# Hiroshi C Watanabe

## List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/9278642/publications.pdf

Version: 2024-02-01

| 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 | Development of QM/MM Method Toward Proton Transfer in Bulk Phase. Seibutsu Butsuri, 2022, 62, 119-121. | 0.0 | 0 |
| 2 | Simulating time evolution with fully optimized single-qubit gates on parametrized quantum circuits. Physical Review A, 2022, 105, . | 1.0 | 8 |
| 3 | 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 |
| 4 | Labelâ€Free Phase Change Detection of Lipid Bilayers Using Nanoscale Diamond Magnetometry. Advanced Quantum Technologies, 2021, 4, 2000106. | 1.8 | 7 |
| 5 | Post-Hartreeâ€“Fock method in quantum chemistry for quantum computer. European Physical Journal: Special Topics, 2021, 230, 1037-1051. | 1.2 | 5 |
| 6 | Applications of quantum computing for investigations of electronic transitions in phenylsulfonyl-carbazole TADF emitters. Npj Computational Materials, 2021, 7, . | 3.5 | 32 |
| 7 | Optimizing Parameterized Quantum Circuits with Free-Axis Selection. , 2021, , . | | 6 |
| 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 | 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 |
| 10 | Improvement of Performance, Stability and Continuity by Modified Size-Consistent Multipartitioning Quantum Mechanical/Molecular Mechanical Method. Molecules, 2018, 23, 1882. | 1.7 | 14 |
| 11 | Structurally conserved channels in cyanobacterial and plant photosystem II. Photosynthesis Research, 2017, 133, 75-85. | 1.6 | 25 |
| 12 | 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 |
| 13 | Origins of Water Molecules in the Photosystem II Crystal Structure. Biochemistry, 2017, 56, 3049-3057. | 1.2 | 63 |
| 14 | 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 |
| 15 | 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 |
| 16 | Electron Transfer Pathways in a Multiheme Cytochrome MtrF. Seibutsu Butsuri, 2017, 57, 151-152. | 0.0 | 0 |
| 17 | Active site structure and absorption spectrum of channelrhodopsin-2 wild-type and C128T mutant. Chemical Science, 2016, 7, 3879-3891. | 3.7 | 40 |
| 18 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | 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 |
| 20 | 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 |
| 21 | Conversion of Channelrhodopsin into a Light-Gated Chloride Channel. Science, 2014, 344, 409-412. | 6.0 | 339 |
| 22 | 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 |
| 23 | QM/MM simulations of vibrational spectra of bacteriorhodopsin and channelrhodopsin-2. Physical Chemistry Chemical Physics, 2013, 15, 6651. | 1.3 | 23 |
| 24 | Rotamer decomposition and protein dynamics: Efficiently analyzing dihedral populations from molecular dynamics. Journal of Computational Chemistry, 2013, 34, 198-205. | 1.5 | 7 |
| 25 | Structural Model of Channelrhodopsin. Journal of Biological Chemistry, 2012, 287, 7456-7466. | 1.6 | 39 |
| 26 | Color Tuning in Binding Pocket Models of the Chlamydomonas-Type Channelrhodopsins. Journal of Physical Chemistry B, 2011, 115, 15119-15128. | 1.2 | 28 |
| 27 | 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 |
| 28 | Theoretical modeling of the Oâ€intermediate structure of bacteriorhodopsin. Proteins: Structure, Function and Bioinformatics, 2009, 75, 53-61. | 1.5 | 5 |
| 29 | Spectral Tuning of Photoactive Yellow Proteinâ€. Photochemistry and Photobiology, 2007, 83, 323-327. | 1.3 | 9 |