Jgvan Magnus Haugaard Olsen

List of Publications by Year in Descending Order

62 papers	2,729 citations	24 h-index	51 g-index
81 ext. papers	3,175 ext. citations	5 avg, IF	5.11 L-index

#	Paper	IF	Citations
62	Efficient Open-Source Implementations of Linear-Scaling Polarizable Embedding: Use Octrees to Save the Trees. *Journal of Chemical Theory and Computation*, **2021**, 17, 3445-3454	6.4	2
61	Harmonic Infrared and Raman Spectra in Molecular Environments Using the Polarizable Embedding Model. *Journal of Chemical Theory and Computation*, **2021**, 17, 3599-3617	6.4	2
60	Frontiers in Multiscale Modeling of Photoreceptor Proteins. *Photochemistry and Photobiology*, **2021**, 97, 243-269	3.6	8
59	The DIRAC code for relativistic molecular calculations. *Journal of Chemical Physics*, **2020**, 152, 204104	3.9	73
58	Two-Photon Absorption Cross-Sections in Fluorescent Proteins Containing Non-canonical Chromophores Using Polarizable QM/MM. *Frontiers in Molecular Biosciences*, **2020**, 7, 111	5.6	1
57	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. *Journal of Chemical Physics*, **2020**, 152, 214115	3.9	24
56	Avoiding Electron Spill-Out in QM/MM Calculations on Excited States with Simple Pseudopotentials. *Journal of Chemical Theory and Computation*, **2020**, 16, 1373-1381	6.4	16
55	MiMiC: Multiscale Modeling in Computational Chemistry. *Frontiers in Molecular Biosciences*, **2020**, 7, 45	5.6	3
54	Molecular Basis of CLC Antiporter Inhibition by Fluoride. *Journal of the American Chemical Society*, **2020**, 142, 7254-7258	16.4	10
53	Cost-Effective Potential for Accurate Polarizable Embedding Calculations in Protein Environments. *Journal of Chemical Theory and Computation*, **2020**, 16, 1162-1174	6.4	7
52	Polarizable Density Embedding for Large Biomolecular Systems. *Journal of Chemical Theory and Computation*, **2020**, 16, 5999-6006	6.4	6
51	Accuracy of Molecular Simulation-Based Predictions of Values: A Metadynamics Study. *Journal of Physical Chemistry Letters*, **2020**, 11, 6373-6381	6.4	14
50	Extreme Scalability of DFT-Based QM/MM MD Simulations Using MiMiC. *Journal of Chemical Theory and Computation*, **2019**, 15, 5601-5613	6.4	20
49	MiMiC: A Novel Framework for Multiscale Modeling in Computational Chemistry. *Journal of Chemical Theory and Computation*, **2019**, 15, 3810-3823	6.4	18
48	CPPE: An Open-Source C++ and Python Library for Polarizable Embedding. *Journal of Chemical Theory and Computation*, **2019**, 15, 6154-6163	6.4	13
47	Response properties of embedded molecules through the polarizable embedding model. *International Journal of Quantum Chemistry*, **2019**, 119, e25717	2.1	22
46	Polarizable Density Embedding Coupled Cluster Method. *Journal of Chemical Theory and Computation*, **2018**, 14, 1351-1360	6.4	15

45	A QM/MM and QM/QM/MM study of Kerr, Cotton-Mouton and Jones linear birefringences in liquid acetonitrile. *Physical Chemistry Chemical Physics*, **2018**, 20, 3831-3840	3.6	3
44	Importance of Accurate Structures for Quantum Chemistry Embedding Methods: Which Strategy Is Better?. *Journal of Chemical Theory and Computation*, **2018**, 14, 4309-4319	6.4	19
43	Polarizable Embedding Combined with the Algebraic Diagrammatic Construction: Tackling Excited States in Biomolecular Systems. *Journal of Chemical Theory and Computation*, **2018**, 14, 4870-4883	6.4	18
42	An averaged polarizable potential for multiscale modeling in phospholipid membranes. *Journal of Computational Chemistry*, **2017**, 38, 601-611	3.5	8
41	Optimization and transferability of non-electrostatic repulsion in the polarizable density embedding model. *Journal of Computational Chemistry*, **2017**, 38, 2108-2117	3.5	3
40	Modeling the absorption spectrum of the permanganate ion in vacuum and in aqueous solution. *Physical Chemistry Chemical Physics*, **2017**, 19, 15870-15875	3.6	9
39	Relativistic Polarizable Embedding. *Journal of Chemical Theory and Computation*, **2017**, 13, 2870-2880	6.4	7
38	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	6.4	14
37	Modeling Electronic Circular Dichroism within the Polarizable Embedding Approach. *Journal of Chemical Theory and Computation*, **2017**, 13, 4442-4451	6.4	9
36	Polarizable Density Embedding: A Solution to the Electron Spill-Out Problem in Multiscale Modeling. *Journal of Physical Chemistry Letters*, **2017**, 8, 5949-5958	6.4	35
35	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	6.4	22
34	Computational Approach for Studying Optical Properties of DNA Systems in Solution. *Journal of Chemical Theory and Computation*, **2016**, 12, 5050-5057	6.4	20
33	Excited states in large molecular systems through polarizable embedding. *Physical Chemistry Chemical Physics*, **2016**, 18, 20234-50	3.6	57
32	Multipole moments for embedding potentials: Exploring different atomic allocation algorithms. *Journal of Computational Chemistry*, **2016**, 37, 1887-96	3.5	4
31	Embedding beyond electrostatics-The role of wave function confinement. *Journal of Chemical Physics*, **2016**, 145, 104102	3.9	17
30	Averaged Solvent Embedding Potential Parameters for Multiscale Modeling of Molecular Properties. *Journal of Chemical Theory and Computation*, **2016**, 12, 1684-95	6.4	32
29	Open-ended response theory with polarizable embedding: multiphoton absorption in biomolecular systems. *Physical Chemistry Chemical Physics*, **2016**, 18, 28339-28352	3.6	19
28	Molecular quantum mechanical gradients within the polarizable embedding approach--application to the internal vibrational Stark shift of acetophenone. *Journal of Chemical Physics*, **2015**, 142, 034119	3.9	15

27	Accuracy of Protein Embedding Potentials: An Analysis in Terms of Electrostatic Potentials. *Journal of Chemical Theory and Computation*, **2015**, 11, 1832-42	6.4	38
26	Analysis of computational models for an accurate study of electronic excitations in GFP. *Physical Chemistry Chemical Physics*, **2015**, 17, 2582-8	3.6	39
25	Polarizable embedding with a multiconfiguration short-range density functional theory linear response method. *Journal of Chemical Physics*, **2015**, 142, 114113	3.9	25
24	Polarizable density embedding: a new QM/QM/MM-based computational strategy. *Journal of Physical Chemistry A*, **2015**, 119, 5344-55	2.8	63
23	Quantifying electron transfer reactions in biological systems: what interactions play the major role?. *Scientific Reports*, **2015**, 5, 18446	4.9	47
22	The Dalton quantum chemistry program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 269-284	7.9	956
21	Photodissociation of OCS: deviations between theory and experiment, and the importance of higher order correlation effects. *Journal of Chemical Physics*, **2014**, 141, 184310	3.9	13
20	Binding free energy based structural dynamics analysis of HIV-1 RT RNase H-inhibitor complexes. *Integrative Biology (United Kingdom)*, **2014**, 6, 1010-22	3.7	17
19	Damped Response Theory in Combination with Polarizable Environments: The Polarizable Embedding Complex Polarization Propagator Method. *Journal of Chemical Theory and Computation*, **2014**, 10, 1164-71	6.4	40
18	Convergence of environment polarization effects in multiscale modeling of excitation energies. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 304-311	2	29
17	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, 981-8	6.4	30
16	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, 2069-80	3.4	17
15	Computational screening of one- and two-photon spectrally tuned channelrhodopsin mutants. *Physical Chemistry Chemical Physics*, **2013**, 15, 7567-76	3.6	25
14	A polarizable embedding DFT study of one-photon absorption in fluorescent proteins. *Physical Chemistry Chemical Physics*, **2013**, 15, 4735-43	3.6	38
13	Amyloid Fibril-Induced Structural and Spectral Modifications in the Thioflavin-T Optical Probe. *Journal of Physical Chemistry Letters*, **2013**, 4, 70-7	6.4	26
12	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, 5440-51	3.6	66
11	Molecular-Level Insight into the Spectral Tuning Mechanism of the DsRed Chromophore. *Journal of Physical Chemistry Letters*, **2012**, 3, 3513-21	6.4	48
10	PERI-CC2: A Polarizable Embedded RI-CC2 Method. *Journal of Chemical Theory and Computation*, **2012**, 8, 3274-83	6.4	66

9	Parallelization of the polarizable embedding scheme for higher-order response functions. *Molecular Physics*, **2012**, 110, 2579-2586	1.7	2
8	Performance of popular XC-functionals for the description of excitation energies in GFP-like chromophore models. *International Journal of Quantum Chemistry*, **2012**, 112, 789-800	2.1	45
7	Solvatochromic shifts vs nanosolvation patterns: Uracil in water as a test case. *Computational and Theoretical Chemistry*, **2011**, 974, 109-116	2	4
6	Molecular Properties through Polarizable Embedding. *Advances in Quantum Chemistry*, **2011**, 61, 107-143	1.4	121
5	Computational protocols for prediction of solute NMR relative chemical shifts. a case study of L-tryptophan in aqueous solution. *Journal of Computational Chemistry*, **2011**, 32, 2853-64	3.5	23
4	Solvation Effects on Electronic Transitions: Exploring the Performance of Advanced Solvent Potentials in Polarizable Embedding Calculations. *Journal of Chemical Theory and Computation*, **2011**, 7, 2209-17	6.4	70
3	Excited States in Solution through Polarizable Embedding. *Journal of Chemical Theory and Computation*, **2010**, 6, 3721-3734	6.4	253
2	Solvatochromic Shifts in Uracil: A Combined MD-QM/MM Study. *Journal of Chemical Theory and Computation*, **2010**, 6, 249-56	6.4	58
1	On the accuracy of molecular simulation-based predictions of koff values: a Metadynamics study		1