Jae Woo Park

List of Publications by Year
in descending order

30 papers	971 citations	471477 17 h-index	477281 29 g-index
31 all docs	31 docs citations	31 times ranked	1208 citing authors

#	Article	IF	Citations
1	A structural remedy toward bright dipolar fluorophores in aqueous media. Chemical Science, 2015, 6, 4335-4342.	7.4	144
2	Analytical Derivative Coupling for Multistate CASPT2 Theory. Journal of Chemical Theory and Computation, 2017, 13, 2561-2570.	5.3	109
3	On-the-Fly CASPT2 Surface-Hopping Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 3676-3683.	5.3	100
4	Multireference Electron Correlation Methods: Journeys along Potential Energy Surfaces. Chemical Reviews, 2020, 120, 5878-5909.	47.7	86
5	Electric Field Keeps Chromophore Planar and Produces High Yield Fluorescence in Green Fluorescent Protein. Journal of the American Chemical Society, 2016, 138, 13619-13629.	13.7	72
6	All-Atom Semiclassical Dynamics Study of Quantum Coherence in Photosynthetic Fennaâ€“Matthewsâ€“Olson Complex. Journal of the American Chemical Society, 2012, 134, 11640-11651.	13.7	61
7	Experimental and theoretical determination of the accurate CH/Ï€ interaction energies in benzeneâ€“alkane clusters: correlation between interaction energy and polarizability. Physical Chemistry Chemical Physics, 2011, 13, 14131.	2.8	52
8	Molecular-Shape-Dependent Luminescent Behavior of Dye Aggregates: Bent versus Linear Benzocoumarins. Crystal Growth and Design, 2014, 14, 6613-6619.	3.0	39
9	Imaginary Shift in CASPT2 Nuclear Gradient and Derivative Coupling Theory. Journal of Chemical Theory and Computation, 2019, 15, 4088-4098.	5.3	30
10	Effect of Chromophore Potential Model on the Description of Excitonâ€“Phonon Interactions. Journal of Physical Chemistry Letters, 2015, 6, 2875-2880.	4.6	27
11	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.	3.0	26
12	Emission shaping in fluorescent proteins: role of electrostatics and Ï€-stacking. Physical Chemistry Chemical Physics, 2016, 18, 3944-3955.	2.8	24
13	Coherent intermolecular proton transfer in the acidâ€“base reaction of excited state pyranine. Physical Chemistry Chemical Physics, 2017, 19, 18243-18251.	2.8	21
14	Single-State Single-Reference and Multistate Multireference Zeroth-Order Hamiltonians in MS-CASPT2 and Conical Intersections. Journal of Chemical Theory and Computation, 2019, 15, 3960-3973.	5.3	21
15	Analytical Gradient Theory for Quasidegenerate N-Electron Valence State Perturbation Theory (QD-NEVPT2). Journal of Chemical Theory and Computation, 2020, 16, 326-339.	5.3	19
16	On the accuracy of retinal protonated Schiff base models. Molecular Physics, 2018, 116, 2583-2590.	1.7	18
17	Analytical Gradient Theory for Strongly Contracted (SC) and Partially Contracted (PC) N-Electron Valence State Perturbation Theory (NEVPT2). Journal of Chemical Theory and Computation, 2019, 15, 5417-5425.	5.3	18
18	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.	2.6	16

#	Article	IF	Citations
19	Second-Order Orbital Optimization with Large Active Spaces Using Adaptive Sampling Configuration Interaction (ASCI) and Its Application to Molecular Geometry Optimization. Journal of Chemical Theory and Computation, 2021, 17, 1522-1534.	5.3	15
20	Towards the Realization of Ab Initio Dynamics at the Speed of Molecular Mechanics: Simulations with Interpolated Diabatic Hamiltonian. ChemPhysChem, 2014, 15, 3183-3193.	2.1	12
21	Analytical First-Order Derivatives of Second-Order Extended Multiconfiguration Quasi-Degenerate Perturbation Theory (XMCQDPT2): Implementation and Application. Journal of Chemical Theory and Computation, 2020, 16, 5562-5571.	5.3	11
22	Constructing polyatomic potential energy surfaces by interpolating diabatic Hamiltonian matrices with demonstration on green fluorescent protein chromophore. Journal of Chemical Physics, 2014, 140, 164112.	3.0	10
23	Diabatic Population Matrix Formalism for Performing Molecular Mechanics Style Simulations with Multiple Electronic States. Journal of Chemical Theory and Computation, 2014, 10, 5238-5253.	5.3	9
24	Near-Exact CASSCF-Level Geometry Optimization with a Large Active Space using Adaptive Sampling Configuration Interaction Self-Consistent Field Corrected with Second-Order Perturbation Theory (ASCI-SCF-PT2). Journal of Chemical Theory and Computation, 2021, 17, 4092-4104.	5.3	9
25	Interpolation for molecular dynamics simulations: from ions in gas phase to proteins in solution. International Journal of Quantum Chemistry, 2016, 116, 573-577.	2.0	7
26	Analytical Gradient Theory for Resolvent-Fitted Second-Order Extended Multiconfiguration Perturbation Theory (XMCQDPT2). Journal of Chemical Theory and Computation, 2021, 17, 6122-6133.	5.3	7
27	Analytical Gradient Theory for Spin-Free State-Averaged Second-Order Driven Similarity Renormalization Group Perturbation Theory (SA-DSRG-MRPT2) and Its Applications for Conical Intersection Optimizations. Journal of Chemical Theory and Computation, 2022, 18, 2233-2245.	5.3	5
28	Nonheme Iron Imido Complexes Bearing a Nonâ€Innocent Ligand: A Synthetic Chameleon Species in Oxidation Reactions. Chemistry - A European Journal, 2021, 27, 17495-17503.	3.3	2
29	Can Adenosine Triarsenate Role as an Energy Carrier?. Bulletin of the Korean Chemical Society, 2013, 34, 361-362.	1.9	1
30	Quantum Chemistry Based Arguments about Singlet Oxygen Formation Trends from Fluorescent Proteins. Rapid Communication in Photoscience, 2016, 5, 18-20.	0.1	0