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	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
2	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
3	Localized Active Space Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 2843-2851.	5.3	6
4	Multiconfiguration Density-Coherence Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 2775-2782.	5.3	12
5	Excited States of Crystalline Point Defects with Multireference Density Matrix Embedding Theory. Journal of Physical Chemistry Letters, 2021, 12, 11688-11694.	4.6	20
6	Periodic Electronic Structure Calculations with the Density Matrix Embedding Theory. Journal of Chemical Theory and Computation, 2020, 16, 130-140.	5.3	40
7	Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	3.0	388
8	Analytic gradients for state-averaged multiconfiguration pair-density functional theory. Journal of Chemical Physics, 2020, 153, 014106.	3.0	16
9	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
10	Variational Localized Active Space Self-Consistent Field Method. Journal of Chemical Theory and Computation, 2020, 16, 4923-4937.	5.3	19
11	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
12	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
13	Merging symmetry projection methods with coupled cluster theory: Lessons from the Lipkin model Hamiltonian. Journal of Chemical Physics, 2017, 146, 054110.	3.0	30
14	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
15	Combining symmetry collective states with coupled-cluster theory: Lessons from the Agassi model Hamiltonian. Physical Review C, 2017, 95, .	2.9	11
16	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
17	General-Order Many-Body Greenâ€™s Function Method. Journal of Chemical Theory and Computation, 2015, 11, 1595-1606.	5.3	61
18	Diagrammatic theories of anharmonic molecular vibrations. International Reviews in Physical Chemistry, 2015, 34, 71-97.	2.3	14

#	Article	IF	Citations
19	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
20	Normal-ordered second-quantized Hamiltonian for molecular vibrations. Journal of Chemical Physics, 2014, 141, 184111.	3.0	12
21	Stochastic many-body perturbation theory for anharmonic molecular vibrations. Journal of Chemical Physics, 2014, 141, 084105.	3.0	14
22	Second-Order Many-Body Perturbation Theory: An Eternal Frontier. Journal of Physical Chemistry A, 2014, 118, 655-672.	2.5	23
23	Second-order many-body perturbation expansions of vibrational Dyson self-energies. Journal of Chemical Physics, 2013, 139, 034111.	3.0	35
24	First-Order Dyson Coordinates and Geometry. Journal of Physical Chemistry A, 2013, 117, 7179-7189.	2.5	13
25	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
26	Size-extensive vibrational self-consistent field methods with anharmonic geometry corrections. Journal of Chemical Physics, 2012, 136, 234109.	3.0	20