Mark R Hoffmann

List of Publications by Year
in descending order

51 papers	1,221 citations	411340 20 h-index	425179 34 g-index
52 all docs	52 docs citations	52 times ranked	952 citing authors

#	Article	IF	Citations
1	Further Development of iCIPT2 for Strongly Correlated Electrons. Journal of Chemical Theory and Computation, 2021, 17, 949-964.	2.3	23
2	Low-Lying Electronic States of the Nickel Dimer. Frontiers in Chemistry, 2021, 9, 678930.	1.8	0
3	Theoretical Calculations of the 242 nm Absorption of Propargyl Radical. Journal of Physical Chemistry A, 2021, 125, 8595-8602.	1.1	1
4	The Ground State Electronic Energy of Benzene. Journal of Physical Chemistry Letters, 2020, 11, 8922-8929.	2.1	90
5	On the development and implementation of multi-CPU parallel versions of accurate, general purpose, methods of multireference perturbation theories. Advances in Quantum Chemistry, 2020, , 105-141.	0.4	3
6	Iterative Configuration Interaction with Selection. Journal of Chemical Theory and Computation, 2020, 16, 2296-2316.	2.3	67
7	Study of iridium silicide monolayers using density functional theory. Journal of Applied Physics, 2018, 123, 074301.	1.1	1
8	Further development of SDSPT2 for strongly correlated electrons. Molecular Physics, 2017, 115, 2696-2707.	0.8	35
9	Accurate Dissociation of Chemical Bonds Using DFT-in-DFT Embedding Theory with External Orbital Orthogonality. Journal of Physical Chemistry A, 2017, 121, 256-264.	1.1	24
10	iVI: An iterative vector interaction method for large eigenvalue problems. Journal of Computational Chemistry, 2017, 38, 2481-2499.	1.5	24
11	An Efficient Storage Format for Storing Configuration Interaction Sparse Matrices on CPU/GPU. , 2017, , .		1
12	iCI: Iterative CI toward full CI. Journal of Chemical Theory and Computation, 2016, 12, 1169-1178.	2.3	123
13	Use of Density Functional Theory Orbitals in the GVVPT2 Variant of Second-Order Multistate Multireference Perturbation Theory. Journal of Physical Chemistry A, 2015, 119, 1548-1553.	1.1	9
14	Relative phase control over tunneling ionization of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow><mml:mo>+</mml:mo></mml:msup></mml:math a synthesized Ï‰-2Ï‰ laser pulse. Physical Review A, 2014, 90, .	1.0	5
15	SDS: the â€˜staticâ€“dynamicâ€“staticâ€™ framework for strongly correlated electrons. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	61
16	Density Differences in Embedding Theory with External Orbital Orthogonality. Journal of Physical Chemistry A, 2014, 118, 9182-9200.	1.1	36
17	Coriolis coupling effect of state-to-state quantum dynamics for HeÂ+ÂHeH+. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	6
18	GVVPT2 multireference perturbation theory study of selenium oxides. Molecular Physics, 2013, 111, 1078-1091.	0.8	4

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19	Generalized Van Vleck perturbation theory study of chlorine monoxide. , 2012, , .		0
20	On the Orthogonality of Orbitals in Subsystem Kohnâ€“Sham Density Functional Theory. Annual Reports in Computational Chemistry, 2012, 8, 53-70.	0.9	27
21	GVVPT2 Multireference Perturbation Theory Description of Diatomic Scandium, Chromium, and Manganese. Journal of Physical Chemistry A, 2012, 116, 4590-4601.	1.1	13
22	Lagrangian approach for geometrical derivatives and nonadiabatic coupling terms in MRCISD. Molecular Physics, 2010, 108, 2703-2716.	0.8	13
23	On the inclusion of triple and quadruple electron excitations into MRCISD for multiple states. Chemical Physics Letters, 2010, 493, 1-10.	1.2	14
24	Embedding theory for excited states. Journal of Chemical Physics, 2010, 133, 044107.	1.2	47
25	Multireference Generalized Van Vleck Perturbation Theory (GVVPT2) Study of the NCO + HCNO Reaction: Insight into Intermediates^{â€}. Journal of Physical Chemistry A, 2010, 114, 8831-8836.	1.1	10
26	MRCISD and GVVPT3 study of the low-lying electronic states of NOâ^'. Molecular Physics, 2009, 107, 889-897.	0.8	2
27	Comparative study of multireference perturbative theories for ground and excited states. Journal of Chemical Physics, 2009, 131, 204104.	1.2	51
28	Thirdâ€order generalized Van Vleck perturbation theory variant of multireference perturbation theory for electron correlation. International Journal of Quantum Chemistry, 2009, 109, 1855-1873.	1.0	8
29	Configuration-Driven Unitary Group Approach for Generalized Van Vleck Variant Multireference Perturbation Theory. Journal of Physical Chemistry A, 2009, 113, 4374-4380.	1.1	46
30	Second-order generalized Van Vleck perturbation theory calculations of potential energy curves for the dissociation of the Câ€“H bond in methane. Molecular Physics, 2007, 105, 2819-2827.	0.8	1
31	Table-CI with macroconfiguration approach for describing electronic states of molecules in intense radiation fields. International Journal of Quantum Chemistry, 2005, 105, 921-928.	1.0	1
32	Macroconfigurations in molecular electronic structure theory. International Journal of Quantum Chemistry, 2004, 99, 210-220.	1.0	36
33	Ground and Low-Lying Excited Electronic States of Difluorodiazirineâ€. Journal of Physical Chemistry A, 2004, 108, 3119-3124.	1.1	12
34	Perturbative triple and quadruple excitation corrections to MRCISD. Chemical Physics Letters, 2003, 372, 674-685.	1.2	11
35	Theoretical study of the ground and first excited singlet state potential energy surfaces of disulphur monoxide (S2O). Molecular Physics, 2003, 101, 1303-1310.	0.8	14
36	Molecular gradients for the second-order generalized Van Vleck variant of multireference perturbation theory. Journal of Chemical Physics, 2003, 119, 651-660.	1.2	26

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37	Low-lying electronic states of difluorodioxirane. Journal of Chemical Physics, 2003, 118, 10065-10072.	1.2	11
38	Explication and revision of generalized Van Vleck perturbation theory for molecular electronic structure. Journal of Chemical Physics, 2002, 117, 4133-4145.	1.2	96
39	Overview: Accurate Description of Low-Lying Electronic States and Potential Energy Surfaces. ACS Symposium Series, 2002, , 1-8.	0.5	4
40	Model Studies of Intersystem Crossing Effects in the O + H₂ Reaction. ACS Symposium Series, 2002, , 329-345.	0.5	7
41	Hamiltonian Matrix Elements for the Table-CI Method Using Genealogical Configuration State Functions. ACS Symposium Series, 2002, , 176-198.	0.5	5
42	Fluorofluoroxydioxirane and Other CF2O3 Isomers. Journal of Physical Chemistry A, 2001, 105, 779-790.	1.1	6
43	Possible use of genealogical spin-adapted functions in the table-CI method. International Journal of Quantum Chemistry, 2001, 81, 130-134.	1.0	9
44	Theoretical Study of 1-Methoxy-2-sulfanylethan-1-yl Cation:Â Insight into Intermediates in Glycosidation Reactions. Journal of Organic Chemistry, 1999, 64, 1247-1253.	1.7	40
45	A Theoretical Study of Substituted Dioxiranes:â€‰ Difluorodioxirane, Fluorofluoroxydioxirane, (Fluoroimino)dioxirane, and Hydrazodioxirane. Journal of Physical Chemistry A, 1999, 103, 521-526.	1.1	18
46	A self-consistent version of quasidegenerate perturbation theory. Journal of Chemical Physics, 1998, 108, 8317-8330.	1.2	45
47	Canonical Van Vleck Quasidegenerate Perturbation Theory with Trigonometric Variables. The Journal of Physical Chemistry, 1996, 100, 6125-6130.	2.9	54
48	A nondiagonal quasidegenerate fourth-order perturbation theory. Journal of Mathematical Chemistry, 1996, 20, 351-364.	0.7	5
49	QUASIDEGENERATE PERTURBATION THEORY USING EFFECTIVE HAMILTONIANS. Advanced Series in Physical Chemistry, 1995, , 1166-1190.	1.5	8
50	Third-order complete active space self-consistent field based generalized Van Vleck perturbation theory. Chemical Physics Letters, 1993, 210, 193-200.	1.2	37
51	A theoretical study of lowâ€‹ying electronic states of aminonitrene, phosphinonitrene, and phosphinocarbene. Journal of Chemical Physics, 1991, 94, 8029-8039.	1.2	25