Young Min Rhee

List of Publications by Year
in descending order

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	Twoâ€dimensional electronic spectrum simulation of simple photosynthetic complex models with semiâ€classical Poisson bracket mapping equation. Bulletin of the Korean Chemical Society, 2022, 43, 355-363.	1.0	2
2	Nearly 100% Exciton Utilization via Hybridized Interâ€and Intramolecular Triplet Exciton Harvesting Channels in Blue Fluorescent Organic Lightâ€Emitting Diodes. Advanced Optical Materials, 2022, 10, .	3.6	11
3	Excited State Proton Transfer of Quinone Cyanine 9: Implications on the Origin of Superâ€Photoacidity. ChemPhotoChem, 2021, 5, 245-252.	1.5	2
4	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
5	Frontiers in Multiscale Modeling of Photoreceptor Proteins. Photochemistry and Photobiology, 2021, 97, 243-269.	1.3	26
6	Theoretical Study on the Degree of CO₂ Activation in CO₂-Coordinated Ni(0) Complexes. ACS Omega, 2021, 6, 7646-7654.	1.6	7
7	Excited State Proton Transfer of Quinone Cyanine 9: Implications on the Origin of Superâ€Photoacidity. ChemPhotoChem, 2021, 5, 186-186.	1.5	1
8	Cooperation between Excitation Energy Transfer and Antisynchronously Coupled Vibrations. Journal of Physical Chemistry B, 2021, 125, 5601-5610.	1.2	7
9	Three States Involving Vibronic Resonance is a Key to Enhancing Reverse Intersystem Crossing Dynamics of an Organoboron-Based Ultrapure Blue Emitter. Jacs Au, 2021, 1, 987-997.	3.6	48
10	Analytical gradients for core-excited states in the algebraic diagrammatic construction (ADC) framework. Journal of Chemical Physics, 2021, 155, 044106.	1.2	4
11	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
12	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
13	Spinâ€“Vibronic Model for Quantitative Prediction of Reverse Intersystem Crossing Rate in Thermally Activated Delayed Fluorescence Systems. Journal of Chemical Theory and Computation, 2020, 16, 621-632.	2.3	53
14	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
15	Effect of Perturbative Vibronic Correction for Weak Fluorescence in Thermally Activated Delayed Fluorescence Systems. Journal of Physical Chemistry A, 2020, 124, 10384-10392.	1.1	7
16	Enhancement of Energy Transfer Efficiency with Structural Control of Multichromophore Lightâ€Harvesting Assembly. Advanced Science, 2020, 7, 2001623.	5.6	6
17	Protein folding from heterogeneous unfolded state revealed by time-resolved X-ray solution scattering. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 14996-15005.	3.3	33
18	Toward monitoring the dissipative vibrational energy flows in open quantum systems by mixed quantumâ€“classical simulations. Journal of Chemical Physics, 2020, 152, 244109.	1.2	5

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19	Two-oscillator mapping modification of the Poisson bracket mapping equation formulation of the quantumâ€“classical Liouville equation. Journal of Chemical Physics, 2020, 153, 214103.	1.2	7
20	Computational Photochemistry. ChemPhotoChem, 2019, 3, 664-665.	1.5	1
21	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
22	Modeling Charge Flux by Interpolating Atomic Partial Charges. Journal of Chemical Information and Modeling, 2019, 59, 2837-2849.	2.5	2
23	Exploring the Possibility of Excited State Ketoâ€Enolate Transformation of the Oxyluciferinâ€Luciferase Complex with QM/MM Free Energy Simulations. ChemPhotoChem, 2019, 3, 804-813.	1.5	2
24	Effect of Underdamped Vibration on Excitation Energy Transfer: Direct Comparison between Two Different Partitioning Schemes. Journal of Physical Chemistry A, 2019, 123, 1186-1197.	1.1	14
25	Excited state energy fluctuations in the Fennaâ€“Matthewsâ€“Olson complex from molecular dynamics simulations with interpolated chromophore potentials. Physical Chemistry Chemical Physics, 2018, 20, 3310-3319.	1.3	31
26	A proton transfer network that generates deprotonated tyrosine is a key to producing reactive oxygen species in phototoxic KillerRed protein. Physical Chemistry Chemical Physics, 2018, 20, 22342-22350.	1.3	9
27	Chargeâ€“dipole interactions in G-quadruplex thrombin-binding aptamer. Physical Chemistry Chemical Physics, 2018, 20, 21068-21074.	1.3	10
28	Coherent intermolecular proton transfer in the acidâ€“base reaction of excited state pyranine. Physical Chemistry Chemical Physics, 2017, 19, 18243-18251.	1.3	21
29	Interpolation for molecular dynamics simulations: from ions in gas phase to proteins in solution. International Journal of Quantum Chemistry, 2016, 116, 573-577.	1.0	7
30	Electric Field Keeps Chromophore Planar and Produces High Yield Fluorescence in Green Fluorescent Protein. Journal of the American Chemical Society, 2016, 138, 13619-13629.	6.6	72
31	How Does Solvation Affect the Binding of Hydrophilic Amino Saccharides to Cucurbit[7]uril with Exceptional Anomeric Selectivity?. Chemistry - A European Journal, 2016, 22, 15791-15799.	1.7	8
32	Constructing an Interpolated Potential Energy Surface of a Large Molecule: A Case Study with Bacteriochlorophyll a Model in the Fennaâ€“Matthewsâ€“Olson Complex. Journal of Chemical Theory and Computation, 2016, 12, 5235-5246.	2.3	23
33	Emission shaping in fluorescent proteins: role of electrostatics and Ï€-stacking. Physical Chemistry Chemical Physics, 2016, 18, 3944-3955.	1.3	24
34	Quantum Chemistry Based Arguments about Singlet Oxygen Formation Trends from Fluorescent Proteins. Rapid Communication in Photoscience, 2016, 5, 18-20.	0.1	0
35	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
36	Highly Sensitive and Selective Biosensors Based on Organic Transistors Functionalized with Cucurbit[6]uril Derivatives. Advanced Functional Materials, 2015, 25, 4882-4888.	7.8	66

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37	A structural remedy toward bright dipolar fluorophores in aqueous media. Chemical Science, 2015, 6, 4335-4342.	3.7	144
38	On Surface Hopping and Time-Reversal. Journal of Physical Chemistry A, 2015, 119, 990-995.	1.1	7
39	Effect of Chromophore Potential Model on the Description of Excitonâ€“Phonon Interactions. Journal of Physical Chemistry Letters, 2015, 6, 2875-2880.	2.1	27
40	N-Heterocyclic Carbene Nitric Oxide Radicals. Journal of the American Chemical Society, 2015, 137, 4642-4645.	6.6	40
41	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
42	Towards the Realization of Ab Initio Dynamics at the Speed of Molecular Mechanics: Simulations with Interpolated Diabatic Hamiltonian. ChemPhysChem, 2014, 15, 3183-3193.	1.0	12
43	Improving long time behavior of Poisson bracket mapping equation: A mapping variable scaling approach. Journal of Chemical Physics, 2014, 141, 124107.	1.2	14
44	Constructing polyatomic potential energy surfaces by interpolating diabatic Hamiltonian matrices with demonstration on green fluorescent protein chromophore. Journal of Chemical Physics, 2014, 140, 164112.	1.2	10
45	Improving long time behavior of Poisson bracket mapping equation: A non-Hamiltonian approach. Journal of Chemical Physics, 2014, 140, 184106.	1.2	38
46	Interpolation of Potential Energy Surfaces for Nonadiabatic Simulations of Biological Systems. Biophysical Journal, 2014, 106, 806a.	0.2	0
47	Mixed Quantum-Classical Study of the Nonadiabatic Dynamics in Photosynthetic Systems. Biophysical Journal, 2014, 106, 806a.	0.2	0
48	Diabatic Population Matrix Formalism for Performing Molecular Mechanics Style Simulations with Multiple Electronic States. Journal of Chemical Theory and Computation, 2014, 10, 5238-5253.	2.3	9
49	Ground-State Elevation Approach To Suppress Side Reactions in Gold-Sensing Systems Based on Alkyne Activation. Organic Letters, 2014, 16, 1374-1377.	2.4	47
50	Simple Method for Hybrid All-Atom and Coarse-Grained Molecular Dynamics Simulations and Its Applications. Biophysical Journal, 2014, 106, 413a.	0.2	0
51	Poly-cyclodextrin and poly-paclitaxel nano-assembly for anticancer therapy. Nature Communications, 2014, 5, 3702.	5.8	184
52	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
53	DNSC: a fluorescent, environmentally sensitive cytidine derivative for the direct detection of GGG triad sequences. Organic and Biomolecular Chemistry, 2013, 11, 5605.	1.5	14
54	Simple Method for Simulating the Mixture of Atomistic and Coarse-Grained Molecular Systems. Journal of Chemical Theory and Computation, 2013, 9, 3728-3739.	2.3	30

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55	Fluorescent peptide indicator displacement assay for monitoring interactions between RNA and RNA binding proteins. Molecular BioSystems, 2013, 9, 948-951.	2.9	5
56	On the pH Dependent Behavior of the Firefly Bioluminescence: Protein Dynamics and Water Content in the Active Pocket. Journal of Physical Chemistry B, 2013, 117, 7260-7269.	1.2	10
57	Can Adenosine Triarsenate Role as an Energy Carrier?. Bulletin of the Korean Chemical Society, 2013, 34, 361-362.	1.0	1
58	Phase Behavior and Conductivity of Sulfonated Block Copolymers Containing Heterocyclic Diazole-Based Ionic Liquids. Macromolecules, 2012, 45, 8702-8713.	2.2	46
59	Interpolated Mechanicsâ€“Molecular Mechanics Study of Internal Rotation Dynamics of the Chromophore Unit in Blue Fluorescent Protein and Its Variants. Journal of Physical Chemistry B, 2012, 116, 11137-11147.	1.2	16
60	Moleculeâ€specific determination of atomic polarizabilities with the polarizable atomic multipole model. Journal of Computational Chemistry, 2012, 33, 1662-1672.	1.5	5
61	All-Atom Semiclassical Dynamics Study of Quantum Coherence in Photosynthetic Fennaâ€“Matthewsâ€“Olson Complex. Journal of the American Chemical Society, 2012, 134, 11640-11651.	6.6	61
62	Studying Interfacial Reactions of Cholesterol Sulfate in an Unsaturated Phosphatidylglycerol Layer with Ozone Using Field Induced Droplet Ionization Mass Spectrometry. Journal of the American Society for Mass Spectrometry, 2012, 23, 141-152.	1.2	17
63	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
64	Mixed Quantum-Classical Description of Excitation Energy Transfer in a Model Fennaâˆ’Matthewsâˆ’Olsen Complex. Journal of Physical Chemistry Letters, 2011, 2, 808-812.	2.1	56
65	Dynamics on the Electronically Excited State Surface of the Bioluminescent Firefly Luciferaseâ€“Oxyluciferin System. Journal of the American Chemical Society, 2011, 133, 12040-12049.	6.6	53
66	Development of force field parameters for oxyluciferin on its electronic ground and excited states. International Journal of Quantum Chemistry, 2011, 111, 4091-4105.	1.0	28
67	Characterization of Vinylgold Intermediates: Goldâ€Mediated Cyclization of Acetylenic Amides. Angewandte Chemie - International Edition, 2011, 50, 11446-11450.	7.2	92
68	On the Mechanism of Irreversible Carbon Dioxide Binding with a Frustrated Lewis Pair: Solventâ€Assisted Frustration and Transitionâ€State Entropic Encouragement. Chemistry - A European Journal, 2011, 17, 6501-6507.	1.7	24
69	Density functional calculations of electronic structure and magnetic properties of the hydrocarbon<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">K</mml:mi><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>picene superconductor near the metal-insulator transition. Physical Review B, 2011, 83, .	1.1	56
70	Condensed phase molecular dynamics using interpolated potential energy surfaces with application to the resolvation process of coumarin 153. Journal of Chemical Physics, 2011, 135, 014107.	1.2	26
71	C₃-Symmetric Cage-like Receptors: Chiral Discrimination of Î±-Chiral Amines in a Confined Space. Organic Letters, 2010, 12, 4228-4231.	2.4	22
72	Dispersionâ€Oriented Soft Interaction in a Frustrated Lewis Pair and the Entropic Encouragement Effect in its Formation. Chemistry - A European Journal, 2009, 15, 13348-13355.	1.7	45

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73	Quartic-Scaling Analytical Gradient of Quasidegenerate Scaled Opposite Spin Second-Order Perturbation Corrections to Single Excitation Configuration Interaction. Journal of Chemical Theory and Computation, 2009, 5, 1224-1236.	2.3	23
74	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. Journal of Physical Chemistry A, 2009, 113, 10564-10576.	1.1	22
75	A Delicate Electronic Balance between Metal and Ligand in [Cuâ^'Pâ^'Cuâ^'P] Diamondoids:Â Oxidation State Dependent Plasticity and the Formation of a Singlet Diradicaloid. Journal of the American Chemical Society, 2008, 130, 3878-3887.	6.6	21
76	Solvent Viscosity Dependence of the Protein Folding Dynamics. Journal of Physical Chemistry B, 2008, 112, 6221-6227.	1.2	29
77	Quasidegenerate scaled opposite spin second order perturbation corrections to single excitation configuration interaction. Journal of Chemical Physics, 2008, 128, 164106.	1.2	43
78	Charged polycyclic aromatic hydrocarbon clusters and the galactic extended red emission. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 5274-5278.	3.3	109
79	Scaled Second-Order Perturbation Corrections to Configuration Interaction Singles:â€‰ Efficient and Reliable Excitation Energy Methods. Journal of Physical Chemistry A, 2007, 111, 5314-5326.	1.1	185
80	An improved algorithm for analytical gradient evaluation in resolution-of-the-identity second-order MÃ¸ller-Plesset perturbation theory: Application to alanine tetrapeptide conformational analysis. Journal of Computational Chemistry, 2007, 28, 839-856.	1.5	134
81	Kinetic Definition of Protein Folding Transition State Ensembles and Reaction Coordinates. Biophysical Journal, 2006, 91, 14-24.	0.2	33
82	The Solvation Interface is a Determining Factor in Peptide Conformational Preferences. Journal of Molecular Biology, 2006, 356, 248-256.	2.0	44
83	Analytical gradient of restricted second-order MÃ¸llerâ€“Plesset correlation energy with the resolution of the identity approximation, applied to the TCNE dimer anion complex. Chemical Physics Letters, 2006, 426, 197-203.	1.2	27
84	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	1.3	2,597
85	On the role of chemical detail in simulating protein folding kinetics. Chemical Physics, 2006, 323, 66-77.	0.9	21
86	How Well Can Simulation Predict Protein Folding Kinetics and Thermodynamics?. Annual Review of Biophysics and Biomolecular Structure, 2005, 34, 43-69.	18.3	225
87	One-Dimensional Reaction Coordinate and the Corresponding Potential of Mean Force from Commitment Probability Distributionâ€. Journal of Physical Chemistry B, 2005, 109, 6780-6786.	1.2	70
88	Dimerization of the p53 Oligomerization Domain: Identification of a Folding Nucleus by Molecular Dynamics Simulations. Journal of Molecular Biology, 2005, 345, 869-878.	2.0	36
89	Does Water Play a Structural Role in the Folding of Small Nucleic Acids?. Biophysical Journal, 2005, 88, 2516-2524.	0.2	95
90	Simulations of the role of water in the protein-folding mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 6456-6461.	3.3	187

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91	Does Native State Topology Determine the RNA Folding Mechanism?. Journal of Molecular Biology, 2004, 337, 789-797.	2.0	44
92	Atomistic protein folding simulations on the submillisecond time scale using worldwide distributed computing. Biopolymers, 2003, 68, 91-109.	1.2	346
93	Insights into Nucleic Acid Conformational Dynamics from Massively Parallel Stochastic Simulations. Biophysical Journal, 2003, 85, 790-803.	0.2	95
94	Multiplexed-Replica Exchange Molecular Dynamics Method for Protein Folding Simulation. Biophysical Journal, 2003, 84, 775-786.	0.2	268
95	Construction of an accurate potential energy surface by interpolation with Cartesian weighting coordinates. Journal of Chemical Physics, 2000, 113, 6021-6024.	1.2	29
96	Dynamic isotope effect on the product energy partitioning in CH2OH+â†'CHO++H2. Journal of Chemical Physics, 1998, 109, 5363-5371.	1.2	11
97	Mode-specific energy analysis for rotating-vibrating triatomic molecules in classical trajectory simulation. Journal of Chemical Physics, 1997, 107, 1394-1402.	1.2	29
98	Potential energy surfaces for polyatomic reactions by interpolation with reaction path weight: CH2OH+â†'CHO++H2 reaction. Journal of Chemical Physics, 1997, 106, 1003-1012.	1.2	43
99	Energy partitioning during the exit channel motion for CH2OH+â†'CHO++H2. Chemical Physics Letters, 1997, 264, 303-308.	1.2	8