

Young Min Rhee

List of Publications by Year in descending order

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99
papers

9,033
citations

126708

33
h-index

39575

94
g-index

104
all docs

104
docs citations

104
times ranked

10357
citing authors

#	ARTICLE	IF	CITATIONS
1	Advances in methods and algorithms in a modern quantum chemistry program package. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 3172-3191.	1.3	2,597
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	0.8	2,561
3	Atomistic protein folding simulations on the submillisecond time scale using worldwide distributed computing. <i>Biopolymers</i> , 2003, 68, 91-109.	1.2	346
4	Multiplexed-Replica Exchange Molecular Dynamics Method for Protein Folding Simulation. <i>Biophysical Journal</i> , 2003, 84, 775-786.	0.2	268
5	How Well Can Simulation Predict Protein Folding Kinetics and Thermodynamics?. <i>Annual Review of Biophysics and Biomolecular Structure</i> , 2005, 34, 43-69.	18.3	225
6	Simulations of the role of water in the protein-folding mechanism. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004, 101, 6456-6461.	3.3	187
7	Scaled Second-Order Perturbation Corrections to Configuration Interaction Singles: Efficient and Reliable Excitation Energy Methods. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5314-5326.	1.1	185
8	Poly-cyclodextrin and poly-paclitaxel nano-assembly for anticancer therapy. <i>Nature Communications</i> , 2014, 5, 3702.	5.8	184
9	A structural remedy toward bright dipolar fluorophores in aqueous media. <i>Chemical Science</i> , 2015, 6, 4335-4342.	3.7	144
10	An improved algorithm for analytical gradient evaluation in resolution-of-the-identity second-order Møller-Plesset perturbation theory: Application to alanine tetrapeptide conformational analysis. <i>Journal of Computational Chemistry</i> , 2007, 28, 839-856.	1.5	134
11	Charged polycyclic aromatic hydrocarbon clusters and the galactic extended red emission. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 5274-5278.	3.3	109
12	Insights into Nucleic Acid Conformational Dynamics from Massively Parallel Stochastic Simulations. <i>Biophysical Journal</i> , 2003, 85, 790-803.	0.2	95
13	Does Water Play a Structural Role in the Folding of Small Nucleic Acids?. <i>Biophysical Journal</i> , 2005, 88, 2516-2524.	0.2	95
14	Characterization of Vinylgold Intermediates: Gold-Mediated Cyclization of Acetylenic Amides. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 11446-11450.	7.2	92
15	Electric Field Keeps Chromophore Planar and Produces High Yield Fluorescence in Green Fluorescent Protein. <i>Journal of the American Chemical Society</i> , 2016, 138, 13619-13629.	6.6	72
16	One-Dimensional Reaction Coordinate and the Corresponding Potential of Mean Force from Commitment Probability Distribution. <i>Journal of Physical Chemistry B</i> , 2005, 109, 6780-6786.	1.2	70
17	Highly Sensitive and Selective Biosensors Based on Organic Transistors Functionalized with Cucurbit[6]uril Derivatives. <i>Advanced Functional Materials</i> , 2015, 25, 4882-4888.	7.8	66
18	All-Atom Semiclassical Dynamics Study of Quantum Coherence in Photosynthetic Fenna-Matthews-Olson Complex. <i>Journal of the American Chemical Society</i> , 2012, 134, 11640-11651.	6.6	61

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19	Mixed Quantum-Classical Description of Excitation Energy Transfer in a Model Fenna-Matthews-Olsen Complex. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 808-812.	2.1	56
20	Density functional calculations of electronic structure and magnetic properties of the hydrocarbon K_3 superconductor near the metal-insulator transition. <i>Physical Review B</i> , 2011, 83, .	1.1	56
21	Dynamics on the Electronically Excited State Surface of the Bioluminescent Firefly Luciferase-Oxyluciferin System. <i>Journal of the American Chemical Society</i> , 2011, 133, 12040-12049.	6.6	53
22	Spin-Vibronic Model for Quantitative Prediction of Reverse Intersystem Crossing Rate in Thermally Activated Delayed Fluorescence Systems. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 621-632.	2.3	53
23	Three States Involving Vibronic Resonance is a Key to Enhancing Reverse Intersystem Crossing Dynamics of an Organoboron-Based Ultrapure Blue Emitter. <i>Jacs Au</i> , 2021, 1, 987-997.	3.6	48
24	Ground-State Elevation Approach To Suppress Side Reactions in Gold-Sensing Systems Based on Alkyne Activation. <i>Organic Letters</i> , 2014, 16, 1374-1377.	2.4	47
25	Phase Behavior and Conductivity of Sulfonated Block Copolymers Containing Heterocyclic Diazole-Based Ionic Liquids. <i>Macromolecules</i> , 2012, 45, 8702-8713.	2.2	46
26	Dispersion-Oriented Soft Interaction in a Frustrated Lewis Pair and the Entropic Encouragement Effect in its Formation. <i>Chemistry - A European Journal</i> , 2009, 15, 13348-13355.	1.7	45
27	Does Native State Topology Determine the RNA Folding Mechanism?. <i>Journal of Molecular Biology</i> , 2004, 337, 789-797.	2.0	44
28	The Solvation Interface is a Determining Factor in Peptide Conformational Preferences. <i>Journal of Molecular Biology</i> , 2006, 356, 248-256.	2.0	44
29	Potential energy surfaces for polyatomic reactions by interpolation with reaction path weight: $CH_2OH + \dot{C}HO + H_2$ reaction. <i>Journal of Chemical Physics</i> , 1997, 106, 1003-1012.	1.2	43
30	Quasidegenerate scaled opposite spin second order perturbation corrections to single excitation configuration interaction. <i>Journal of Chemical Physics</i> , 2008, 128, 164106.	1.2	43
31	<i>N</i> -Heterocyclic Carbene Nitric Oxide Radicals. <i>Journal of the American Chemical Society</i> , 2015, 137, 4642-4645.	6.6	40
32	Improving long time behavior of Poisson bracket mapping equation: A non-Hamiltonian approach. <i>Journal of Chemical Physics</i> , 2014, 140, 184106.	1.2	38
33	Dimerization of the p53 Oligomerization Domain: Identification of a Folding Nucleus by Molecular Dynamics Simulations. <i>Journal of Molecular Biology</i> , 2005, 345, 869-878.	2.0	36
34	Kinetic Definition of Protein Folding Transition State Ensembles and Reaction Coordinates. <i>Biophysical Journal</i> , 2006, 91, 14-24.	0.2	33
35	Protein folding from heterogeneous unfolded state revealed by time-resolved X-ray solution scattering. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 14996-15005.	3.3	33
36	Excited state energy fluctuations in the Fenna-Matthews-Olson complex from molecular dynamics simulations with interpolated chromophore potentials. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 3310-3319.	1.3	31

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37	Simple Method for Simulating the Mixture of Atomistic and Coarse-Grained Molecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3728-3739.	2.3	30
38	Mode-specific energy analysis for rotating-vibrating triatomic molecules in classical trajectory simulation. <i>Journal of Chemical Physics</i> , 1997, 107, 1394-1402.	1.2	29
39	Construction of an accurate potential energy surface by interpolation with Cartesian weighting coordinates. <i>Journal of Chemical Physics</i> , 2000, 113, 6021-6024.	1.2	29
40	Solvent Viscosity Dependence of the Protein Folding Dynamics. <i>Journal of Physical Chemistry B</i> , 2008, 112, 6221-6227.	1.2	29
41	Development of force field parameters for oxyluciferin on its electronic ground and excited states. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 4091-4105.	1.0	28
42	Analytical gradient of restricted second-order Møller-Plesset correlation energy with the resolution of the identity approximation, applied to the TCNE dimer anion complex. <i>Chemical Physics Letters</i> , 2006, 426, 197-203.	1.2	27
43	Effect of Chromophore Potential Model on the Description of Exciton-Phonon Interactions. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 2875-2880.	2.1	27
44	Condensed phase molecular dynamics using interpolated potential energy surfaces with application to the resolution process of coumarin 153. <i>Journal of Chemical Physics</i> , 2011, 135, 014107.	1.2	26
45	Frontiers in Multiscale Modeling of Photoreceptor Proteins. <i>Photochemistry and Photobiology</i> , 2021, 97, 243-269.	1.3	26
46	On the Mechanism of Irreversible Carbon Dioxide Binding with a Frustrated Lewis Pair: Solvent-Assisted Frustration and Transition State Entropic Encouragement. <i>Chemistry - A European Journal</i> , 2011, 17, 6501-6507.	1.7	24
47	Emission shaping in fluorescent proteins: role of electrostatics and π -stacking. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 3944-3955.	1.3	24
48	Quartic-Scaling Analytical Gradient of Quasidegenerate Scaled Opposite Spin Second-Order Perturbation Corrections to Single Excitation Configuration Interaction. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1224-1236.	2.3	23
49	Constructing an Interpolated Potential Energy Surface of a Large Molecule: A Case Study with Bacteriochlorophyll <i>a</i> Model in the Fenna-Matthews-Olson Complex. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5235-5246.	2.3	23
50	Performance of Quasi-Degenerate Scaled Opposite Spin Perturbation Corrections to Single Excitation Configuration Interaction for Excited State Structures and Excitation Energies with Application to the Stokes Shift of 9-Methyl-9,10-dihydro-9-silaphenanthrene. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10564-10576.	1.1	22
51	<i>C</i> ₃ -Symmetric Cage-like Receptors: Chiral Discrimination of Δ -Chiral Amines in a Confined Space. <i>Organic Letters</i> , 2010, 12, 4228-4231.	2.4	22
52	On the role of chemical detail in simulating protein folding kinetics. <i>Chemical Physics</i> , 2006, 323, 66-77.	0.9	21
53	A Delicate Electronic Balance between Metal and Ligand in [Cu ^{II} P ^{III} Cu ^{II} P] Diamondoids: A Oxidation State Dependent Plasticity and the Formation of a Singlet Diradicaloid. <i>Journal of the American Chemical Society</i> , 2008, 130, 3878-3887.	6.6	21
54	Coherent intermolecular proton transfer in the acid-base reaction of excited state pyranine. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 18243-18251.	1.3	21

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55	Studying Interfacial Reactions of Cholesterol Sulfate in an Unsaturated Phosphatidylglycerol Layer with Ozone Using Field Induced Droplet Ionization Mass Spectrometry. <i>Journal of the American Society for Mass Spectrometry</i> , 2012, 23, 141-152.	1.2	17
56	Interpolated Mechanicsâ€”Molecular Mechanics Study of Internal Rotation Dynamics of the Chromophore Unit in Blue Fluorescent Protein and Its Variants. <i>Journal of Physical Chemistry B</i> , 2012, 116, 11137-11147.	1.2	16
57	DNSC: a fluorescent, environmentally sensitive cytidine derivative for the direct detection of GGG triad sequences. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 5605.	1.5	14
58	Improving long time behavior of Poisson bracket mapping equation: A mapping variable scaling approach. <i>Journal of Chemical Physics</i> , 2014, 141, 124107.	1.2	14
59	Effect of Underdamped Vibration on Excitation Energy Transfer: Direct Comparison between Two Different Partitioning Schemes. <i>Journal of Physical Chemistry A</i> , 2019, 123, 1186-1197.	1.1	14
60	Towards the Realization of Ab Initio Dynamics at the Speed of Molecular Mechanics: Simulations with Interpolated Diabatic Hamiltonian. <i>ChemPhysChem</i> , 2014, 15, 3183-3193.	1.0	12
61	Dynamic isotope effect on the product energy partitioning in $\text{CH}_2\text{OH}+\hat{\text{t}}^+\text{CHO}++\text{H}_2$. <i>Journal of Chemical Physics</i> , 1998, 109, 5363-5371.	1.2	11
62	Nearly 100% Exciton Utilization via Hybridized Interâ€”and Intramolecular Triplet Exciton Harvesting Channels in Blue Fluorescent Organic Lightâ€”Emitting Diodes. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	11
63	On the pH Dependent Behavior of the Firefly Bioluminescence: Protein Dynamics and Water Content in the Active Pocket. <i>Journal of Physical Chemistry B</i> , 2013, 117, 7260-7269.	1.2	10
64	Constructing polyatomic potential energy surfaces by interpolating diabatic Hamiltonian matrices with demonstration on green fluorescent protein chromophore. <i>Journal of Chemical Physics</i> , 2014, 140, 164112.	1.2	10
65	Chargeâ€”dipole interactions in G-quadruplex thrombin-binding aptamer. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21068-21074.	1.3	10
66	Diabatic Population Matrix Formalism for Performing Molecular Mechanics Style Simulations with Multiple Electronic States. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5238-5253.	2.3	9
67	A proton transfer network that generates deprotonated tyrosine is a key to producing reactive oxygen species in phototoxic KillerRed protein. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 22342-22350.	1.3	9
68	Energy partitioning during the exit channel motion for $\text{CH}_2\text{OH}+\hat{\text{t}}^+\text{CHO}++\text{H}_2$. <i>Chemical Physics Letters</i> , 1997, 264, 303-308.	1.2	8
69	How Does Solvation Affect the Binding of Hydrophilic Amino Saccharides to Cucurbit[7]uril with Exceptional Anomeric Selectivity?. <i>Chemistry - A European Journal</i> , 2016, 22, 15791-15799.	1.7	8
70	On Surface Hopping and Time-Reversal. <i>Journal of Physical Chemistry A</i> , 2015, 119, 990-995.	1.1	7
71	Interpolation for molecular dynamics simulations: from ions in gas phase to proteins in solution. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 573-577.	1.0	7
72	Effect of Perturbative Vibronic Correction for Weak Fluorescence in Thermally Activated Delayed Fluorescence Systems. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10384-10392.	1.1	7

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73	Theoretical Study on the Degree of CO ₂ Activation in CO ₂ -Coordinated Ni(0) Complexes. ACS Omega, 2021, 6, 7646-7654.	1.6	7
74	Cooperation between Excitation Energy Transfer and Antisynchronously Coupled Vibrations. Journal of Physical Chemistry B, 2021, 125, 5601-5610.	1.2	7
75	Two-oscillator mapping modification of the Poisson bracket mapping equation formulation of the quantum-classical Liouville equation. Journal of Chemical Physics, 2020, 153, 214103.	1.2	7
76	Enhancement of Energy Transfer Efficiency with Structural Control of Multichromophore Light-Harvesting Assembly. Advanced Science, 2020, 7, 2001623.	5.6	6
77	Behavior of Poisson Bracket Mapping Equation in Studying Excitation Energy Transfer Dynamics of Cryptophyte Phycocyanin 645 Complex. Bulletin of the Korean Chemical Society, 2012, 33, 933-940.	1.0	6
78	Molecule-specific determination of atomic polarizabilities with the polarizable atomic multipole model. Journal of Computational Chemistry, 2012, 33, 1662-1672.	1.5	5
79	Fluorescent peptide indicator displacement assay for monitoring interactions between RNA and RNA binding proteins. Molecular BioSystems, 2013, 9, 948-951.	2.9	5
80	Toward monitoring the dissipative vibrational energy flows in open quantum systems by mixed quantum-classical simulations. Journal of Chemical Physics, 2020, 152, 244109.	1.2	5
81	Computational elucidations on the role of vibrations in energy transfer processes of photosynthetic complexes. Physical Chemistry Chemical Physics, 2021, 23, 26623-26639.	1.3	5
82	Analytical gradients for core-excited states in the algebraic diagrammatic construction (ADC) framework. Journal of Chemical Physics, 2021, 155, 044106.	1.2	4
83	Uncovering the Conformational Distribution of a Small Protein with Nanoparticle-Aided Cryo-Electron Microscopy Sampling. Journal of Physical Chemistry Letters, 2021, 12, 6565-6573.	2.1	4
84	Efficiently Transplanting Potential Energy Interpolation Database between Two Systems: Bacteriochlorophyll Case with FMO and LH2 Complexes. Journal of Chemical Information and Modeling, 2019, 59, 4228-4238.	2.5	3
85	Modeling Charge Flux by Interpolating Atomic Partial Charges. Journal of Chemical Information and Modeling, 2019, 59, 2837-2849.	2.5	2
86	Exploring the Possibility of Excited State Keto-Enolate Transformation of the Oxyluciferin-Luciferase Complex with QM/MM Free Energy Simulations. ChemPhotoChem, 2019, 3, 804-813.	1.5	2
87	Free energy level correction by Monte Carlo resampling with weighted histogram analysis method. Chinese Journal of Chemical Physics, 2020, 33, 183-195.	0.6	2
88	Excited State Proton Transfer of Quinone Cyanine 9: Implications on the Origin of Super-Photoacidity. ChemPhotoChem, 2021, 5, 245-252.	1.5	2
89	Two-dimensional electronic spectrum simulation of simple photosynthetic complex models with semi-classical Poisson bracket mapping equation. Bulletin of the Korean Chemical Society, 2022, 43, 355-363.	1.0	2
90	Computational Photochemistry. ChemPhotoChem, 2019, 3, 664-665.	1.5	1

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91	Considering both small and large scale motions of vascular endothelial growth factor (VEGF) is crucial for reliably predicting its binding affinities to DNA aptamers. RSC Advances, 2021, 11, 9315-9326.	1.7	1
92	Excited State Proton Transfer of Quinone Cyanine 9: Implications on the Origin of Superacidity. ChemPhotoChem, 2021, 5, 186-186.	1.5	1
93	Can Adenosine Triarsenate Role as an Energy Carrier?. Bulletin of the Korean Chemical Society, 2013, 34, 361-362.	1.0	1
94	Interpolation of Potential Energy Surfaces for Nonadiabatic Simulations of Biological Systems. Biophysical Journal, 2014, 106, 806a.	0.2	0
95	Mixed Quantum-Classical Study of the Nonadiabatic Dynamics in Photosynthetic Systems. Biophysical Journal, 2014, 106, 806a.	0.2	0
96	Simple Method for Hybrid All-Atom and Coarse-Grained Molecular Dynamics Simulations and Its Applications. Biophysical Journal, 2014, 106, 413a.	0.2	0
97	Organic Electronics: Highly Sensitive and Selective Biosensors Based on Organic Transistors Functionalized with Cucurbit[6]uril Derivatives (Adv. Funct. Mater. 30/2015). Advanced Functional Materials, 2015, 25, 4920-4920.	7.8	0
98	Excitonic Energy Transfer of Cryptophyte Phycocyanin 645 Complex in Physiological Temperature by Reduced Hierarchical Equation of Motion. Bulletin of the Korean Chemical Society, 2014, 35, 858-864.	1.0	0
99	Quantum Chemistry Based Arguments about Singlet Oxygen Formation Trends from Fluorescent Proteins. Rapid Communication in Photoscience, 2016, 5, 18-20.	0.1	0