

Seunghoon Lee

List of Publications by Citations

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25
papers

283
citations

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h-index

16
g-index

27
ext. papers

414
ext. citations

4.5
avg, IF

4.01
L-index

#	Paper	IF	Citations
25	The Ground State Electronic Energy of Benzene. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 8922-8924	6.4	52
24	Eliminating spin-contamination of spin-flip time dependent density functional theory within linear response formalism by the use of zeroth-order mixed-reference (MR) reduced density matrix. <i>Journal of Chemical Physics</i> , 2018 , 149, 104101	3.9	39
23	Design of singlet fission chromophores with cyclic (alkyl)(amino) carbene building blocks. <i>Journal of Chemical Physics</i> , 2019 , 150, 234306	3.9	24
22	Efficient implementations of analytic energy gradient for mixed-reference spin-flip time-dependent density functional theory (MRSF-TDDFT). <i>Journal of Chemical Physics</i> , 2019 , 150, 184111	3.9	21
21	Conical Intersections in Organic Molecules: Benchmarking Mixed-Reference Spin-Flip Time-Dependent DFT (MRSF-TD-DFT) vs Spin-Flip TD-DFT. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 6455-6462	2.8	20
20	Performance Analysis and Optimization of Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT) for Vertical Excitation Energies and Singlet-Triplet Energy Gaps. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 7991-8000	2.8	17
19	Fast Overlap Evaluations for Nonadiabatic Molecular Dynamics Simulations: Applications to SF-TDDFT and TDDFT. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 882-891	6.4	13
18	Shedding new light on an old molecule: quinophthalone displays uncommon N-to-O excited state intramolecular proton transfer (ESIPT) between photobases. <i>Scientific Reports</i> , 2017 , 7, 3863	4.9	10
17	Diboron- and Diaza-Doped Anthracenes and Phenanthrenes: Their Electronic Structures for Being Singlet Fission Chromophores. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 8159-8172	2.8	10
16	Impact of the Dynamic Electron Correlation on the Unusually Long Excited-State Lifetime of Thymine. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 4339-4346	6.4	9
15	Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT) as a Simple yet Accurate Method for Diradicals and Diradicaloids. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 848-859	6.4	8
14	Computation of Molecular Ionization Energies Using an Ensemble Density Functional Theory Method. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 4489-4504	6.4	7
13	Computation of Molecular Electron Affinities Using an Ensemble Density Functional Theory Method. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 7795-7804	2.8	7
12	Externally Corrected CCSD with Renormalized Perturbative Triples (R-ecCCSD(T)) and the Density Matrix Renormalization Group and Selected Configuration Interaction External Sources. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 3414-3425	6.4	7
11	Optimization of Three State Conical Intersections by Adaptive Penalty Function Algorithm in Connection with the Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory Method (MRSF-TDDFT). <i>Journal of Physical Chemistry A</i> , 2021 , 125, 1994-2006	2.8	6
10	Fast and Accurate Computation of Nonadiabatic Coupling Matrix Elements Using the Truncated Leibniz Formula and Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 4722-4728	6.4	6
9	How Beneficial Is the Account of Doubly-Excited Configurations in Linear Response Theory?. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 975-984	6.4	6

8	Internal Conversion between Bright (1) and Dark (2) States in s-Butadiene and s-Hexatriene. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 9720-9729	6.4	4
7	New Method for Constant- NPT Molecular Dynamics. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 1689-1698	6.2	3
6	Structural or population dynamics: what is revealed by the time-resolved photoelectron spectroscopy of 1,3-cyclohexadiene? A study with an ensemble density functional theory method. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 17567-17573	3.6	3
5	FOLD: a method to optimize power in meta-analysis of genetic association studies with overlapping subjects. <i>Bioinformatics</i> , 2017 , 33, 3947-3954	7.2	2
4	Exploring Dyson Orbitals and Their Electron Binding Energies for Conceptualizing Excited States from Response Methodology. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 9963-9972	6.4	2
3	Description of Sudden Polarization in the Excited Electronic States with an Ensemble Density Functional Theory Method. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 5123-5139	6.4	2
2	Signatures of Conical Intersection Dynamics in the Time-Resolved Photoelectron Spectrum of Furan: Theoretical Modeling with an Ensemble Density Functional Theory Method. <i>International Journal of Molecular Sciences</i> , 2021 , 22,	6.3	1
1	Resummation of the Brillouin-Wigner Perturbation Series. <i>Bulletin of the Korean Chemical Society</i> , 2018 , 39, 347-355	1.2	