

# Gerrit Groenhof

## List of Publications by Year in descending order

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77  
papers

17,981  
citations

108046

37  
h-index

73587

79  
g-index

90  
all docs

90  
docs citations

90  
times ranked

24550  
citing authors

#	ARTICLE	IF	CITATIONS
1	The Photocycle of Bacteriophytochrome Is Initiated by Counterclockwise Chromophore Isomerization. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 4538-4542.	2.1	7
2	Controlling Exciton Propagation in Organic Crystals through Strong Coupling to Plasmonic Nanoparticle Arrays. <i>ACS Photonics</i> , 2022, 9, 2263-2272.	3.2	18
3	Identifying Vibrations that Control Non-adiabatic Relaxation of Polaritons in Strongly Coupled Molecule-Cavity Systems. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 6259-6267.	2.1	10
4	Ultrafast structural changes within a photosynthetic reaction centre. <i>Nature</i> , 2021, 589, 310-314.	13.7	47
5	Covalent and non-covalent coupling of a Au <sub>102</sub> nanocluster with a fluorophore: energy transfer, quenching and intracellular pH sensing. <i>Nanoscale Advances</i> , 2021, 3, 6649-6658.	2.2	7
6	Multi-scale dynamics simulations of molecular polaritons: The effect of multiple cavity modes on polariton relaxation. <i>Journal of Chemical Physics</i> , 2021, 154, 104112.	1.2	50
7	Effect of molecular Stokes shift on polariton dynamics. <i>Journal of Chemical Physics</i> , 2021, 154, 154303.	1.2	23
8	Photoactive Yellow Protein Chromophore Photoisomerizes around a Single Bond if the Double Bond Is Locked. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 2177-2181.	2.1	4
9	Observe while it happens: catching photoactive proteins in the act with non-adiabatic molecular dynamics simulations. <i>Current Opinion in Structural Biology</i> , 2020, 61, 106-112.	2.6	6
10	GROMEX: A Scalable and Versatile Fast Multipole Method for Biomolecular Simulation. <i>Lecture Notes in Computational Science and Engineering</i> , 2020, , 517-543.	0.1	2
11	The primary structural photoresponse of phytochrome proteins captured by a femtosecond X-ray laser. <i>ELife</i> , 2020, 9, .	2.8	78
12	Tracking Polariton Relaxation with Multiscale Molecular Dynamics Simulations. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 5476-5483.	2.1	100
13	Exploring fast proton transfer events associated with lateral proton diffusion on the surface of membranes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 2443-2451.	3.3	45
14	Protonation of the Biliverdin IX <sub>β</sub> Chromophore in the Red and Far-Red Photoactive States of a Bacteriophytochrome. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2325-2334.	1.2	25
15	Theory for the stationary polariton response in the presence of vibrations. <i>Physical Review B</i> , 2019, 100, .	1.1	7
16	Excitation-Wavelength-Dependent Photocycle Initiation Dynamics Resolve Heterogeneity in the Photoactive Yellow Protein from <i>Halorhodospira halophila</i> . <i>Biochemistry</i> , 2018, 57, 1733-1747.	1.2	7
17	Molecular Mechanism of ATP Hydrolysis in an ABC Transporter. <i>ACS Central Science</i> , 2018, 4, 1334-1343.	5.3	65
18	Aluminum Plasmonics: Fabrication and Characterization of Broadly Tunable Plasmonic Surfaces for Plasmon Molecule Strong-Coupling and Fluorescence Enhancement. <i>NATO Science for Peace and Security Series B: Physics and Biophysics</i> , 2018, , 429-430.	0.2	0

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19	Is ATP Hydrolysis the Power Stroke in ABC Transporters?. <i>Biophysical Journal</i> , 2018, 114, 148a.	0.2	0
20	Coherent Light Harvesting through Strong Coupling to Confined Light. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4848-4851.	2.1	63
21	Accurate Three States Model for Amino Acids with Two Chemically Coupled Titrating Sites in Explicit Solvent Atomistic Constant pH Simulations and p <i>K<sub>a</sub></i> Calculations. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 147-160.	2.3	27
22	Dynamics of Strongly Coupled Modes between Surface Plasmon Polaritons and Photoactive Molecules: The Effect of the Stokes Shift. <i>ACS Photonics</i> , 2017, 4, 28-37.	3.2	42
23	Multiscale Molecular Dynamics Simulations of Polaritonic Chemistry. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4324-4335.	2.3	123
24	Exploring Strategies for Labeling Viruses with Gold Nanoclusters through Non-equilibrium Molecular Dynamics Simulations. <i>Bioconjugate Chemistry</i> , 2017, 28, 2327-2339.	1.8	9
25	Dynamic Stabilization of the Ligand-Metal Interface in Atomically Precise Gold Nanoclusters Au <sub>68</sub> and Au <sub>144</sub> Protected by <i>meta</i> -Mercaptobenzoic Acid. <i>ACS Nano</i> , 2017, 11, 11872-11879.	7.3	37
26	Cationic and Anionic Impact on the Electronic Structure of Liquid Water. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3759-3764.	2.1	26
27	The Low Barrier Hydrogen Bond in the Photoactive Yellow Protein: A Vacuum Artifact Absent in the Crystal and Solution. <i>Journal of the American Chemical Society</i> , 2016, 138, 16620-16631.	6.6	18
28	Acid-Base Properties and Surface Charge Distribution of the Water-Soluble Au <sub>102</sub> ( <i>p</i> -MBA) <sub>44</sub> Nanocluster. <i>Journal of Physical Chemistry C</i> , 2016, 120, 10041-10050.	1.5	47
29	Femtosecond structural dynamics drives the trans/cis isomerization in photoactive yellow protein. <i>Science</i> , 2016, 352, 725-729.	6.0	348
30	The room temperature crystal structure of a bacterial phytochrome determined by serial femtosecond crystallography. <i>Scientific Reports</i> , 2016, 6, 35279.	1.6	39
31	Hydrogen Bond Fluctuations Control Photochromism in a Reversibly Photo-switchable Fluorescent Protein. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 576-578.	7.2	35
32	Charge-Neutral Constant pH Molecular Dynamics Simulations Using a Parsimonious Proton Buffer. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1040-1051.	2.3	44
33	A Unified AMBER-Compatible Molecular Mechanics Force Field for Thiolate-Protected Gold Nanoclusters. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1342-1350.	2.3	76
34	New QM/MM implementation of the DFTB3 method in the gromacs package. <i>Journal of Computational Chemistry</i> , 2015, 36, 1978-1989.	1.5	45
35	Room temperature crystal structure of the fast switching M159T mutant of the fluorescent protein dronpa. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015, 83, 397-402.	1.5	8
36	The Lineshape of the Electronic Spectrum of the Green Fluorescent Protein Chromophore, Part II: Solution Phase. <i>ChemPhysChem</i> , 2014, 15, 3246-3257.	1.0	27

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37	On the use of reduced active space in CASSCF calculations. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 6-13.	1.1	12
38	Explicit proton transfer in classical molecular dynamics simulations. <i>Journal of Computational Chemistry</i> , 2014, 35, 657-671.	1.5	37
39	Quantifying Artifacts in Ewald Simulations of Inhomogeneous Systems with a Net Charge. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 381-390.	2.3	176
40	Anomalous Surface Diffusion of Protons on Lipid Membranes. <i>Biophysical Journal</i> , 2014, 107, 76-87.	0.2	55
41	Visualizing a protein quake with time-resolved X-ray scattering at a free-electron laser. <i>Nature Methods</i> , 2014, 11, 923-926.	9.0	173
42	Thermodynamics of hydronium and hydroxide surface solvation. <i>Chemical Science</i> , 2014, 5, 1745.	3.7	56
43	Weak intermolecular interactions promote blue luminescence of protonated 2,2'-dipyridylamine salts. <i>Journal of Materials Chemistry C</i> , 2014, 2, 8285-8294.	2.7	14
44	Steering the excited state dynamics of a photoactive yellow protein chromophore analogue with external electric fields. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 120-125.	1.1	8
45	The Lineshape of the Electronic Spectrum of the Green Fluorescent Protein Chromophore, Part I: Gas Phase. <i>ChemPhysChem</i> , 2014, 15, 3236-3245.	1.0	16
46	Force Distribution Analysis of Mechanochemically Reactive Dimethylcyclobutene. <i>ChemPhysChem</i> , 2013, 14, 2687-2697.	1.0	15
47	Combined QM/MM Investigation on the Light-Driven Electron-Induced Repair of the (6 <sup>4</sup> ) Thymine Dimer Catalyzed by DNA Photolyase. <i>Journal of Physical Chemistry B</i> , 2013, 117, 10071-10079.	1.2	24
48	Solving Chemical Problems with a Mixture of Quantum-Mechanical and Molecular Mechanics Calculations: Nobel Prize in Chemistry 2013. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 12489-12491.	7.2	6
49	Constant pH simulations with the coarse-grained MARTINI model – Application to oleic acid aggregates. <i>Canadian Journal of Chemistry</i> , 2013, 91, 839-846.	0.6	59
50	Introduction to QM/MM Simulations. <i>Methods in Molecular Biology</i> , 2013, 924, 43-66.	0.4	85
51	Control Mechanisms of Photoisomerization in Protonated Schiff Bases. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1005-1011.	2.1	18
52	Core hole screening and decay rates of double core ionized first row hydrides. <i>Journal of Chemical Physics</i> , 2013, 138, 164304.	1.2	13
53	Auger spectrum of a water molecule after single and double core ionization. <i>Journal of Chemical Physics</i> , 2012, 136, 144304.	1.2	46
54	Photochemical reactions in biological systems: probing the effect of the environment by means of hybrid quantum chemistry/molecular mechanics simulations. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 7912.	1.3	50

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55	Evaluating nonpolarizable nucleic acid force fields: A systematic comparison of the nucleobases hydration free energies and chloroform-water partition coefficients. <i>Journal of Computational Chemistry</i> , 2012, 33, 2225-2232.	1.5	25
56	Constant pH Molecular Dynamics in Explicit Solvent with $\lambda$ -Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1962-1978.	2.3	163
57	Controlling the Photoreactivity of the Photoactive Yellow Protein Chromophore by Substituting at the <i>p</i> -Coumaric Acid Group. <i>Journal of Physical Chemistry B</i> , 2011, 115, 7021-7028.	1.2	28
58	Promiscuity of Carbonic Anhydrase II. Unexpected Ester Hydrolysis of Carbohydrate-Based Sulfamate Inhibitors. <i>Journal of the American Chemical Society</i> , 2011, 133, 18452-18462.	6.6	38
59	g_membed: Efficient insertion of a membrane protein into an equilibrated lipid bilayer with minimal perturbation. <i>Journal of Computational Chemistry</i> , 2010, 31, 2169-2174.	1.5	355
60	Computer Simulations of Photobiological Processes: The Effect of the Protein Environment. <i>Advances in Quantum Chemistry</i> , 2010, , 181-212.	0.4	12
61	Molecular Basis of the Light-driven Switching of the Photochromic Fluorescent Protein Padron. <i>Journal of Biological Chemistry</i> , 2010, 285, 14603-14609.	1.6	65
62	Light-Induced Structural Changes in a Photosynthetic Reaction Center Caught by Laue Diffraction. <i>Science</i> , 2010, 328, 630-633.	6.0	103
63	Inclusion of ionization states of ligands in affinity calculations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 76, 138-150.	1.5	10
64	From fast light-activated processes in biomolecules to large-scale aggregation of membrane proteins: molecular dynamics simulations at different time and length scales. <i>Chemistry Central Journal</i> , 2009, 3, .	2.6	0
65	Hydrogen Bonding Controls Excited-State Decay of the Photoactive Yellow Protein Chromophore. <i>Journal of the American Chemical Society</i> , 2009, 131, 13580-13581.	6.6	75
66	Constant pH Simulations In Explicit Solvent Using The Lambda-Dynamics Approach. <i>Biophysical Journal</i> , 2009, 96, 574a.	0.2	0
67	Approximate switching algorithms for trajectory surface hopping. <i>Chemical Physics</i> , 2008, 351, 111-116.	0.9	54
68	Arginine52 Controls the Photoisomerization Process in Photoactive Yellow Protein. <i>Journal of the American Chemical Society</i> , 2008, 130, 3250-3251.	6.6	80
69	Chromophore Protonation State Controls Photoswitching of the Fluoroprotein asFP595. <i>PLoS Computational Biology</i> , 2008, 4, e1000034.	1.5	98
70	Ultrafast Deactivation Channel for Thymine Dimerization. <i>Journal of the American Chemical Society</i> , 2007, 129, 10996-10997.	6.6	125
71	Ultrafast Deactivation of an Excited Cytosine-Guanine Base Pair in DNA. <i>Journal of the American Chemical Society</i> , 2007, 129, 6812-6819.	6.6	164
72	Photoswitching of the Fluorescent Protein asFP595: Mechanism, Proton Pathways, and Absorption Spectra. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 530-536.	7.2	95

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73	The planar conformation of a strained proline ring: A QM/MM study. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 64, 700-710.	1.5	15
74	GROMACS: Fast, flexible, and free. <i>Journal of Computational Chemistry</i> , 2005, 26, 1701-1718.	1.5	13,676
75	Photoactivation of the Photoactive Yellow Protein: Why Photon Absorption Triggers a Trans-to-Cis Isomerization of the Chromophore in the Protein. <i>Journal of the American Chemical Society</i> , 2004, 126, 4228-4233.	6.6	265
76	Signal transduction in the photoactive yellow protein. II. Proton transfer initiates conformational changes. <i>Proteins: Structure, Function and Bioinformatics</i> , 2002, 48, 212-219.	1.5	36
77	Signal transduction in the photoactive yellow protein. I. Photon absorption and the isomerization of the chromophore. <i>Proteins: Structure, Function and Bioinformatics</i> , 2002, 48, 202-211.	1.5	64