Nanna Holmgaard List

List of Publications by Year
in descending order

39	1,264	331259	360668
papers	citations	21 h-index	35 g-index

46	46	46	1357
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Benchmarking two-photon absorption cross sections: performance of CC2 and CAM-B3LYP. Physical Chemistry Chemical Physics, 2015, 17, 19306-19314.	1.3	160
2	Excited states in large molecular systems through polarizable embedding. Physical Chemistry Chemical Physics, 2016, 18, 20234-20250.	1.3	78
3	Local electric fields and molecular properties in heterogeneous environments through polarizable embedding. Physical Chemistry Chemical Physics, 2016, 18, 10070-10080.	1.3	60
4	Molecular-Level Insight into the Spectral Tuning Mechanism of the DsRed Chromophore. Journal of Physical Chemistry Letters, 2012, 3, 3513-3521.	2.1	54
5	Direct observation of ultrafast hydrogen bond strengthening in liquid water. Nature, 2021, 596, 531-535.	13.7	53
6	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
7	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
8	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
9	Beyond the electric-dipole approximation: A formulation and implementation of molecular response theory for the description of absorption of electromagnetic field radiation. Journal of Chemical Physics, 2015, 142, 244111.	1.2	48
10	The multi-configuration self-consistent field method within a polarizable embedded framework. Journal of Chemical Physics, 2013, 139, 044101.	1.2	46
11	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. Journal of Chemical Physics, 2020, 152, 214115.	1.2	45
12	Averaged Solvent Embedding Potential Parameters for Multiscale Modeling of Molecular Properties. Journal of Chemical Theory and Computation, 2016, 12, 1684-1695.	2.3	42
13	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
14	Origin of DNA-Induced Circular Dichroism in a Minor-Groove Binder. Journal of the American Chemical Society, 2017, 139, 14947-14953.	6.6	38
15	VeloxChem: A Pythonâ€driven densityâ€functional theory program for spectroscopy simulations in highâ€performance computing environments. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1457.	6.2	34
16	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
17	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
18	Probing competing relaxation pathways in malonaldehyde with transient X-ray absorption spectroscopy. Chemical Science, 2020, 11, 4180-4193.	3.7	29

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19	Resolving the ultrafast dynamics of the anionic green fluorescent protein chromophore in water. Chemical Science, 2021, 12, 11347-11363.	3.7	28
20	Rotationally averaged linear absorption spectra beyond the electric-dipole approximation. Molecular Physics, 2017, 115, 63-74.	0.8	24
21	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
22	Open-ended response theory with polarizable embedding: multiphoton absorption in biomolecular systems. Physical Chemistry Chemical Physics, 2016, 18, 28339-28352.	1.3	23
23	Internal conversion of the anionic GFP chromophore: in and out of the I-twisted S₁/S₀ conical intersection seam. Chemical Science, 2022, 13, 373-385.	3.7	23
24	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
25	Lanczos-driven coupledâ€“cluster damped linear response theory for molecules in polarizable environments. Journal of Chemical Physics, 2014, 141, 244107.	1.2	19
26	Embedding beyond electrostaticsâ€”The role of wave function confinement. Journal of Chemical Physics, 2016, 145, 104102.	1.2	19
27	Design of new fluorescent cholesterol and ergosterol analogs: Insights from theory. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 2188-2199.	1.4	17
28	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
29	Beyond the electric-dipole approximation in simulations of x-ray absorption spectroscopy: Lessons from relativistic theory. Journal of Chemical Physics, 2020, 152, 184110.	1.2	17
30	How Far Does a Receptor Influence Vibrational Properties of an Odorant?. PLoS ONE, 2016, 11, e0152345.	1.1	15
31	A Unified Framework for the Polarizable Embedding and Continuum Methods Within Multiconfigurational Self-consistent Field Theory. Advances in Quantum Chemistry, 2013, 66, 195-238.	0.4	12
32	An averaged polarizable potential for multiscale modeling in phospholipid membranes. Journal of Computational Chemistry, 2017, 38, 601-611.	1.5	12
33	A quantum-mechanical perspective on linear response theory within polarizable embedding. Journal of Chemical Physics, 2017, 146, 234101.	1.2	12
34	Computational Approach to Evaluation of Optical Properties of Membrane Probes. Journal of Chemical Theory and Computation, 2017, 13, 719-726.	2.3	11
35	Identifying the Hamiltonian structure in linear response theory. Journal of Chemical Physics, 2014, 140, 224103.	1.2	10
36	Steric and Electronic Origins of Fluorescence in GFP and GFP-like Proteins. Journal of the American Chemical Society, 2022, 144, 12732-12746.	6.6	8

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37	Harmonic Infrared and Raman Spectra in Molecular Environments Using the Polarizable Embedding Model. Journal of Chemical Theory and Computation, 2021, 17, 3599-3617.	2.3	6
38	Probing chirality across the electromagnetic spectrum with the full semi-classical lightâ€“matter interaction. Journal of Chemical Physics, 2022, 156, 054113.	1.2	4
39	Predictions of Pre-edge Features in Time-Resolved Near-Edge X-ray Absorption Fine Structure Spectroscopy from Holeâ€“Hole Tammâ€“Dancoff-Approximated Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 7120-7133.	2.3	3