

# Joonho Lee

## List of Publications by Citations

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41  
papers

1,034  
citations

16  
h-index

31  
g-index

44  
ext. papers

1,569  
ext. citations

5.7  
avg, IF

5.23  
L-index

#	Paper	IF	Citations
41	A deterministic alternative to the full configuration interaction quantum Monte Carlo method. <i>Journal of Chemical Physics</i> , <b>2016</b> , 145, 044112	3.9	161
40	Generalized Unitary Coupled Cluster Wave functions for Quantum Computation. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 311-324	6.4	118
39	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , <b>2021</b> , 155, 084801	3.9	115
38	Embedded mean-field theory. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 568-80	6.4	77
37	Regularized Orbital-Optimized Second-Order Møller-Plesset Perturbation Theory: A Reliable Fifth-Order-Scaling Electron Correlation Model with Orbital Energy Dependent Regularizers. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 5203-5219	6.4	56
36	Coupled-Cluster Valence-Bond Singles and Doubles for Strongly Correlated Systems: Block-Tensor Based Implementation and Application to Oligoacenes. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 602-615	6.4	46
35	QMCPACK: Advances in the development, efficiency, and application of auxiliary field and real-space variational and diffusion quantum Monte Carlo. <i>Journal of Chemical Physics</i> , <b>2020</b> , 152, 174103	3.9	44
34	A non-orthogonal variational quantum eigensolver. <i>New Journal of Physics</i> , <b>2020</b> , 22, 073009	2.9	34
33	Distinguishing artificial and essential symmetry breaking in a single determinant: approach and application to the C <sub>60</sub> , C <sub>70</sub> , and C <sub>84</sub> fullerenes. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 4763-4778	3.6	31
32	Two single-reference approaches to singlet biradicaloid problems: Complex, restricted orbitals and approximate spin-projection combined with regularized orbital-optimized Møller-Plesset perturbation theory. <i>Journal of Chemical Physics</i> , <b>2019</b> , 150, 244106	3.9	30
31	Halogen- $\pi$ Interactions between Benzene and X/CX (X = Cl, Br): Assessment of Various Density Functionals with Respect to CCSD(T). <i>Journal of Physical Chemistry A</i> , <b>2016</b> , 120, 9305-9314	2.8	29
30	Excited states via coupled cluster theory without equation-of-motion methods: Seeking higher roots with application to doubly excited states and double core hole states. <i>Journal of Chemical Physics</i> , <b>2019</b> , 151, 214103	3.9	26
29	Systematically Improvable Tensor Hypercontraction: Interpolative Separable Density-Fitting for Molecules Applied to Exact Exchange, Second- and Third-Order Møller-Plesset Perturbation Theory. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 243-263	6.4	25
28	Third-Order Møller-Plesset Perturbation Theory Made Useful? Choice of Orbitals and Scaling Greatly Improves Accuracy for Thermochemistry, Kinetics, and Intermolecular Interactions. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 4170-4176	6.4	24
27	Utilizing Essential Symmetry Breaking in Auxiliary-Field Quantum Monte Carlo: Application to the Spin Gaps of the C <sub>60</sub> Fullerene and an Iron Porphyrin Model Complex. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 3019-3027	6.4	20
26	Limit of metastability for liquid and vapor phases of water. <i>Physical Review Letters</i> , <b>2014</b> , 112, 157802	7.4	17
25	A phaseless auxiliary-field quantum Monte Carlo perspective on the uniform electron gas at finite temperatures: Issues, observations, and benchmark study. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 064103	3.9	15

24	Kohn-Sham Density Functional Theory with Complex, Spin-Restricted Orbitals: Accessing a New Class of Densities without the Symmetry Dilemma. <i>Physical Review Letters</i> , <b>2019</b> , 123, 113001	7.4	13
23	Even More Efficient Quantum Computations of Chemistry Through Tensor Hypercontraction. <i>PRX Quantum</i> , <b>2021</b> , 2,	6.1	13
22	An auxiliary-Field quantum Monte Carlo perspective on the ground state of the dense uniform electron gas: An investigation with Hartree-Fock trial wavefunctions. <i>Journal of Chemical Physics</i> , <b>2019</b> , 151, 064122	3.9	11
21	Open-shell coupled-cluster valence-bond theory augmented with an independent amplitude approximation for three-pair correlations: Application to a model oxygen-evolving complex and single molecular magnet. <i>Journal of Chemical Physics</i> , <b>2018</b> , 149, 244121	3.9	11
20	Making many-body interactions nearly pairwise additive: The polarized many-body expansion approach. <i>Journal of Chemical Physics</i> , <b>2019</b> , 151, 194101	3.9	10
19	Unbiasing fermionic quantum Monte Carlo with a quantum computer.. <i>Nature</i> , <b>2022</b> , 603, 416-420	50.4	10
18	Adsorption of Carbon Tetrahalides on Coronene and Graphene. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 14968-14974	3.8	9
17	The performance of phaseless auxiliary-field quantum Monte Carlo on the ground state electronic energy of benzene. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 126101	3.9	9
16	Virtual Distillation for Quantum Error Mitigation. <i>Physical Review X</i> , <b>2021</b> , 11,	9.1	9
15	Revealing the nature of electron correlation in transition metal complexes with symmetry breaking and chemical intuition. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 194109	3.9	9
14	Stochastic resolution-of-the-identity auxiliary-field quantum Monte Carlo: Scaling reduction without overhead. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 044131	3.9	8
13	Energy Decomposition Analysis for Interactions of Radicals: Theory and Implementation at the MP2 Level with Application to Hydration of Halogenated Benzene Cations and Complexes between CO <sub>2</sub> and Pyridine and Imidazole. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 9621-9633	2.8	8
12	A non-perturbative pairwise-additive analysis of charge transfer contributions to intermolecular interaction energies. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 928-943	3.6	7
11	Regularized Second-Order Møller-Plesset Theory: A More Accurate Alternative to Conventional MP2 for Noncovalent Interactions and Transition Metal Thermochemistry for the Same Computational Cost.. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 12084-12097	6.4	6
10	Polishing the Gold Standard: The Role of Orbital Choice in CCSD(T) Vibrational Frequency Prediction. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 742-755	6.4	6
9	Spectral Functions from Auxiliary-Field Quantum Monte Carlo without Analytic Continuation: The Extended Koopmans Theorem Approach. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 3372-3387	6.4	5
8	What the foundations of quantum computer science teach us about chemistry. <i>Journal of Chemical Physics</i> , <b>2021</b> , 155, 150901	3.9	4
7	Approaching the basis set limit in Gaussian-orbital-based periodic calculations with transferability: Performance of pure density functionals for simple semiconductors. <i>Journal of Chemical Physics</i> , <b>2021</b> , 155, 164102	3.9	4

6	Constrained-path auxiliary-field quantum Monte Carlo for coupled electrons and phonons. <i>Physical Review B</i> , <b>2021</b> , 103,	3.3	3
5	Compressing Many-Body Fermion Operators under Unitary Constraints.. <i>Journal of Chemical Theory and Computation</i> , <b>2022</b> ,	6.4	3
4	Molecular Mechanics Simulations and Improved Tight-Binding Hamiltonians for Artificial Light Harvesting Systems: Predicting Geometric Distributions, Disorder, and Spectroscopy of Chromophores in a Protein Environment. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 12292-12301	3.4	2
3	Exploring the Limits of Second- and Third-Order Møller-Plesset Perturbation Theories for Noncovalent Interactions: Revisiting MP2.5 and Assessing the Importance of Regularization and Reference Orbitals. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 5582-5599	6.4	2
2	Selected configuration interaction wave functions in phaseless auxiliary field quantum Monte Carlo.. <i>Journal of Chemical Physics</i> , <b>2022</b> , 156, 174111	3.9	2
1	Exploring spin symmetry-breaking effects for static field ionization of atoms: Is there an analog to the Coulson-Fischer point in bond dissociation?. <i>Journal of Chemical Physics</i> , <b>2021</b> , 155, 014309	3.9	1