Mark R Hoffmann

List of Publications by Year
in descending order

51 papers	1,221 citations	361413 20 h-index	377865 34 g-index
52 all docs	52 docs citations	52 times ranked	821 citing authors

#	Article	IF	Citations
1	iCI: Iterative CI toward full CI. Journal of Chemical Theory and Computation, 2016, 12, 1169-1178.	5.3	123
2	Explication and revision of generalized Van Vleck perturbation theory for molecular electronic structure. Journal of Chemical Physics, 2002, 117, 4133-4145.	3.0	96
3	The Ground State Electronic Energy of Benzene. Journal of Physical Chemistry Letters, 2020, 11, 8922-8929.	4.6	90
4	Iterative Configuration Interaction with Selection. Journal of Chemical Theory and Computation, 2020, 16, 2296-2316.	5.3	67
5	SDS: the â€˜staticâ€“dynamicâ€“staticâ€™ framework for strongly correlated electrons. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	61
6	Canonical Van Vleck Quasidegenerate Perturbation Theory with Trigonometric Variables. The Journal of Physical Chemistry, 1996, 100, 6125-6130.	2.9	54
7	Comparative study of multireference perturbative theories for ground and excited states. Journal of Chemical Physics, 2009, 131, 204104.	3.0	51
8	Embedding theory for excited states. Journal of Chemical Physics, 2010, 133, 044107.	3.0	47
9	Configuration-Driven Unitary Group Approach for Generalized Van Vleck Variant Multireference Perturbation Theory. Journal of Physical Chemistry A, 2009, 113, 4374-4380.	2.5	46
10	A self-consistent version of quasidegenerate perturbation theory. Journal of Chemical Physics, 1998, 108, 8317-8330.	3.0	45
11	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.	3.2	40
12	Third-order complete active space self-consistent field based generalized Van Vleck perturbation theory. Chemical Physics Letters, 1993, 210, 193-200.	2.6	37
13	Macroconfigurations in molecular electronic structure theory. International Journal of Quantum Chemistry, 2004, 99, 210-220.	2.0	36
14	Density Differences in Embedding Theory with External Orbital Orthogonality. Journal of Physical Chemistry A, 2014, 118, 9182-9200.	2.5	36
15	Further development of SDSPT2 for strongly correlated electrons. Molecular Physics, 2017, 115, 2696-2707.	1.7	35
16	On the Orthogonality of Orbitals in Subsystem Kohnâ€“Sham Density Functional Theory. Annual Reports in Computational Chemistry, 2012, 8, 53-70.	1.7	27
17	Molecular gradients for the second-order generalized Van Vleck variant of multireference perturbation theory. Journal of Chemical Physics, 2003, 119, 651-660.	3.0	26
18	A theoretical study of lowâ€lying electronic states of aminonitrene, phosphinonitrene, and phosphinocarbene. Journal of Chemical Physics, 1991, 94, 8029-8039.	3.0	25

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19	Accurate Dissociation of Chemical Bonds Using DFT-in-DFT Embedding Theory with External Orbital Orthogonality. Journal of Physical Chemistry A, 2017, 121, 256-264.	2.5	24
20	iVI: An iterative vector interaction method for large eigenvalue problems. Journal of Computational Chemistry, 2017, 38, 2481-2499.	3.3	24
21	Further Development of iCIPT2 for Strongly Correlated Electrons. Journal of Chemical Theory and Computation, 2021, 17, 949-964.	5.3	23
22	A Theoretical Study of Substituted Dioxiranes:â€‰ Difluorodioxirane, Fluorofluoroxydioxirane, (Fluoroimino)dioxirane, and Hydrazodioxirane. Journal of Physical Chemistry A, 1999, 103, 521-526.	2.5	18
23	Theoretical study of the ground and first excited singlet state potential energy surfaces of disulphur monoxide (S2O). Molecular Physics, 2003, 101, 1303-1310.	1.7	14
24	On the inclusion of triple and quadruple electron excitations into MRCISD for multiple states. Chemical Physics Letters, 2010, 493, 1-10.	2.6	14
25	Lagrangian approach for geometrical derivatives and nonadiabatic coupling terms in MRCISD. Molecular Physics, 2010, 108, 2703-2716.	1.7	13
26	GVVPT2 Multireference Perturbation Theory Description of Diatomic Scandium, Chromium, and Manganese. Journal of Physical Chemistry A, 2012, 116, 4590-4601.	2.5	13
27	Ground and Low-Lying Excited Electronic States of Difluorodiazirineâ€. Journal of Physical Chemistry A, 2004, 108, 3119-3124.	2.5	12
28	Perturbative triple and quadruple excitation corrections to MRCISD. Chemical Physics Letters, 2003, 372, 674-685.	2.6	11
29	Low-lying electronic states of difluorodioxirane. Journal of Chemical Physics, 2003, 118, 10065-10072.	3.0	11
30	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.	2.5	10
31	Possible use of genealogical spin-adapted functions in the table-CI method. International Journal of Quantum Chemistry, 2001, 81, 130-134.	2.0	9
32	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.	2.5	9
33	QUASIDEGENERATE PERTURBATION THEORY USING EFFECTIVE HAMILTONIANS. Advanced Series in Physical Chemistry, 1995, , 1166-1190.	1.5	8
34	Thirdâ€order generalized Van Vleck perturbation theory variant of multireference perturbation theory for electron correlation. International Journal of Quantum Chemistry, 2009, 109, 1855-1873.	2.0	8
35	Model Studies of Intersystem Crossing Effects in the O + H₂ Reaction. ACS Symposium Series, 2002, , 329-345.	0.5	7
36	Fluorofluoroxydioxirane and Other CF2O3 Isomers. Journal of Physical Chemistry A, 2001, 105, 779-790.	2.5	6

#	Article	IF	Citations
37	Coriolis coupling effect of state-to-state quantum dynamics for HeÂ+ÂHeH+. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	6
38	A nondiagonal quasidegenerate fourth-order perturbation theory. Journal of Mathematical Chemistry, 1996, 20, 351-364.	1.5	5
39	Hamiltonian Matrix Elements for the Table-CI Method Using Genealogical Configuration State Functions. ACS Symposium Series, 2002, , 176-198.	0.5	5
40	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:mat a synthesized Ï‰-2Ï‰ laser pulse. Physical Review A, 2014, 90, .	2.5	5
41	Overview: Accurate Description of Low-Lying Electronic States and Potential Energy Surfaces. ACS Symposium Series, 2002, , 1-8.	0.5	4
42	GVVPT2 multireference perturbation theory study of selenium oxides. Molecular Physics, 2013, 111, 1078-1091.	1.7	4
43	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.	0.8	3
44	MRCISD and GVVPT3 study of the low-lying electronic states of NOâ^'. Molecular Physics, 2009, 107, 889-897.	1.7	2
45	Table-CI with macroconfiguration approach for describing electronic states of molecules in intense radiation fields. International Journal of Quantum Chemistry, 2005, 105, 921-928.	2.0	1
46	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.	1.7	1
47	An Efficient Storage Format for Storing Configuration Interaction Sparse Matrices on CPU/GPU. , 2017, , .		1
48	Study of iridium silicide monolayers using density functional theory. Journal of Applied Physics, 2018, 123, 074301.	2.5	1
49	Theoretical Calculations of the 242 nm Absorption of Propargyl Radical. Journal of Physical Chemistry A, 2021, 125, 8595-8602.	2.5	1
50	Generalized Van Vleck perturbation theory study of chlorine monoxide. , 2012, , .		0
51	Low-Lying Electronic States of the Nickel Dimer. Frontiers in Chemistry, 2021, 9, 678930.	3.6	0