Casper Steinmann

List of Publications by Year
in descending order

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28 papers	705 citations	516215 16 h-index	552369 26 g-index
35 all docs	35 docs citations	35 times ranked	788 citing authors

#	Article	IF	Citations
1	Effective Fragment Molecular Orbital Method: A Merger of the Effective Fragment Potential and Fragment Molecular Orbital Methods^{â€}. Journal of Physical Chemistry A, 2010, 114, 8705-8712.	1.1	80
2	Polarizable Density Embedding: A New QM/QM/MM-Based Computational Strategy. Journal of Physical Chemistry A, 2015, 119, 5344-5355.	1.1	78
3	Fully Integrated Effective Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2013, 9, 2235-2249.	2.3	56
4	A third-generation dispersion and third-generation hydrogen bonding corrected PM6 method: PM6-D3H+. PeerJ, 2014, 2, e449.	0.9	46
5	FragIt: A Tool to Prepare Input Files for Fragment Based Quantum Chemical Calculations. PLoS ONE, 2012, 7, e44480.	1.1	39
6	Improving solvation energy predictions using the SMD solvation method and semiempirical electronic structure methods. Journal of Chemical Physics, 2018, 149, 104102.	1.2	39
7	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
8	Response properties of embedded molecules through the polarizable embedding model. International Journal of Quantum Chemistry, 2019, 119, e25717.	1.0	37
9	Mapping Enzymatic Catalysis Using the Effective Fragment Molecular Orbital Method: Towards all ab initio Biochemistry. PLoS ONE, 2013, 8, e60602.	1.1	33
10	The Effective Fragment Molecular Orbital Method for Fragments Connected by Covalent Bonds. PLoS ONE, 2012, 7, e41117.	1.1	28
11	Computational Approach for Studying Optical Properties of DNA Systems in Solution. Journal of Chemical Theory and Computation, 2016, 12, 5050-5057.	2.3	26
12	Relative Ligand-Binding Free Energies Calculated from Multiple Short QM/MM MD Simulations. Journal of Chemical Theory and Computation, 2018, 14, 3228-3237.	2.3	23
13	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
14	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
15	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
16	Inhibitor Ranking through QM Based Chelation Calculations for Virtual Screening of HIV-1 RNase H Inhibition. PLoS ONE, 2014, 9, e98659.	1.1	17
17	Interface of the Polarizable Continuum Model of Solvation with Semi-Empirical Methods in the GAMESS Program. PLoS ONE, 2013, 8, e67725.	1.1	13
18	Using a genetic algorithm to find molecules with good docking scores. PeerJ Physical Chemistry, 0, 3, e18.	0.0	13

#	Article	IF	Citations
19	An averaged polarizable potential for multiscale modeling in phospholipid membranes. Journal of Computational Chemistry, 2017, 38, 601-611.	1.5	12
20	Modeling Electronic Circular Dichroism within the Polarizable Embedding Approach. Journal of Chemical Theory and Computation, 2017, 13, 4442-4451.	2.3	12
21	Cost-Effective Potential for Accurate Polarizable Embedding Calculations in Protein Environments. Journal of Chemical Theory and Computation, 2020, 16, 1162-1174.	2.3	12
22	Computational Approach to Evaluation of Optical Properties of Membrane Probes. Journal of Chemical Theory and Computation, 2017, 13, 719-726.	2.3	11
23	Hybrid RHF/MP2 Geometry Optimizations with the Effective Fragment Molecular Orbital Method. PLoS ONE, 2014, 9, e88800.	1.1	11
24	Mapping Interaction Energies in Chorismate Mutase with the Fragment Molecular Orbital Method. Journal of Physical Chemistry A, 2017, 121, 1797-1807.	1.1	9
25	A computational method for the systematic screening of reaction barriers in enzymes: searching forBacillus circulansxylanase mutants with greater activity towards a synthetic substrate. PeerJ, 2013, 1, e111.	0.9	7
26	The augâ€ccâ€pVTZâ€¦ basis set for the pâ€block fourthâ€row elements Ga, Ge, As, Se, and Br. Magnetic Resonance in Chemistry, 2021, 59, 1134-1145.	1.1	6
27	Supramolecular Complexes of Plant Neurotoxin Veratridine with Cyclodextrins and Their Antidote-like Effect on Neuro-2a Cell Viability. Pharmaceutics, 2022, 14, 598.	2.0	2
28	Combining polarizable embedding with the Frenkel exciton model: applications to absorption spectra with overlapping soluteâ€“solvent bands. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	0