Hiroshi C Watanabe

List of Publications by Year in descending order

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29	899	686830 13	552369 26
papers	citations	h-index	g-index

35	35	35	1231
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Conversion of Channelrhodopsin into a Light-Gated Chloride Channel. Science, 2014, 344, 409-412.	6.0	339
2	Origins of Water Molecules in the Photosystem II Crystal Structure. Biochemistry, 2017, 56, 3049-3057.	1.2	63
3	Towards an Understanding of Channelrhodopsin Function: Simulations Lead to Novel Insights of the Channel Mechanism. Journal of Molecular Biology, 2013, 425, 1795-1814.	2.0	62
4	Size-Consistent Multipartitioning QM/MM: A Stable and Efficient Adaptive QM/MM Method. Journal of Chemical Theory and Computation, 2014, 10, 4242-4252.	2.3	55
5	Electron transfer pathways in a multiheme cytochrome MtrF. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2916-2921.	3.3	41
6	Active site structure and absorption spectrum of channelrhodopsin-2 wild-type and C128T mutant. Chemical Science, 2016, 7, 3879-3891.	3.7	40
7	Structural Model of Channelrhodopsin. Journal of Biological Chemistry, 2012, 287, 7456-7466.	1.6	39
8	Quantitative Analysis of QM/MM Boundary Artifacts and Correction in Adaptive QM/MM Simulations. Journal of Chemical Theory and Computation, 2019, 15, 3917-3928.	2.3	32
9	Applications of quantum computing for investigations of electronic transitions in phenylsulfonyl-carbazole TADF emitters. Npj Computational Materials, 2021, 7, .	3.5	32
10	Color Tuning in Binding Pocket Models of the Chlamydomonas-Type Channelrhodopsins. Journal of Physical Chemistry B, 2011, 115, 15119-15128.	1.2	28
11	Structurally conserved channels in cyanobacterial and plant photosystem II. Photosynthesis Research, 2017, 133, 75-85.	1.6	25
12	QM/MM simulations of vibrational spectra of bacteriorhodopsin and channelrhodopsin-2. Physical Chemistry Chemical Physics, 2013, 15, 6651.	1.3	23
13	Molecular mechanism of long-range synergetic color tuning between multiple amino acid residues in conger rhodopsin. Biophysics (Nagoya-shi, Japan), 2010, 6, 67-78.	0.4	15
14	Improvement of Performance, Stability and Continuity by Modified Size-Consistent Multipartitioning Quantum Mechanical/Molecular Mechanical Method. Molecules, 2018, 23, 1882.	1.7	14
15	An adaptive quantum mechanics/molecular mechanics method for the infrared spectrum of water: incorporation of the quantum effect between solute and solvent. Physical Chemistry Chemical Physics, 2016, 18, 7318-7333.	1.3	12
16	Cation solvation with quantum chemical effects modeled by a size-consistent multi-partitioning quantum mechanics/molecular mechanics method. Physical Chemistry Chemical Physics, 2017, 19, 17985-17997.	1.3	10
17	Spectral Tuning of Photoactive Yellow Proteinâ€. Photochemistry and Photobiology, 2007, 83, 323-327.	1.3	9
18	Mutational analysis of the conserved carboxylates of anion channelrhodopsin-2 (ACR2) expressed in Escherichia coli and their roles in anion transport. Biophysics and Physicobiology, 2018, 15, 179-188.	0.5	9

#	Article	IF	Citations
19	Simulating time evolution with fully optimized single-qubit gates on parametrized quantum circuits. Physical Review A, 2022, 105, .	1.0	8
20	Rotamer decomposition and protein dynamics: Efficiently analyzing dihedral populations from molecular dynamics. Journal of Computational Chemistry, 2013, 34, 198-205.	1.5	7
21	Proton transfer in bulk water using the full adaptive QM/MM method: integration of solute- and solvent-adaptive approaches. Physical Chemistry Chemical Physics, 2021, 23, 8344-8360.	1.3	7
22	Labelâ€Free Phase Change Detection of Lipid Bilayers Using Nanoscale Diamond Magnetometry. Advanced Quantum Technologies, 2021, 4, 2000106.	1.8	7
23	Optimizing Parameterized Quantum Circuits with Free-Axis Selection. , 2021, , .		6
24	Theoretical modeling of the Oâ€intermediate structure of bacteriorhodopsin. Proteins: Structure, Function and Bioinformatics, 2009, 75, 53-61.	1.5	5
25	Post-Hartreeâ€“Fock method in quantum chemistry for quantum computer. European Physical Journal: Special Topics, 2021, 230, 1037-1051.	1.2	5
26	Thermal fluctuations enable rapid proteinâ€“protein associations in aqueous solution by lowering the reaction barrier. Chemical Physics Letters, 2016, 643, 114-118.	1.2	3
27	Reply to Breuer et al.: Molecular dynamics simulations do not provide functionally relevant values of redox potential in MtrF. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E10029-E10030.	3.3	3
28	Electron Transfer Pathways in a Multiheme Cytochrome MtrF. Seibutsu Butsuri, 2017, 57, 151-152.	0.0	0
29	Development of QM/MM Method Toward Proton Transfer in Bulk Phase. Seibutsu Butsuri, 2022, 62, 119-121.	0.0	0