	10
71	Synthesis, biological evaluation and molecular modelling studies of 4-anilinoquinazoline derivatives as protein kinase inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , 2014 , 22, 1909-15	3.4	10
70	The Reaction of Oxy Hemoglobin with Nitrite: Mechanism, Antioxidant-Modulated Effect, and Implications for Blood Substitute Evaluation. <i>Molecules</i> , 2018 , 23,	4.8	9
69	Computational assignment of redox states to Coulomb blockade diamonds. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 17473-8	3.6	9
68	Chelation-Induced Quenching of Two-Photon Absorption of Azacrown Ether Substituted Distyryl Benzene for Metal Ion Sensing. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 778-88	6.4	9
67	Modeling Electronic Circular Dichroism within the Polarizable Embedding Approach. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 4442-4451	6.4	9

66	Benchmarking the multipole shielding polarizability/reaction field approach to solvation against QM/MM: applications to the shielding constants of N-methylacetamide. <i>Journal of Chemical Physics</i> , 2011 , 134, 044514	3.9	9
65	An averaged polarizable potential for multiscale modeling in phospholipid membranes. <i>Journal of Computational Chemistry</i> , 2017 , 38, 601-611	3.5	8
64	Very Strong Binding for a Neutral Calix[4]pyrrole Receptor Displaying Positive Allosteric Binding. <i>Journal of Organic Chemistry</i> , 2017 , 82, 2123-2128	4.2	8
63	Structural design of intrinsically fluorescent oxysterols. <i>Chemistry and Physics of Lipids</i> , 2018 , 212, 26-34	3.7	8
62	The Second-Order Polarization Propagator Approximation (SOPPA) method coupled to the polarizable continuum model. <i>Computational and Theoretical Chemistry</i> , 2014 , 1040-1041, 54-60	2	8
61	Binding Mechanism and Magnetic Properties of a Multifunctional Spin Label for Targeted EPR Imaging of Amyloid Proteins: Insight from Atomistic Simulations and First-Principles Calculations. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 4766-74	6.4	8
60	Design, synthesis, and biologic evaluation of novel galloyl derivatives as HIV-1 RNase H inhibitors. <i>Chemical Biology and Drug Design</i> , 2019 , 93, 582-589	2.9	8
59	Frontiers in Multiscale Modeling of Photoreceptor Proteins. <i>Photochemistry and Photobiology</i> , 2021 , 97, 243-269	3.6	8
58	Relativistic Polarizable Embedding. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 2870-2880	6.4	7
57	Determination of rate constants for the uptake process involving SO ₂ and an aerosol particle. A quantum mechanics/molecular mechanics and quantum statistical investigation. <i>Chemical Physics</i> , 2008 , 348, 21-30	2.3	7
56	Binding and intracellular transport of 25-hydroxycholesterol by Niemann-Pick C2 protein. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2020 , 1862, 183063	3.8	7
55	Modeling of Magnetic Circular Dichroism and UV/Vis Absorption Spectra Using Fluctuating Charges or Polarizable Embedding within a Resonant-Convergent Response Theory Formalism. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 6391-6404	6.4	7
54	Modeling magnetic circular dichroism within the polarizable embedding approach. <i>Theoretical Chemistry Accounts</i> , 2018 , 137, 1	1.9	6
53	Dual mechanism of HIV-1 integrase and RNase H inhibition by diketo derivatives: a computational study. <i>RSC Advances</i> , 2014 , 4, 38672-38681	3.7	6
52	Simulations of light absorption of carbon particles in nanoaerosol clusters. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 1879-86	2.8	6
51	Coordination-driven switching of a preorganized and cooperative calix[4]pyrrole receptor. <i>Chemistry - A European Journal</i> , 2013 , 19, 2768-75	4.8	6
50	Polarizable Density Embedding for Large Biomolecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 5999-6006	6.4	6
49	One- and two-photon solvatochromism of the fluorescent dye Nile Red and its CF, F and Br-substituted analogues. <i>Photochemical and Photobiological Sciences</i> , 2020 , 19, 1382-1391	4.2	6

48	Rational design of novel fluorescent analogues of cholesterol: a "step-by-step" computational study. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 15487-15503	3.6	5
47	Discovery of a Potent Adenine-Benzyltriazolo-Pleuromutilin Conjugate with Pronounced Antibacterial Activity against MRSA. <i>Journal of Medicinal Chemistry</i> , 2020 , 63, 15693-15708	8.3	5
46	Rational Design of Nile Red Analogs for Sensing in Membranes. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 10424-10432	3.4	5
45	Membrane organization and intracellular transport of a fluorescent analogue of 27-hydroxycholesterol. <i>Chemistry and Physics of Lipids</i> , 2020 , 233, 105004	3.7	5
44	Nitrogen -Edge X-ray Absorption Spectra of Ammonium and Ammonia in Water Solution: Assessing the Performance of Polarizable Embedding Coupled Cluster Methods. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 8865-8871	6.4	5
43	Ultramild protein-mediated click chemistry creates efficient oligonucleotide probes for targeting and detecting nucleic acids. <i>ChemBioChem</i> , 2015 , 16, 1163-7	3.8	4
42	Multipole moments for embedding potentials: Exploring different atomic allocation algorithms. <i>Journal of Computational Chemistry</i> , 2016 , 37, 1887-96	3.5	4
41	Computational Characterization of a Cholesterol-Based Molecular Rotor in Lipid Membranes. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 7313-7326	3.4	4
40	EPR spin Hamiltonian parameters of encapsulated spin-labels: impact of the hydrogen bonding topology. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 2427-34	3.6	4
39	How Crucial Are Finite Temperature and Solvent Effects on Structure and Absorption Spectra of Si10?. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 26618-26624	3.8	4
38	Solvatochromic shifts vs nanosolvation patterns: Uracil in water as a test case. <i>Computational and Theoretical Chemistry</i> , 2011 , 974, 109-116	2	4
37	The coupling constant polarizability and hyperpolarizability of 1J(NH) in N-methylacetamide, and its application for the multipole spin-spin coupling constant polarizability/reaction field approach to solvation. <i>Journal of Computational Chemistry</i> , 2011 , 32, 3168-74	3.5	4
36	Substituted 9-Diethylaminobenzo[<i>b</i>]phenoxazin-5-ones (Nile Red Analogues): Synthesis and Photophysical Properties. <i>Journal of Organic Chemistry</i> , 2021 , 86, 1471-1488	4.2	4
35	Binding affinity models for Falcipain inhibition based on the Linear Interaction Energy method. <i>Journal of Molecular Graphics and Modelling</i> , 2016 , 70, 236-245	2.8	4
34	Preparation of organocobalt(iii) complexes via O activation. <i>Dalton Transactions</i> , 2021 , 50, 4819-4829	4.3	4
33	Optimization and transferability of non-electrostatic repulsion in the polarizable density embedding model. <i>Journal of Computational Chemistry</i> , 2017 , 38, 2108-2117	3.5	3
32	A comparative study of binding affinities for 6,7-dimethoxy-4-pyrrolidylquinazolines as phosphodiesterase 10A inhibitors using the linear interaction energy method. <i>Journal of Molecular Graphics and Modelling</i> , 2015 , 61, 44-52	2.8	3
31	One-Photon Absorption Properties from a Hybrid Polarizable Density Embedding/Complex Polarization Propagator Approach for Polarizable Solutions. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 2145-2154	6.4	3

30	Basis set error estimation for DFT calculations of electronic g-tensors for transition metal complexes. <i>Journal of Computational Chemistry</i> , 2014 , 35, 1809-14	3.5	3
29	Biochemical and Computational Analysis of the Substrate Specificities of Cfr and RlmN Methyltransferases. <i>PLoS ONE</i> , 2015 , 10, e0145655	3.7	3
28	Gauge-origin independent magnetizabilities from hybrid quantum mechanics/molecular mechanics models: Theory and applications to liquid water. <i>Chemical Physics Letters</i> , 2007 , 442, 322-328	2.5	3
27	Actin Peptide-Based Inhibitors of Histidine Methyltransferase SETD3. <i>ChemMedChem</i> , 2021 , 16, 2695-2702	3.7	3
26	Photophysical investigation of two emissive nucleosides exhibiting gigantic stokes shifts. <i>Photochemical and Photobiological Sciences</i> , 2019 , 18, 1858-1865	4.2	2
25	Multiscale Modeling of the Active Site of [Fe] Hydrogenase: The H ₂ Binding Site in Open and Closed Protein Conformations. <i>Angewandte Chemie</i> , 2015 , 127, 6344-6348	3.6	2
24	The chemistry of Coulomb blockade diamonds for 1,4-diamino-benzene. <i>Chemical Physics</i> , 2015 , 459, 40-44	2.3	2
23	Mechanistic Insight into Lipid Binding to Yeast Niemann Pick Type C2 Protein. <i>Biochemistry</i> , 2020 , 59, 4407-4420	3.2	2
22	Modeling the Sterol-Binding Domain of Aster-A Provides Insight into Its Multiligand Specificity. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 2268-2281	6.1	2
21	Hole Hopping through Cytochrome P450. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 3065-3073	3.4	2
20	Comparison between theoretically and experimentally determined electronic properties: applications to two-photon singlet oxygen sensitizers. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 1906-1916	2.8	2
19	Parallelization of the polarizable embedding scheme for higher-order response functions. <i>Molecular Physics</i> , 2012 , 110, 2579-2586	1.7	2
18	Modelling spectroscopic properties of large molecular systems. The combined Density Functional Theory/Molecular Mechanics approach. <i>Journal of Computational Methods in Sciences and Engineering</i> , 2008 , 7, 135-158	0.3	2
17	Polarizable Embedding as a Tool to Address Light-Responsive Biological Systems. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2021 , 143-195	0.7	2
16	Efficient Open-Source Implementations of Linear-Scaling Polarizable Embedding: Use Octrees to Save the Trees. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 3445-3454	6.4	2
15	Harmonic Infrared and Raman Spectra in Molecular Environments Using the Polarizable Embedding Model. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 3599-3617	6.4	2
14	Computational Modeling Explains the Multi Sterol Ligand Specificity of the N-Terminal Domain of Niemann-Pick C1-Like 1 Protein. <i>ACS Omega</i> , 2019 , 4, 20894-20904	3.9	2
13	Computational and photophysical characterization of a Laurdan malononitrile derivative. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 9139-9146	3.6	2

12	Importance of Ile71 in β -actin on histidine methyltransferase SETD3 catalysis.. <i>Organic and Biomolecular Chemistry</i> , 2022 ,	3.9	1
11	Computational Characterization of Novel Malononitrile Variants of Laurdan with Improved Photophysical Properties for Sensing in Membranes. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 9526-9534	3.4	1
10	Photophysical and Structural Characterization of Intrinsically Fluorescent Sterol Aggregates. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 5838-5852	3.4	1
9	Modeling One- and Two-Photon Excitation of 4?-(Hydroxymethyl)-4,5?,8-trimethylpsoralen in Complex with DNA: Solving Electron Spill-Out Problems in Polarizable QM/MM Calculations. <i>Advanced Theory and Simulations</i> , 2021 , 4, 2000294	3.5	1
8	Fast Approximate but Accurate QM/MM Interactions for Polarizable Embedding.. <i>Journal of Chemical Theory and Computation</i> , 2021 ,	6.4	1
7	Direct observation of nystatin binding to the plasma membrane of living cells. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2021 , 1863, 183528	3.8	0
6	Modeling environmental effects in two-photon circular dichroism calculations. <i>Theoretical Chemistry Accounts</i> , 2021 , 140, 1	1.9	0
5	Combining polarizable embedding with the Frenkel exciton model: applications to absorption spectra with overlapping solute-solvent bands. <i>Theoretical Chemistry Accounts</i> , 2019 , 138, 1	1.9	
4	Relaxation Dynamics of the Triazene Compound Berenil in DNA-Minor-Groove Confinement after Photoexcitation. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 5203-5211	6.4	
3	THE (HYPER)POLARIZABILITIES OF LIQUID WATER MODELLED USING COUPLED CLUSTER/MOLECULAR MECHANICS RESPONSE THEORY METHODS 2006 , 215-281		
2	Computational analysis of altered one- and two-photon CD of sterols inside a protein binding pocket. <i>Theoretical Chemistry Accounts</i> , 2022 , 141, 1	1.9	
1	Linear Response Theory in Connection to Density Functional Theory/Molecular Dynamics and Coupled Cluster/Molecular Dynamics Methods. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2008 , 349-380	0.7	