Mark R Hoffmann

List of Publications by Citations

50 papers	989 citations	18 h-index	30 g-index
52 ext. papers	1,096 ext. citations	2.8 avg, IF	4.69 L-index

#	Paper	IF	Citations
50	iCI: Iterative CI toward full CI. *Journal of Chemical Theory and Computation*, **2016**, 12, 1169-78	6.4	90
49	Explication and revision of generalized Van Vleck perturbation theory for molecular electronic structure. *Journal of Chemical Physics*, **2002**, 117, 4133-4145	3.9	88
48	The Ground State Electronic Energy of Benzene. *Journal of Physical Chemistry Letters*, **2020**, 11, 8922-8929	6.4	52
47	Canonical Van Vleck Quasidegenerate Perturbation Theory with Trigonometric Variables. *The Journal of Physical Chemistry*, **1996**, 100, 6125-6130		51
46	Comparative study of multireference perturbative theories for ground and excited states. *Journal of Chemical Physics*, **2009**, 131, 204104	3.9	48
45	SDS: the Static-Dynamic-Static framework for strongly correlated electrons. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	46
44	Configuration-driven unitary group approach for generalized Van Vleck variant multireference perturbation theory. *Journal of Physical Chemistry A*, **2009**, 113, 4374-80	2.8	44
43	A self-consistent version of quasidegenerate perturbation theory. *Journal of Chemical Physics*, **1998**, 108, 8317-8330	3.9	44
42	Embedding theory for excited states. *Journal of Chemical Physics*, **2010**, 133, 044107	3.9	39
41	Third-order complete active space self-consistent field based generalized Van Vleck perturbation theory. *Chemical Physics Letters*, **1993**, 210, 193-200	2.5	37
40	Theoretical Study of 1-Methoxy-2-sulfanylethan-1-yl Cation: Insight into Intermediates in Glycosidation Reactions. *Journal of Organic Chemistry*, **1999**, 64, 1247-1253	4.2	35
39	Iterative Configuration Interaction with Selection. *Journal of Chemical Theory and Computation*, **2020**, 16, 2296-2316	6.4	34
38	Macroconfigurations in molecular electronic structure theory. *International Journal of Quantum Chemistry*, **2004**, 99, 210-220	2.1	34
37	Density differences in embedding theory with external orbital orthogonality. *Journal of Physical Chemistry A*, **2014**, 118, 9182-200	2.8	30
36	Further development of SDSPT2 for strongly correlated electrons. *Molecular Physics*, **2017**, 115, 2696-2707	1.7	26
35	Molecular gradients for the second-order generalized Van Vleck variant of multireference perturbation theory. *Journal of Chemical Physics*, **2003**, 119, 651-660	3.9	23
34	A theoretical study of low-lying electronic states of aminonitrene, phosphinonitrene, and phosphinocarbene. *Journal of Chemical Physics*, **1991**, 94, 8029-8039	3.9	23

33	On the Orthogonality of Orbitals in Subsystem Kohn–Sham Density Functional Theory. *Annual Reports in Computational Chemistry*, **2012**, 8, 53-70	1.8	20
32	iVI: An iterative vector interaction method for large eigenvalue problems. *Journal of Computational Chemistry*, **2017**, 38, 2481-2499	3.5	16
31	Accurate Dissociation of Chemical Bonds Using DFT-in-DFT Embedding Theory with External Orbital Orthogonality. *Journal of Physical Chemistry A*, **2017**, 121, 256-264	2.8	15
30	A Theoretical Study of Substituted Dioxiranes: Difluorodioxirane, Fluorofluoroxydioxirane, (Fluoroimino)dioxirane, and Hydrazodioxirane. *Journal of Physical Chemistry A*, **1999**, 103, 521-526	2.8	15
29	On the inclusion of triple and quadruple electron excitations into MRCISD for multiple states. *Chemical Physics Letters*, **2010**, 493, 1-10	2.5	14
28	GVVPT2 multireference perturbation theory description of diatomic scandium, chromium, and manganese. *Journal of Physical Chemistry A*, **2012**, 116, 4590-601	2.8	12
27	Lagrangian approach for geometrical derivatives and nonadiabatic coupling terms in MRCISD. *Molecular Physics*, **2010**, 108, 2703-2716	1.7	12
26	Ground and Low-Lying Excited Electronic States of Difluorodiazirine. *Journal of Physical Chemistry A*, **2004**, 108, 3119-3124	2.8	11
25	Perturbative triple and quadruple excitation corrections to MRCISD. *Chemical Physics Letters*, **2003**, 372, 674-685	2.5	11
24	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	11
23	Low-lying electronic states of difluorodioxirane. *Journal of Chemical Physics*, **2003**, 118, 10065-10072	3.9	11
22	Use of density functional theory orbitals in the GVVPT2 variant of second-order multistate multireference perturbation theory. *Journal of Physical Chemistry A*, **2015**, 119, 1548-53	2.8	9
21	Multireference generalized Van Vleck perturbation theory (GVVPT2) study of the NCO + HCNO reaction: insight into intermediates. *Journal of Physical Chemistry A*, **2010**, 114, 8831-6	2.8	9
20	Possible use of genealogical spin-adapted functions in the table-CI method. *International Journal of Quantum Chemistry*, **2001**, 81, 130-134	2.1	9
19	Third-order generalized Van Vleck perturbation theory variant of multireference perturbation theory for electron correlation. *International Journal of Quantum Chemistry*, **2009**, 109, 1855-1873	2.1	8
18	QUASIDEGENERATE PERTURBATION THEORY USING EFFECTIVE HAMILTONIANS. *Advanced Series in Physical Chemistry*, **1995**, 1166-1190		8
17	Model Studies of Intersystem Crossing Effects in the O + H2 Reaction. *ACS Symposium Series*, **2002**, 329-345	3.4	7
16	Further Development of iCIPT2 for Strongly Correlated Electrons. *Journal of Chemical Theory and Computation*, **2021**, 17, 949-964	6.4	7

15	Fluorofluoroxydioxirane and Other CF2O3 Isomers. *Journal of Physical Chemistry A*, **2001**, 105, 779-790	2.8	6
14	Coriolis coupling effect of state-to-state quantum dynamics for He + HeH+. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	5
13	Hamiltonian Matrix Elements for the Table-CI Method Using Genealogical Configuration State Functions. *ACS Symposium Series*, **2002**, 176-198	0.4	5
12	GVVPT2 multireference perturbation theory study of selenium oxides. *Molecular Physics*, **2013**, 111, 1078-1091	1.7	4
11	A nondiagonal quasidegenerate fourth-order perturbation theory. *Journal of Mathematical Chemistry*, **1996**, 20, 351-364	2.1	4
10	Relative phase control over tunneling ionization of H2+ with a synthesized □2□laser pulse. *Physical Review A*, **2014**, 90,	2.6	3
9	Overview: Accurate Description of Low-Lying Electronic States and Potential Energy Surfaces. *ACS Symposium Series*, **2002**, 1-8	0.4	3
8	MRCISD and GVVPT3 study of the low-lying electronic states of NO□*Molecular Physics*, **2009**, 107, 889-897	1.7	2
7	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	1.4	1
6	An Efficient Storage Format for Storing Configuration Interaction Sparse Matrices on CPU/GPU **2017**,		1
5	Second-order generalized Van Vleck perturbation theory calculations of potential energy curves for the dissociation of the C□H bond in methane. *Molecular Physics*, **2007**, 105, 2819-2827	1.7	1
4	Table-CI with macroconfiguration approach for describing electronic states of molecules in intense radiation fields. *International Journal of Quantum Chemistry*, **2005**, 105, 921-928	2.1	1
3	Study of iridium silicide monolayers using density functional theory. *Journal of Applied Physics*, **2018** , 123, 074301	2.5	0
2	Low-Lying Electronic States of the Nickel Dimer. *Frontiers in Chemistry*, **2021**, 9, 678930	5	
1	Theoretical Calculations of the 242 nm Absorption of Propargyl Radical. *Journal of Physical Chemistry A*, **2021**, 125, 8595-8602	2.8	