Matthew R Hermes

List of Publications by Year
in descending order

26 papers	920 citations	567281 15 h-index	501196 28 g-index
28 all docs	28 docs citations	28 times ranked	611 citing authors

#	Article	IF	Citations
1	Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	3.0	388
2	General-Order Many-Body Greenâ€™s Function Method. Journal of Chemical Theory and Computation, 2015, 11, 1595-1606.	5.3	61
3	Multiconfigurational Self-Consistent Field Theory with Density Matrix Embedding: The Localized Active Space Self-Consistent Field Method. Journal of Chemical Theory and Computation, 2019, 15, 972-986.	5.3	55
4	Periodic Electronic Structure Calculations with the Density Matrix Embedding Theory. Journal of Chemical Theory and Computation, 2020, 16, 130-140.	5.3	40
5	Second-order many-body perturbation expansions of vibrational Dyson self-energies. Journal of Chemical Physics, 2013, 139, 034111.	3.0	35
6	Convergence Acceleration of Parallel Monte Carlo Second-Order Many-Body Perturbation Calculations Using Redundant Walkers. Journal of Chemical Theory and Computation, 2013, 9, 4396-4402.	5.3	32
7	Merging symmetry projection methods with coupled cluster theory: Lessons from the Lipkin model Hamiltonian. Journal of Chemical Physics, 2017, 146, 054110.	3.0	30
8	Finite-temperature coupled-cluster, many-body perturbation, and restricted and unrestricted Hartreeâ€“Fock study on one-dimensional solids: Luttinger liquids, Peierls transitions, and spin- and charge-density waves. Journal of Chemical Physics, 2015, 143, 102818.	3.0	24
9	Second-Order Many-Body Perturbation Theory: An Eternal Frontier. Journal of Physical Chemistry A, 2014, 118, 655-672.	2.5	23
10	A New Mixing of Nonlocal Exchange and Nonlocal Correlation with Multiconfiguration Pair-Density Functional Theory. Journal of Physical Chemistry Letters, 2020, 11, 10158-10163.	4.6	21
11	Size-extensive vibrational self-consistent field methods with anharmonic geometry corrections. Journal of Chemical Physics, 2012, 136, 234109.	3.0	20
12	Excited States of Crystalline Point Defects with Multireference Density Matrix Embedding Theory. Journal of Physical Chemistry Letters, 2021, 12, 11688-11694.	4.6	20
13	Variational Localized Active Space Self-Consistent Field Method. Journal of Chemical Theory and Computation, 2020, 16, 4923-4937.	5.3	19
14	Electronic structure of strongly correlated systems: recent developments in multiconfiguration pair-density functional theory and multiconfiguration nonclassical-energy functional theory. Chemical Science, 2022, 13, 7685-7706.	7.4	18
15	Analytic gradients for state-averaged multiconfiguration pair-density functional theory. Journal of Chemical Physics, 2020, 153, 014106.	3.0	16
16	Stochastic many-body perturbation theory for anharmonic molecular vibrations. Journal of Chemical Physics, 2014, 141, 084105.	3.0	14
17	Diagrammatic theories of anharmonic molecular vibrations. International Reviews in Physical Chemistry, 2015, 34, 71-97.	2.3	14
18	First-Order Dyson Coordinates and Geometry. Journal of Physical Chemistry A, 2013, 117, 7179-7189.	2.5	13

#	Article	IF	Citations
19	Normal-ordered second-quantized Hamiltonian for molecular vibrations. Journal of Chemical Physics, 2014, 141, 184111.	3.0	12
20	Multiconfiguration Density-Coherence Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 2775-2782.	5.3	12
21	Combining symmetry collective states with coupled-cluster theory: Lessons from the Agassi model Hamiltonian. Physical Review C, 2017, 95, .	2.9	11
22	Spin-State Ordering in Metal-Based Compounds Using the Localized Active Space Self-Consistent Field Method. Journal of Physical Chemistry Letters, 2019, 10, 5507-5513.	4.6	11
23	Analytic gradients for multiconfiguration pair-density functional theory with density fitting: Development and application to geometry optimization in the ground and excited states. Journal of Chemical Physics, 2021, 154, 074108.	3.0	8
24	Stochastic algorithm for size-extensive vibrational self-consistent field methods on fully anharmonic potential energy surfaces. Journal of Chemical Physics, 2014, 141, 244111.	3.0	6
25	Low-rank canonical-tensor decomposition of potential energy surfaces: application to grid-based diagrammatic vibrational Green's function theory. Molecular Physics, 2017, 115, 2120-2134.	1.7	6
26	Localized Active Space Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 2843-2851.	5.3	6