Daniel Kats

List of Publications by Year
in descending order

40 papers	1,920 citations	361296 20 h-index	289141 40 g-index
40 all docs	40 docs citations	40 times ranked	1114 citing authors

#	Article	IF	Citations
1	Full configuration interaction quantum Monte Carlo treatment of fragments embedded in a periodic mean field. Journal of Chemical Physics, 2022, 156, 154107.	1.2	8
2	Spin Purification in Full-CI Quantum Monte Carlo via a First-Order Penalty Approach. Journal of Physical Chemistry A, 2022, 126, 2050-2060.	1.1	8
3	FCIQMC-Tailored Distinguishable Cluster Approach: Open-Shell Systems. Journal of Chemical Theory and Computation, 2022, , .	2.3	4
4	Combined unitary and symmetric group approach applied to low-dimensional Heisenberg spin systems. Physical Review B, 2022, 105, .	1.1	9
5	Description of excited states in photochemistry with theoretical methods. ChemistrySelect, 2021, 6, .	0.7	2
6	Towards efficient and accurate ab initio solutions to periodic systems via transcorrelation and coupled cluster theory. Physical Review Research, 2021, 3, .	1.3	16
7	Accuracy of the distinguishable cluster approximation for triple excitations for open-shell molecules and excited states. Journal of Chemical Physics, 2021, 155, 064101.	1.2	6
8	Transcorrelated coupled cluster methods. Journal of Chemical Physics, 2021, 155, 191101.	1.2	17
9	Fragment-Based Restricted Active Space Configuration Interaction with Second-Order Corrections Embedded in Periodic Hartreeâ€“Fock Wave Function. Journal of Chemical Theory and Computation, 2020, 16, 7100-7108.	2.3	11
10	FCIQMC-Tailored Distinguishable Cluster Approach. Journal of Chemical Theory and Computation, 2020, 16, 5621-5634.	2.3	22
11	The Molpro quantum chemistry package. Journal of Chemical Physics, 2020, 152, 144107.	1.2	603
12	Role of Valence and Semicore Electron Correlation on Spin Gaps in Fe(II)-Porphyrins. Journal of Chemical Theory and Computation, 2019, 15, 1492-1497.	2.3	51
13	Multi-state local complete active space second-order perturbation theory using pair natural orbitals (PNO-MS-CASPT2). Journal of Chemical Physics, 2019, 150, 214107.	1.2	17
14	Toward fast and accurate ab initio calculation of magnetic exchange in polynuclear lanthanide complexes. Physical Chemistry Chemical Physics, 2019, 21, 9769-9778.	1.3	12
15	On the distinguishable cluster approximation for triple excitations. Journal of Chemical Physics, 2019, 150, 151101.	1.2	17
16	Perturbation Expansion of Internally Contracted Coupled-Cluster Theory up to Third Order. Journal of Chemical Theory and Computation, 2019, 15, 2291-2305.	2.3	14
17	Orbital-Optimized Distinguishable Cluster Theory with Explicit Correlation. Journal of Chemical Theory and Computation, 2019, 15, 13-17.	2.3	12
18	Embedded Multireference Coupled Cluster Theory. Journal of Chemical Theory and Computation, 2018, 14, 693-709.	2.3	30

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19	Improving the distinguishable cluster results: spin-component scaling. Molecular Physics, 2018, 116, 1435-1442.	0.8	15
20	Particleâ€“hole symmetry in many-body theories of electron correlation. Molecular Physics, 2018, 116, 1496-1503.	0.8	9
21	Relaxing Constrained Amplitudes: Improved F12 Treatments of Orbital Optimization and Coreâ€“Valence Correlation Energies. Journal of Chemical Theory and Computation, 2018, 14, 5435-5440.	2.3	6
22	Speeding up local correlation methods: System-inherent domains. Journal of Chemical Physics, 2016, 145, 014103.	1.2	13
23	Local complete active space second-order perturbation theory using pair natural orbitals (PNO-CASPT2). Journal of Chemical Physics, 2016, 145, 124115.	1.2	79
24	The distinguishable cluster approach from a screened Coulomb formalism. Journal of Chemical Physics, 2016, 144, 044102.	1.2	31
25	Accurate thermochemistry from explicitly correlated distinguishable cluster approximation. Journal of Chemical Physics, 2015, 142, 064111.	1.2	55
26	Communication: The distinguishable cluster approximation. II. The role of orbital relaxation. Journal of Chemical Physics, 2014, 141, 061101.	1.2	50
27	Speeding up local correlation methods. Journal of Chemical Physics, 2014, 141, 244101.	1.2	24
28	Local CC2 response method based on the Laplace transform: Orbital-relaxed first-order properties for excited states. Journal of Chemical Physics, 2013, 139, 084111.	1.2	23
29	Sparse tensor framework for implementation of general local correlation methods. Journal of Chemical Physics, 2013, 138, 144101.	1.2	52
30	Communication: The distinguishable cluster approximation. Journal of Chemical Physics, 2013, 139, 021102.	1.2	98
31	Application of Hermitian time-dependent coupled-cluster responseAnsÃtzeof second order to excitation energies and frequency-dependent dipole polarizabilities. Physical Review A, 2012, 86, .	1.0	28
32	Second-order variational coupled-cluster linear-response method: A Hermitian time-dependent theory. Physical Review A, 2011, 83, .	1.0	19
33	Local Approximations for an Efficient and Accurate Treatment of Electron Correlation and Electron Excitations in Molecules. Challenges and Advances in Computational Chemistry and Physics, 2011, , 345-407.	0.6	27
34	Local CC2 response method for triplet states based on Laplace transform: Excitation energies and first-order properties. Journal of Chemical Physics, 2010, 133, 244110.	1.2	66
35	Local Time-Dependent Coupled Cluster Response for Properties of Excited States in Large Molecules. Zeitschrift Fur Physikalische Chemie, 2010, 224, 601-616.	1.4	24
36	A multistate local coupled cluster CC2 response method based on the Laplace transform. Journal of Chemical Physics, 2009, 131, 124117.	1.2	109

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37	Comment on â€œMinimax approximation for the decomposition of energy denominators in Laplace-transformed MÃ¸llerâ€“Plesset perturbation theoriesâ€•[J. Chem. Phys. 129, 044112 (2008)]. Journal of Chemical Physics, 2009, 130, 127101.	1.2	15
38	On the use of the Laplace transform in local correlation methods. Physical Chemistry Chemical Physics, 2008, 10, 3430.	1.3	54
39	Transition strengths and first-order properties of excited states from local coupled cluster CC2 response theory with density fitting. Journal of Chemical Physics, 2007, 127, 064107.	1.2	98
40	Local CC2 electronic excitation energies for large molecules with density fitting. Journal of Chemical Physics, 2006, 125, 104106.	1.2	166