Peter Reinholdt

List of Publications by Year in descending order

32 papers	412 citations	840119 11 h-index	794141 19 g-index
41 all docs	41 docs citations	41 times ranked	673 citing authors

#	Article	IF	Citations
1	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
2	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. Journal of Chemical Physics, 2020, 152, 214115.	1.2	45
3	Response properties of embedded molecules through the polarizable embedding model. International Journal of Quantum Chemistry, 2019, 119, e25717.	1.0	37
4	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
5	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
6	CPPE: An Open-Source C++ and Python Library for Polarizable Embedding. Journal of Chemical Theory and Computation, 2019, 15, 6154-6163.	2.3	20
7	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
8	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
9	One- and two-photon solvatochromism of the fluorescent dye Nile Red and its CF3, F and Br-substituted analogues. Photochemical and Photobiological Sciences, 2020, 19, 1382-1391.	1.6	15
10	Modeling of Magnetic Circular Dichroism and UV/Vis Absorption Spectra Using Fluctuating Charges or Polarizable Embedding within a Resonant-Convergent Response Theory Formalism. Journal of Chemical Theory and Computation, 2018, 14, 6391-6404.	2.3	12
11	Cost-Effective Potential for Accurate Polarizable Embedding Calculations in Protein Environments. Journal of Chemical Theory and Computation, 2020, 16, 1162-1174.	2.3	12
12	Binding and intracellular transport of 25-hydroxycholesterol by Niemann-Pick C2 protein. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183063.	1.4	11
13	Nitrogen K-Edge X-ray Absorption Spectra of Ammonium and Ammonia in Water Solution: Assessing the Performance of Polarizable Embedding Coupled Cluster Methods. Journal of Physical Chemistry Letters, 2021, 12, 8865-8871.	2.1	11
14	Polarizable Density Embedding for Large Biomolecular Systems. Journal of Chemical Theory and Computation, 2020, 16, 5999-6006.	2.3	10
15	Rational Design of Nile Red Analogs for Sensing in Membranes. Journal of Physical Chemistry B, 2019, 123, 10424-10432.	1.2	9
16	Mechanistic Insight into Lipid Binding to Yeast Niemann Pick Type C2 Protein. Biochemistry, 2020, 59, 4407-4420.	1.2	9
17	Membrane organization and intracellular transport of a fluorescent analogue of 27-hydroxycholesterol. Chemistry and Physics of Lipids, 2020, 233, 105004.	1.5	8
18	Direct observation of nystatin binding to the plasma membrane of living cells. Biochimica Et Biophysica Acta - Biomembranes, 2021, 1863, 183528.	1.4	8

#	Article	IF	Citations
19	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.	2.3	7
20	Rational design of novel fluorescent analogues of cholesterol: a â€œstep-by-stepâ€•computational study. Physical Chemistry Chemical Physics, 2019, 21, 15487-15503.	1.3	6
21	Cubes on a string: a series of linear coordination polymers with cubane-like nodes and dicarboxylate linkers. Nanoscale, 2020, 12, 11601-11611.	2.8	6
22	Fast Approximate but Accurate QM/MM Interactions for Polarizable Embedding. Journal of Chemical Theory and Computation, 2022, 18, 344-356.	2.3	6
23	A comparative study of binding affinities for 6,7-dimethoxy-4-pyrrolidylquinazolines as phosphodiesterase 10A inhibitors using the linear interaction energy method. Journal of Molecular Graphics and Modelling, 2015, 61, 44-52.	1.3	5
24	Computational Characterization of a Cholesterol-Based Molecular Rotor in Lipid Membranes. Journal of Physical Chemistry B, 2019, 123, 7313-7326.	1.2	5
25	Modeling the Sterol-Binding Domain of Aster-A Provides Insight into Its Multiligand Specificity. Journal of Chemical Information and Modeling, 2020, 60, 2268-2281.	2.5	4
26	Modeling Oneâ€•and Twoâ€Photon Excitation of 4â€²â€(Hydroxymethyl)â€4,5â€²,8â€trimethylpsoralen in Complex with DNA: Solving Electron Spillâ€Out Problems in Polarizable QM/MM Calculations. Advanced Theory and Simulations, 2021, 4, 2000294.	1.3	4
27	Photophysical and Structural Characterization of Intrinsically Fluorescent Sterol Aggregates. Journal of Physical Chemistry B, 2021, 125, 5838-5852.	1.2	4
28	Polarizable Embedding as a Tool to Address Light-Responsive Biological Systems. Challenges and Advances in Computational Chemistry and Physics, 2021, , 143-195.	0.6	3
29	Mechanism behind Polysorbatesâ€™ Inhibitory Effect on P-Glycoprotein. Molecular Pharmaceutics, 2022, , .	2.3	3
30	Computational Characterization of Novel Malononitrile Variants of Laurdan with Improved Photophysical Properties for Sensing in Membranes. Journal of Physical Chemistry B, 2020, 124, 9526-9534.	1.2	2
31	Computational and photophysical characterization of a Laurdan malononitrile derivative. Physical Chemistry Chemical Physics, 2021, 23, 9139-9146.	1.3	2
32	Relaxation Dynamics of the Triazene Compound Berenil in DNA-Minor-Groove Confinement after Photoexcitation. Journal of Chemical Theory and Computation, 2020, 16, 5203-5211.	2.3	1