Seunghoon Lee

List of Publications by Year in Descending Order

25 papers	283 citations	9 h-index	16 g-index
27 ext. papers	414 ext. citations	4.5 avg, IF	4.01 L-index

#	Paper	IF	Citations
25	Exploring Dyson Orbitals and Their Electron Binding Energies for Conceptualizing Excited States from Response Methodology. *Journal of Physical Chemistry Letters*, **2021**, 12, 9963-9972	6.4	2
24	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). *Journal of Physical Chemistry A*, **2021**, 125, 1994-2006	2.8	6
23	Signatures of Conical Intersection Dynamics in the Time-Resolved Photoelectron Spectrum of Furan: Theoretical Modeling with an Ensemble Density Functional Theory Method. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	1
22	Impact of the Dynamic Electron Correlation on the Unusually Long Excited-State Lifetime of Thymine. *Journal of Physical Chemistry Letters*, **2021**, 12, 4339-4346	6.4	9
21	Fast and Accurate Computation of Nonadiabatic Coupling Matrix Elements Using the Truncated Leibniz Formula and Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory. *Journal of Physical Chemistry Letters*, **2021**, 12, 4722-4728	6.4	6
20	Externally Corrected CCSD with Renormalized Perturbative Triples (R-ecCCSD(T)) and the Density Matrix Renormalization Group and Selected Configuration Interaction External Sources. *Journal of Chemical Theory and Computation*, **2021**, 17, 3414-3425	6.4	7
19	Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT) as a Simple yet Accurate Method for Diradicals and Diradicaloids. *Journal of Chemical Theory and Computation*, **2021**, 17, 848-859	6.4	8
18	Description of Sudden Polarization in the Excited Electronic States with an Ensemble Density Functional Theory Method. *Journal of Chemical Theory and Computation*, **2021**, 17, 5123-5139	6.4	2
17	Internal Conversion between Bright (1) and Dark (2) States in s--Butadiene and s--Hexatriene. *Journal of Physical Chemistry Letters*, **2021**, 12, 9720-9729	6.4	4
16	How Beneficial Is the Account of Doubly-Excited Configurations in Linear Response Theory?. *Journal of Chemical Theory and Computation*, **2021**, 17, 975-984	6.4	6
15	Computation of Molecular Ionization Energies Using an Ensemble Density Functional Theory Method. *Journal of Chemical Theory and Computation*, **2020**, 16, 4489-4504	6.4	7
14	The Ground State Electronic Energy of Benzene. *Journal of Physical Chemistry Letters*, **2020**, 11, 8922-8929	6.4	52
13	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. *Physical Chemistry Chemical Physics*, **2020**, 22, 17567-17573	3.6	3
12	Diboron- and Diaza-Doped Anthracenes and Phenanthrenes: Their Electronic Structures for Being Singlet Fission Chromophores. *Journal of Physical Chemistry A*, **2020**, 124, 8159-8172	2.8	10
11	Computation of Molecular Electron Affinities Using an Ensemble Density Functional Theory Method. *Journal of Physical Chemistry A*, **2020**, 124, 7795-7804	2.8	7
10	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. *Journal of Physical Chemistry A*, **2019**, 123, 7991-8000	2.8	17
9	Efficient implementations of analytic energy gradient for mixed-reference spin-flip time-dependent density functional theory (MRSF-TDDFT). *Journal of Chemical Physics*, **2019**, 150, 184111	3.9	21

8	Design of singlet fission chromophores with cyclic (alkyl)(amino) carbene building blocks. *Journal of Chemical Physics*, **2019**, 150, 234306	3.9	24
7	New Method for Constant- NPT Molecular Dynamics. *Journal of Physical Chemistry A*, **2019**, 123, 1689-1698	2.8	3
6	Conical Intersections in Organic Molecules: Benchmarking Mixed-Reference Spin-Flip Time-Dependent DFT (MRSF-TD-DFT) vs Spin-Flip TD-DFT. *Journal of Physical Chemistry A*, **2019**, 123, 6455-6462	2.8	20
5	Fast Overlap Evaluations for Nonadiabatic Molecular Dynamics Simulations: Applications to SF-TDDFT and TDDFT. *Journal of Chemical Theory and Computation*, **2019**, 15, 882-891	6.4	13
4	Resummation of the Brillouin-Wigner Perturbation Series. *Bulletin of the Korean Chemical Society*, **2018**, 39, 347-355	1.2	
3	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. *Journal of Chemical Physics*, **2018**, 149, 104101	3.9	39
2	Shedding new light on an old molecule: quinophthalone displays uncommon N-to-O excited state intramolecular proton transfer (ESIPT) between photobases. *Scientific Reports*, **2017**, 7, 3863	4.9	10
1	FOLD: a method to optimize power in meta-analysis of genetic association studies with overlapping subjects. *Bioinformatics*, **2017**, 33, 3947-3954	7.2	2