Joonho Lee

List of Publications by Year in Descending Order

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	Compressing Many-Body Fermion Operators under Unitary Constraints.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	3
40	Unbiasing fermionic quantum Monte Carlo with a quantum computer.. *Nature*, **2022**, 603, 416-420	50.4	10
39	Selected configuration interaction wave functions in phaseless auxiliary field quantum Monte Carlo.. *Journal of Chemical Physics*, **2022**, 156, 174111	3.9	2
38	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.. *Journal of Physical Chemistry Letters*, **2021**, 12, 12084-12097	6.4	6
37	Virtual Distillation for Quantum Error Mitigation. *Physical Review X*, **2021**, 11,	9.1	9
36	What the foundations of quantum computer science teach us about chemistry. *Journal of Chemical Physics*, **2021**, 155, 150901	3.9	4
35	Approaching the basis set limit in Gaussian-orbital-based periodic calculations with transferability: Performance of pure density functionals for simple semiconductors. *Journal of Chemical Physics*, **2021**, 155, 164102	3.9	4
34	Constrained-path auxiliary-field quantum Monte Carlo for coupled electrons and phonons. *Physical Review B*, **2021**, 103,	3.3	3
33	Spectral Functions from Auxiliary-Field Quantum Monte Carlo without Analytic Continuation: The Extended KoopmansSTheorem Approach. *Journal of Chemical Theory and Computation*, **2021**, 17, 3372-3387	6.4	5
32	Revealing the nature of electron correlation in transition metal complexes with symmetry breaking and chemical intuition. *Journal of Chemical Physics*, **2021**, 154, 194109	3.9	9
31	Even More Efficient Quantum Computations of Chemistry Through Tensor Hypercontraction. *PRX Quantum*, **2021**, 2,	6.1	13
30	A non-perturbative pairwise-additive analysis of charge transfer contributions to intermolecular interaction energies. *Physical Chemistry Chemical Physics*, **2021**, 23, 928-943	3.6	7
29	Polishing the Gold Standard: The Role of Orbital Choice in CCSD(T) Vibrational Frequency Prediction. *Journal of Chemical Theory and Computation*, **2021**, 17, 742-755	6.4	6
28	A phaseless auxiliary-field quantum Monte Carlo perspective on the uniform electron gas at finite temperatures: Issues, observations, and benchmark study. *Journal of Chemical Physics*, **2021**, 154, 064109	3.9	15
27	Exploring spin symmetry-breaking effects for static field ionization of atoms: Is there an analog to the Coulson-Fischer point in bond dissociation?. *Journal of Chemical Physics*, **2021**, 155, 014309	3.9	1
26	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
25	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. *Journal of Chemical Theory and Computation*, **2021**, 17, 5582-5599	6.4	2

24	Stochastic resolution-of-the-identity auxiliary-field quantum Monte Carlo: Scaling reduction without overhead. *Journal of Chemical Physics*, **2020**, 153, 044131	3.9	8
23	The performance of phaseless auxiliary-field quantum Monte Carlo on the ground state electronic energy of benzene. *Journal of Chemical Physics*, **2020**, 153, 126101	3.9	9
22	QMCPACK: Advances in the development, efficiency, and application of auxiliary field and real-space variational and diffusion quantum Monte Carlo. *Journal of Chemical Physics*, **2020**, 152, 174105	3.9	44
21	A non-orthogonal variational quantum eigensolver. *New Journal of Physics*, **2020**, 22, 073009	2.9	34
20	Systematically Improvable Tensor Hypercontraction: Interpolative Separable Density-Fitting for Molecules Applied to Exact Exchange, Second- and Third-Order M□ller-Plesset Perturbation Theory. *Journal of Chemical Theory and Computation*, **2020**, 16, 243-263	6.4	25
19	Utilizing Essential Symmetry Breaking in Auxiliary-Field Quantum Monte Carlo: Application to the Spin Gaps of the C Fullerene and an Iron Porphyrin Model Complex. *Journal of Chemical Theory and Computation*, **2020**, 16, 3019-3027	6.4	20
18	An auxiliary-Field quantum Monte Carlo perspective on the ground state of the dense uniform electron gas: An investigation with Hartree-Fock trial wavefunctions. *Journal of Chemical Physics*, **2019**, 151, 064122	3.9	11
17	Kohn-Sham Density Functional Theory with Complex, Spin-Restricted Orbitals: Accessing a New Class of Densities without the Symmetry Dilemma. *Physical Review Letters*, **2019**, 123, 113001	7.4	13
16	Distinguishing artificial and essential symmetry breaking in a single determinant: approach and application to the C, C, and C fullerenes. *Physical Chemistry Chemical Physics*, **2019**, 21, 4763-4778	3.6	31
15	Two single-reference approaches to singlet biradicaloid problems: Complex, restricted orbitals and approximate spin-projection combined with regularized orbital-optimized M□ller-Plesset perturbation theory. *Journal of Chemical Physics*, **2019**, 150, 244106	3.9	30
14	Third-Order M□ller-Plesset Perturbation Theory Made Useful? Choice of Orbitals and Scaling Greatly Improves Accuracy for Thermochemistry, Kinetics, and Intermolecular Interactions. *Journal of Physical Chemistry Letters*, **2019**, 10, 4170-4176	6.4	24
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□ and Pyridine and Imidazole. *Journal of Physical Chemistry A*, **2019**, 123, 9621-9633	2.8	8
12	Making many-body interactions nearly pairwise additive: The polarized many-body expansion approach. *Journal of Chemical Physics*, **2019**, 151, 194101	3.9	10
11	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. *Journal of Chemical Physics*, **2019**, 151, 214103	3.9	26
10	Generalized Unitary Coupled Cluster Wave functions for Quantum Computation. *Journal of Chemical Theory and Computation*, **2019**, 15, 311-324	6.4	118
9	Regularized Orbital-Optimized Second-Order M□ller-Plesset Perturbation Theory: A Reliable Fifth-Order-Scaling Electron Correlation Model with Orbital Energy Dependent Regularizers. *Journal of Chemical Theory and Computation*, **2018**, 14, 5203-5219	6.4	56
8	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. *Journal of Physical Chemistry B*, **2018**, 122, 12292-12301	3.4	2
7	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. *Journal of Chemical Physics*, **2018**, 149, 244121	3.9	11

6	Coupled-Cluster Valence-Bond Singles and Doubles for Strongly Correlated Systems: Block-Tensor Based Implementation and Application to Oligoacenes. *Journal of Chemical Theory and Computation* , **2017**, 13, 602-615	6.4	46
5	Adsorption of Carbon Tetrahalides on Coronene and Graphene. *Journal of Physical Chemistry C*, **2017**, 121, 14968-14974	3.8	9
4	Halogen-Interactions between Benzene and X/CX (X = Cl, Br): Assessment of Various Density Functionals with Respect to CCSD(T). *Journal of Physical Chemistry A*, **2016**, 120, 9305-9314	2.8	29
3	A deterministic alternative to the full configuration interaction quantum Monte Carlo method. *Journal of Chemical Physics*, **2016**, 145, 044112	3.9	161
2	Embedded mean-field theory. *Journal of Chemical Theory and Computation*, **2015**, 11, 568-80	6.4	77
1	Limit of metastability for liquid and vapor phases of water. *Physical Review Letters*, **2014**, 112, 157802	7.4	17