

Jae Woo Park

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

29
papers

700
citations

14
h-index

26
g-index

31
ext. papers

848
ext. citations

7.8
avg, IF

5.02
L-index

#	Paper	IF	Citations
29	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). <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 4092-4104	6.4	0
28	Second-Order Orbital Optimization with Large Active Spaces Using Adaptive Sampling Configuration Interaction (ASCI) and Its Application to Molecular Geometry Optimization. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 1522-1534	6.4	7
27	Nonheme Iron Imido Complexes Bearing a Non-Innocent Ligand: A Synthetic Chameleon Species in Oxidation Reactions. <i>Chemistry - A European Journal</i> , 2021 , 27, 17495-17503	4.8	1
26	Analytical Gradient Theory for Resolvent-Fitted Second-Order Extended Multiconfiguration Perturbation Theory (XMCQDPT2). <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 6122-6133	6.4	0
25	Multireference Electron Correlation Methods: Journeys along Potential Energy Surfaces. <i>Chemical Reviews</i> , 2020 , 120, 5878-5909	68.1	44
24	Analytical Gradient Theory for Quasidegenerate -Electron Valence State Perturbation Theory (QD-NEVPT2). <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 326-339	6.4	12
23	Analytical First-Order Derivatives of Second-Order Extended Multiconfiguration Quasi-Degenerate Perturbation Theory (XMCQDPT2): Implementation and Application. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 5562-5571	6.4	3
22	Analytical Gradient Theory for Strongly Contracted (SC) and Partially Contracted (PC) -Electron Valence State Perturbation Theory (NEVPT2). <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 5417-5425	6.4	13
21	Imaginary Shift in CASPT2 Nuclear Gradient and Derivative Coupling Theory. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 4088-4098	6.4	17
20	Single-State Single-Reference and Multistate Multireference Zeroth-Order Hamiltonians in MS-CASPT2 and Conical Intersections. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 3960-3973	6.4	10
19	On the accuracy of retinal protonated Schiff base models. <i>Molecular Physics</i> , 2018 , 116, 2583-2590	1.7	13
18	Analytical Derivative Coupling for Multistate CASPT2 Theory. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 2561-2570	6.4	71
17	Coherent intermolecular proton transfer in the acid-base reaction of excited state pyranine. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 18243-18251	3.6	16
16	On-the-Fly CASPT2 Surface-Hopping Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 3676-3683	6.4	76
15	Emission shaping in fluorescent proteins: role of electrostatics and π -stacking. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 3944-55	3.6	19
14	Quantum Chemistry Based Arguments about Singlet Oxygen Formation Trends from Fluorescent Proteins. <i>Rapid Communication in Photoscience</i> , 2016 , 5, 18-20		
13	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	2.1	6

12	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	16.4	51
11	Effect of Chromophore Potential Model on the Description of Exciton-Phonon Interactions. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 2875-80	6.4	26
10	A structural remedy toward bright dipolar fluorophores in aqueous media. <i>Chemical Science</i> , 2015 , 6, 4335-4342	9.4	109
9	Diabatic Population Matrix Formalism for Performing Molecular Mechanics Style Simulations with Multiple Electronic States. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 5238-53	6.4	8
8	Towards the realization of ab initio dynamics at the speed of molecular mechanics: simulations with interpolated diabatic Hamiltonian. <i>ChemPhysChem</i> , 2014 , 15, 3183-93	3.2	10
7	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	3.9	10
6	Molecular-Shape-Dependent Luminescent Behavior of Dye Aggregates: Bent versus Linear Benzocoumarins. <i>Crystal Growth and Design</i> , 2014 , 14, 6613-6619	3.5	32
5	Can Adenosine Triarsenate Role as an Energy Carrier?. <i>Bulletin of the Korean Chemical Society</i> , 2013 , 34, 361-362	1.2	1
4	Interpolated mechanics-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, 11137-47	3.4	15
3	All-atom semiclassical dynamics study of quantum coherence in photosynthetic Fenna-Matthews-Olson complex. <i>Journal of the American Chemical Society</i> , 2012 , 134, 11640-51	16.4	58
2	Experimental and theoretical determination of the accurate CH/π interaction energies in benzene-alkane clusters: correlation between interaction energy and polarizability. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 14131-41	3.6	46
1	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	3.9	26