Gerrit Groenhof

List of Publications by Year
in descending order

77 papers	17,981 citations	94269 37 h-index	64668 79 g-index
90 all docs	90 docs citations	90 times ranked	21695 citing authors

#	Article	IF	Citations
1	GROMACS: Fast, flexible, and free. Journal of Computational Chemistry, 2005, 26, 1701-1718.	1.5	13,676
2	g_membed: Efficient insertion of a membrane protein into an equilibrated lipid bilayer with minimal perturbation. Journal of Computational Chemistry, 2010, 31, 2169-2174.	1.5	355
3	Femtosecond structural dynamics drives the trans/cis isomerization in photoactive yellow protein. Science, 2016, 352, 725-729.	6.0	348
4	Photoactivation of the Photoactive Yellow Protein:Â Why Photon Absorption Triggers a Trans-to-Cis Isomerization of the Chromophore in the Protein. Journal of the American Chemical Society, 2004, 126, 4228-4233.	6.6	265
5	Quantifying Artifacts in Ewald Simulations of Inhomogeneous Systems with a Net Charge. Journal of Chemical Theory and Computation, 2014, 10, 381-390.	2.3	176
6	Visualizing a protein quake with time-resolved X-ray scattering at a free-electron laser. Nature Methods, 2014, 11, 923-926.	9.0	173
7	Ultrafast Deactivation of an Excited Cytosineâ"Guanine Base Pair in DNA. Journal of the American Chemical Society, 2007, 129, 6812-6819.	6.6	164
8	Constant pH Molecular Dynamics in Explicit Solvent with Î»-Dynamics. Journal of Chemical Theory and Computation, 2011, 7, 1962-1978.	2.3	163
9	Ultrafast Deactivation Channel for Thymine Dimerization. Journal of the American Chemical Society, 2007, 129, 10996-10997.	6.6	125
10	Multiscale Molecular Dynamics Simulations of Polaritonic Chemistry. Journal of Chemical Theory and Computation, 2017, 13, 4324-4335.	2.3	123
11	Light-Induced Structural Changes in a Photosynthetic Reaction Center Caught by Laue Diffraction. Science, 2010, 328, 630-633.	6.0	103
12	Tracking Polariton Relaxation with Multiscale Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2019, 10, 5476-5483.	2.1	100
13	Chromophore Protonation State Controls Photoswitching of the Fluoroprotein asFP595. PLoS Computational Biology, 2008, 4, e1000034.	1.5	98
14	Photoswitching of the Fluorescent Protein asFP595: Mechanism, Proton Pathways, and Absorption Spectra. Angewandte Chemie - International Edition, 2007, 46, 530-536.	7.2	95
15	Introduction to QM/MM Simulations. Methods in Molecular Biology, 2013, 924, 43-66.	0.4	85
16	Arginine52 Controls the Photoisomerization Process in Photoactive Yellow Protein. Journal of the American Chemical Society, 2008, 130, 3250-3251.	6.6	80
17	The primary structural photoresponse of phytochrome proteins captured by a femtosecond X-ray laser. ELife, 2020, 9, .	2.8	78
18	A Unified AMBER-Compatible Molecular Mechanics Force Field for Thiolate-Protected Gold Nanoclusters. Journal of Chemical Theory and Computation, 2016, 12, 1342-1350.	2.3	76

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19	Hydrogen Bonding Controls Excited-State Decay of the Photoactive Yellow Protein Chromophore. Journal of the American Chemical Society, 2009, 131, 13580-13581.	6.6	75
20	Molecular Basis of the Light-driven Switching of the Photochromic Fluorescent Protein Padron. Journal of Biological Chemistry, 2010, 285, 14603-14609.	1.6	65
21	Molecular Mechanism of ATP Hydrolysis in an ABC Transporter. ACS Central Science, 2018, 4, 1334-1343.	5.3	65
22	Signal transduction in the photoactive yellow protein. I. Photon absorption and the isomerization of the chromophore. Proteins: Structure, Function and Bioinformatics, 2002, 48, 202-211.	1.5	64
23	Coherent Light Harvesting through Strong Coupling to Confined Light. Journal of Physical Chemistry Letters, 2018, 9, 4848-4851.	2.1	63
24	Constant pH simulations with the coarse-grained MARTINI model â€" Application to oleic acid aggregates. Canadian Journal of Chemistry, 2013, 91, 839-846.	0.6	59
25	Thermodynamics of hydronium and hydroxide surface solvation. Chemical Science, 2014, 5, 1745.	3.7	56
26	Anomalous Surface Diffusion of Protons on Lipid Membranes. Biophysical Journal, 2014, 107, 76-87.	0.2	55
27	Approximate switching algorithms for trajectory surface hopping. Chemical Physics, 2008, 351, 111-116.	0.9	54
28	Photochemical reactions in biological systems: probing the effect of the environment by means of hybrid quantum chemistry/molecular mechanics simulations. Physical Chemistry Chemical Physics, 2012, 14, 7912.	1.3	50
29	Multi-scale dynamics simulations of molecular polaritons: The effect of multiple cavity modes on polariton relaxation. Journal of Chemical Physics, 2021, 154, 104112.	1.2	50
30	Acidâ€"Base Properties and Surface Charge Distribution of the Water-Soluble Au₁₀₂(pMBA)₄₄ Nanocluster. Journal of Physical Chemistry C, 2016, 120, 10041-10050.	1.5	47
31	Ultrafast structural changes within a photosynthetic reaction centre. Nature, 2021, 589, 310-314.	13.7	47
32	Auger spectrum of a water molecule after single and double core ionization. Journal of Chemical Physics, 2012, 136, 144304.	1.2	46
33	New QM/MM implementation of the DFTB3 method in the gromacs package. Journal of Computational Chemistry, 2015, 36, 1978-1989.	1.5	45
34	Exploring fast proton transfer events associated with lateral proton diffusion on the surface of membranes. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 2443-2451.	3.3	45
35	Charge-Neutral Constant pH Molecular Dynamics Simulations Using a Parsimonious Proton Buffer. Journal of Chemical Theory and Computation, 2016, 12, 1040-1051.	2.3	44
36	Dynamics of Strongly Coupled Modes between Surface Plasmon Polaritons and Photoactive Molecules: The Effect of the Stokes Shift. ACS Photonics, 2017, 4, 28-37.	3.2	42

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37	The room temperature crystal structure of a bacterial phytochrome determined by serial femtosecond crystallography. Scientific Reports, 2016, 6, 35279.	1.6	39
38	Promiscuity of Carbonic Anhydrase II. Unexpected Ester Hydrolysis of Carbohydrate-Based Sulfamate Inhibitors. Journal of the American Chemical Society, 2011, 133, 18452-18462.	6.6	38
39	Explicit proton transfer in classical molecular dynamics simulations. Journal of Computational Chemistry, 2014, 35, 657-671.	1.5	37
40	Dynamic Stabilization of the Ligandâ€“Metal Interface in Atomically Precise Gold Nanoclusters Au₆₈ and Au₁₄₄ Protected by meta-Mercaptobenzoic Acid. ACS Nano, 2017, 11, 11872-11879.	7.3	37
41	Signal transduction in the photoactive yellow protein. II. Proton transfer initiates conformational changes. Proteins: Structure, Function and Bioinformatics, 2002, 48, 212-219.	1.5	36
42	Hydrogen Bond Fluctuations Control Photochromism in a Reversibly Photoâ€Šswitchable Fluorescent Protein. Angewandte Chemie - International Edition, 2016, 55, 576-578.	7.2	35
43	Controlling the Photoreactivity of the Photoactive Yellow Protein Chromophore by Substituting at the p-Coumaric Acid Group. Journal of Physical Chemistry B, 2011, 115, 7021-7028.	1.2	28
44	The Lineshape of the Electronic Spectrum of the Green Fluorescent Protein Chromophore, Part II: Solution Phase. ChemPhysChem, 2014, 15, 3246-3257.	1.0	27
45	Accurate Three States Model for Amino Acids with Two Chemically Coupled Titrating Sites in Explicit Solvent Atomistic Constant pH Simulations and pK_a Calculations. Journal of Chemical Theory and Computation, 2017, 13, 147-160.	2.3	27
46	Cationic and Anionic Impact on the Electronic Structure of Liquid Water. Journal of Physical Chemistry Letters, 2017, 8, 3759-3764.	2.1	26
47	Evaluating nonpolarizable nucleic acid force fields: A systematic comparison of the nucleobases hydration free energies and chloroformâ€toâ€water partition coefficients. Journal of Computational Chemistry, 2012, 33, 2225-2232.	1.5	25
48	Protonation of the Biliverdin IXÎ± Chromophore in the Red and Far-Red Photoactive States of a Bacteriophytochrome. Journal of Physical Chemistry B, 2019, 123, 2325-2334.	1.2	25
49	Combined QM/MM Investigation on the Light-Driven Electron-Induced Repair of the (6â€“4) Thymine Dimer Catalyzed by DNA Photolyase. Journal of Physical Chemistry B, 2013, 117, 10071-10079.	1.2	24
50	Effect of molecular Stokes shift on polariton dynamics. Journal of Chemical Physics, 2021, 154, 154303.	1.2	23
51	Control Mechanisms of Photoisomerization in Protonated Schiff Bases. Journal of Physical Chemistry Letters, 2013, 4, 1005-1011.	2.1	18
52	The Low Barrier Hydrogen Bond in the Photoactive Yellow Protein: A Vacuum Artifact Absent in the Crystal and Solution. Journal of the American Chemical Society, 2016, 138, 16620-16631.	6.6	18
53	Controlling Exciton Propagation in Organic Crystals through Strong Coupling to Plasmonic Nanoparticle Arrays. ACS Photonics, 2022, 9, 2263-2272.	3.2	18
54	The Lineshape of the Electronic Spectrum of the Green Fluorescent Protein Chromophore, Part I: Gas Phase. ChemPhysChem, 2014, 15, 3236-3245.	1.0	16

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55	The planar conformation of a strained proline ring: A QM/MM study. Proteins: Structure, Function and Bioinformatics, 2006, 64, 700-710.	1.5	15
56	Force Distribution Analysis of Mechanochemically Reactive Dimethylcyclobutene. ChemPhysChem, 2013, 14, 2687-2697.	1.0	15
57	Weak intermolecular interactions promote blue luminescence of protonated 2,2â€²-dipyridylamine salts. Journal of Materials Chemistry C, 2014, 2, 8285-8294.	2.7	14
58	Core hole screening and decay rates of double core ionized first row hydrides. Journal of Chemical Physics, 2013, 138, 164304.	1.2	13
59	Computer Simulations of Photobiological Processes: The Effect of the Protein Environment. Advances in Quantum Chemistry, 2010, , 181-212.	0.4	12
60	On the use of reduced active space in CASSCF calculations. Computational and Theoretical Chemistry, 2014, 1040-1041, 6-13.	1.1	12
61	Inclusion of ionization states of ligands in affinity calculations. Proteins: Structure, Function and Bioinformatics, 2009, 76, 138-150.	1.5	10
62	Identifying Vibrations that Control Non-adiabatic Relaxation of Polaritons in Strongly Coupled Moleculeâ€“Cavity Systems. Journal of Physical Chemistry Letters, 2022, 13, 6259-6267.	2.1	10
63	Exploring Strategies for Labeling Viruses with Gold Nanoclusters through Non-equilibrium Molecular Dynamics Simulations. Bioconjugate Chemistry, 2017, 28, 2327-2339.	1.8	9
64	Steering the excited state dynamics of a photoactive yellow protein chromophore analogue with external electric fields. Computational and Theoretical Chemistry, 2014, 1040-1041, 120-125.	1.1	8
65	Room temperature crystal structure of the fast switching M159T mutant of the fluorescent protein dronpa. Proteins: Structure, Function and Bioinformatics, 2015, 83, 397-402.	1.5	8
66	Excitation-Wavelength-Dependent Photocycle Initiation Dynamics Resolve Heterogeneity in the Photoactive Yellow Protein from Halorhodospira halophila. Biochemistry, 2018, 57, 1733-1747.	1.2	7
67	Theory for the stationary polariton response in the presence of vibrations. Physical Review B, 2019, 100, .	1.1	7
68	Covalent and non-covalent coupling of a Au₁₀₂ nanocluster with a fluorophore: energy transfer, quenching and intracellular pH sensing. Nanoscale Advances, 2021, 3, 6649-6658.	2.2	7
69	The Photocycle of Bacteriophytochrome Is Initiated by Counterclockwise Chromophore Isomerization. Journal of Physical Chemistry Letters, 2022, 13, 4538-4542.	2.1	7
70	Solving Chemical Problems with a Mixture of Quantumâ€Mechanical and Molecular Mechanics Calculations: Nobel Prize in Chemistry 2013. Angewandte Chemie - International Edition, 2013, 52, 12489-12491.	7.2	6
71	Observe while it happens: catching photoactive proteins in the act with non-adiabatic molecular dynamics simulations. Current Opinion in Structural Biology, 2020, 61, 106-112.	2.6	6
72	Photoactive Yellow Protein Chromophore Photoisomerizes around a Single Bond if the Double Bond Is Locked. Journal of Physical Chemistry Letters, 2020, 11, 2177-2181.	2.1	4

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73	GROMEX: A Scalable and Versatile Fast Multipole Method for Biomolecular Simulation. Lecture Notes in Computational Science and Engineering, 2020, , 517-543.	0.1	2
74	From fast light-activated processes in biomolecules to large-scale aggregation of membrane proteins: molecular dynamics simulations at different time and length scales. Chemistry Central Journal, 2009, 3, .	2.6	0
75	Constant pH Simulations In Explicit Solvent Using The Lambda-Dynamics Approach. Biophysical Journal, 2009, 96, 574a.	0.2	0
76	Aluminum Plasmonics: Fabrication and Characterization of Broadly Tunable Plasmonic Surfaces for Plasmon Molecule Strong-Coupling and Fluorescence Enhancement. NATO Science for Peace and Security Series B: Physics and Biophysics, 2018, , 429-430.	0.2	0
77	Is ATP Hydrolysis the Power Stroke in ABC Transporters?. Biophysical Journal, 2018, 114, 148a.	0.2	0