Joshua J Goings

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3744419/publications.pdf

Version: 2024-02-01

33	1,100	361413	395702
papers	citations	20 h-index	33 g-index

38	38	38	957
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Exploring Potential Energy Surfaces Using Reinforcement Machine Learning. Journal of Chemical Information and Modeling, 2022, 62, 3169-3179.	5.4	6
2	Reinforcement Learning Configuration Interaction. Journal of Chemical Theory and Computation, 2021, 17, 5482-5491.	5.3	9
3	Determination of the SmO+ bond energy by threshold photodissociation of the cryogenically cooled ion. Journal of Chemical Physics, 2021, 155, 174303.	3.0	15
4	The Chronus Quantum software package. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1436.	14.6	66
5	Formation of an unusual glutamine tautomer in a blue light using flavin photocycle characterizes the light-adapted state. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 26626-26632.	7.1	34
6	Nonequilibrium Dynamics of Proton-Coupled Electron Transfer in Proton Wires: Concerted but Asynchronous Mechanisms. ACS Central Science, 2020, 6, 1594-1601.	11.3	20
7	Role of Intact Hydrogen-Bond Networks in Multiproton-Coupled Electron Transfer. Journal of the American Chemical Society, 2020, 142, 21842-21851.	13.7	23
8	Proton-coupled electron transfer across benzimidazole bridges in bioinspired proton wires. Chemical Science, 2020, 11, 3820-3828.	7.4	23
9	Proton-Coupled Electron Transfer Drives Long-Range Proton Translocation in Bioinspired Systems. Journal of the American Chemical Society, 2019, 141, 14057-14061.	13.7	33
10	Early Photocycle of Slr1694 Blue-Light Using Flavin Photoreceptor Unraveled through Adiabatic Excited-State Quantum Mechanical/Molecular Mechanical Dynamics. Journal of the American Chemical Society, 2019, 141, 20470-20479.	13.7	33
11	Electron-Coupled Double Proton Transfer in the Slr1694 BLUF Photoreceptor: A Multireference Electronic Structure Study. Journal of Physical Chemistry B, 2019, 123, 439-447.	2.6	23
12	Orientation-dependent imaging of electronically excited quantum dots. Journal of Chemical Physics, 2018, 148, 064701.	3.0	13
13	Current development of noncollinear electronic structure theory. International Journal of Quantum Chemistry, 2018, 118, e25398.	2.0	22
14	Realâ€time timeâ€dependent electronic structure theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1341.	14.6	122
15	Propensity for Proton Relay and Electrostatic Impact of Protein Reorganization in Slr1694 BLUF Photoreceptor. Journal of the American Chemical Society, 2018, 140, 15241-15251.	13.7	25
16	Controlling Proton-Coupled Electron Transfer in Bioinspired Artificial Photosynthetic Relays. Journal of the American Chemical Society, 2018, 140, 15450-15460.	13.7	52
17	Two-Component Noncollinear Time-Dependent Spin Density Functional Theory for Excited State Calculations. Journal of Chemical Theory and Computation, 2017, 13, 2591-2603.	5.3	66
18	Real time propagation of the exact two component time-dependent density functional theory. Journal of Chemical Physics, 2016, 145, 104107.	3.0	71

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19	Can Quantized Vibrational Effects Be Obtained from Ehrenfest Mixed Quantum-Classical Dynamics?. Journal of Physical Chemistry Letters, 2016, 7, 5193-5197.	4.6	6
20	An atomic orbital based real-time time-dependent density functional theory for computing electronic circular dichroism band spectra. Journal of Chemical Physics, 2016, 144, 234102.	3.0	41
21	Quantum confinement effects on optical transitions in nanodiamonds containing nitrogen vacancies. Physical Review B, 2016, 94, .	3.2	36
22	Direct Atomic-Orbital-Based Relativistic Two-Component Linear Response Method for Calculating Excited-State Fine Structures. Journal of Chemical Theory and Computation, 2016, 12, 3711-3718.	5.3	51
23	Accelerating Real-Time Time-Dependent Density Functional Theory with a Nonrecursive Chebyshev Expansion of the Quantum Propagator. Journal of Chemical Theory and Computation, 2016, 12, 5333-5338.	5.3	18
24	Viewpoints on the 2016 Theory and Applications of Computational Chemistry Conference. Journal of Physical Chemistry A, 2016, 120, 8485-8487.	2.5	1
25	Approximate singly excited states from a two-component Hartree-Fock reference. Journal of Chemical Physics, 2015, 143, 144106.	3.0	10
26	Ab initio two-component Ehrenfest dynamics. Journal of Chemical Physics, 2015, 143, 114105.	3.0	31
27	Imaging Excited Orbitals of Quantum Dots: Experiment and Electronic Structure Theory. Journal of the American Chemical Society, 2015, 137, 14743-14750.	13.7	18
28	Stability of the complex generalized Hartree-Fock equations. Journal of Chemical Physics, 2015, 142, 154109.	3.0	29
29	Energy-Specific Equation-of-Motion Coupled-Cluster Methods for High-Energy Excited States: Application to K-edge X-ray Absorption Spectroscopy. Journal of Chemical Theory and Computation, 2015, 11, 4146-4153.	5.3	92
30	Assessment of low-scaling approximations to the equation of motion coupled-cluster singles and doubles equations. Journal of Chemical Physics, 2014, 141, 164116.	3.0	45
31	Ab initio non-relativistic spin dynamics. Journal of Chemical Physics, 2014, 141, 214111.	3.0	20
32	Theoretical Characterization of Conduction-Band Electrons in Photodoped and Aluminum-Doped Zinc Oxide (AZO) Quantum Dots. Journal of Physical Chemistry C, 2014, 118, 26584-26590.	3.1	31
33	Sorption of H2to Open Metal Sites in a Metalâ€“Organic Framework: A Symmetry-Adapted Perturbation Theory Analysis. Journal of Physical Chemistry A, 2014, 118, 7411-7417.	2.5	13