Jir Pittner

List of Publications by Year in Descending Order

66 papers	2,397 citations	29 h-index	47 g-index
68 ext. papers	2,561 ext. citations	3.6 avg, IF	5.09 L-index

#	Paper	IF	Citations
66	Theoretical Investigation of the Effect of Alkylation and Bromination on Intersystem Crossing in BODIPY-Based Photosensitizers. *Journal of Physical Chemistry B*, **2021**, 125, 11617-11627	3.4	1
65	Variational quantum eigensolver for approximate diagonalization of downfolded Hamiltonians using generalized unitary coupled cluster ansatz. *Quantum Science and Technology*, **2021**, 6, 034008	5.5	7
64	Toward DMRG-tailored coupled cluster method in the 4c-relativistic domain. *Journal of Chemical Physics*, **2020**, 152, 174107	3.9	8
63	Near-Linear Scaling in DMRG-Based Tailored Coupled Clusters: An Implementation of DLPNO-TCCSD and DLPNO-TCCSD(T). *Journal of Chemical Theory and Computation*, **2020**, 16, 3028-3040	6.4	7
62	Ground state of the Fe(ii)-porphyrin model system corresponds to quintet: a DFT and DMRG-based tailored CC study. *Physical Chemistry Chemical Physics*, **2020**, 22, 17033-17037	3.6	10
61	Toward the efficient local tailored coupled cluster approximation and the peculiar case of oxo-Mn(Salen). *Journal of Chemical Physics*, **2019**, 151, 084112	3.9	11
60	Perturbative triples correction to domain-based local pair natural orbital variants of Mukherjee's state specific coupled cluster method. *Physical Chemistry Chemical Physics*, **2019**, 21, 5022-5038	3.6	7
59	Quantum information-based analysis of electron-deficient bonds. *Journal of Chemical Physics*, **2019**, 150, 204117	3.9	5
58	Photophysics of BODIPY-Based Photosensitizer for Photodynamic Therapy: Surface Hopping and Classical Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2019**, 15, 5046-5057	6.4	8
57	Numerical and Theoretical Aspects of the DMRG-TCC Method Exemplified by the Nitrogen Dimer. *Journal of Chemical Theory and Computation*, **2019**, 15, 2206-2220	6.4	25
56	Domain-Based Local Pair Natural Orbital Version of Mukherjee's State-Specific Coupled Cluster Method. *Journal of Chemical Theory and Computation*, **2018**, 14, 1370-1382	6.4	24
55	The Intricate Case of Tetramethyleneethane: A Full Configuration Interaction Quantum Monte Carlo Benchmark and Multireference Coupled Cluster Studies. *Journal of Chemical Theory and Computation*, **2018**, 14, 2439-2445	6.4	24
54	Orientation of Laurdan in Phospholipid Bilayers Influences Its Fluorescence: Quantum Mechanics and Classical Molecular Dynamics Study. *Molecules*, **2018**, 23,	4.8	12
53	An Isolated Molecule of Iron(II) Phthalocyanin Exhibits Quintet Ground-State: A Nexus between Theory and Experiment. *Chemistry - A European Journal*, **2018**, 24, 13413-13417	4.8	7
52	A new approach to molecular dynamics with non-adiabatic and spin-orbit effects with applications to QM/MM simulations of thiophene and selenophene. *Journal of Chemical Physics*, **2017**, 146, 114101	3.9	19
51	A MRCC study of the isomerisation of cyclopropane. *Molecular Physics*, **2017**, 115, 2743-2754	1.7	6
50	Quantum chemistry beyond Born□Oppenheimer approximation on a quantum computer: A simulated phase estimation study. *International Journal of Quantum Chemistry*, **2016**, 116, 1328-1336	2.1	21

49	Perturbative universal state-selective correction for state-specific multi-reference coupled cluster methods. *Journal of Chemical Physics*, **2016**, 145, 164106	3.9	6
48	Coupled Cluster Method with Single and Double Excitations Tailored by Matrix Product State Wave Functions. *Journal of Physical Chemistry Letters*, **2016**, 7, 4072-4078	6.4	59
47	A Local Pair Natural Orbital-Based Multireference Mukherjee's Coupled Cluster Method. *Journal of Chemical Theory and Computation*, **2015**, 11, 3104-14	6.4	53
46	Iterative universal state selective correction for the Brillouin-Wigner multireference coupled-cluster theory. *Journal of Chemical Physics*, **2015**, 142, 114106	3.9	5
45	Surface Hopping Dynamics with Correlated Single-Reference Methods: 9H-Adenine as a Case Study. *Journal of Chemical Theory and Computation*, **2014**, 10, 1395-405	6.4	139
44	Fluorescence of PRODAN in water: A computational QM/MM MD study. *Chemical Physics Letters*, **2014**, 597, 57-62	2.5	11
43	Quantum Computing Approach to Nonrelativistic and Relativistic Molecular Energy Calculations. *Advances in Chemical Physics*, **2014**, 107-136		2
42	Newton-X: a surface-hopping program for nonadiabatic molecular dynamics. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 26-33	7.9	280
41	Adiabatic state preparation study of methylene. *Journal of Chemical Physics*, **2014**, 140, 214111	3.9	30
40	Coupled Cluster Theories for Strongly Correlated Molecular Systems. *Springer Series in Solid-state Sciences*, **2013**, 237-271	0.4	2
39	Perturbative triples correction for explicitly correlated Mukherjee's state-specific coupled cluster method. *Molecular Physics*, **2013**, 111, 2477-2488	1.7	10
38	An explicitly correlated Mukherjee's state specific coupled cluster method: development and pilot applications. *Physical Chemistry Chemical Physics*, **2012**, 14, 4753-62	3.6	25
37	Parallel Implementation of Multireference Coupled-Cluster Theories Based on the Reference-Level Parallelism. *Journal of Chemical Theory and Computation*, **2012**, 8, 487-97	6.4	23
36	Towards large-scale calculations with State-Specific Multireference Coupled Cluster methods: Studies on dodecane, naphthynes, and polycarbenes. *Chemical Physics Letters*, **2012**, 542, 128-133	2.5	11
35	Relativistic quantum chemistry on quantum computers. *Physical Review A*, **2012**, 85,	2.6	25
34	Multireference coupled cluster study of the oxyallyl diradical. *Chemical Physics*, **2012**, 401, 203-207	2.3	12
33	Universal state-selective corrections to multi-reference coupled-cluster theories with single and double excitations. *Journal of Chemical Physics*, **2012**, 136, 124102	3.9	19
32	Communication: Application of state-specific multireference coupled cluster methods to core-level excitations. *Journal of Chemical Physics*, **2012**, 137, 171101	3.9	34

31	Surface hopping dynamics using a locally diabatic formalism: charge transfer in the ethylene dimer cation and excited state dynamics in the 2-pyridone dimer. *Journal of Chemical Physics*, **2012**, 137, 22A514	3.9	139
30	Implementation of the multireference Brillouin-Wigner and Mukherjee's coupled cluster methods with non-iterative triple excitations utilizing reference-level parallelism. *Journal of Chemical Physics* , **2012**, 137, 094112	3.9	16
29	Nonadiabatic molecular dynamics study of the cis-trans photoisomerization of azobenzene excited to the S1 state. *Journal of Physical Chemistry A*, **2011**, 115, 11136-43	2.8	97
28	Absorption and fluorescence of PRODAN in phospholipid bilayers: a combined quantum mechanics and classical molecular dynamics study. *Journal of Physical Chemistry A*, **2011**, 115, 11428-37	2.8	41
27	Multireference F12 coupled cluster theory: The Brillouin-Wigner approach with single and double excitations. *Chemical Physics Letters*, **2011**, 511, 418-423	2.5	29
26	Massively parallel implementation of the multireference Brillouin□Wigner CCSD method. *Chemical Physics Letters*, **2011**, 514, 347-351	2.5	21
25	Multireference state-specific Mukherjee's coupled cluster method with noniterative triexcitations using uncoupled approximation. *Journal of Chemical Physics*, **2011**, 134, 154106	3.9	43
24	Multireference Coupled-Cluster Methods: Recent Developments. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 455-489	0.7	33
23	Uncoupled multireference state-specific Mukherjee's coupled cluster method with triexcitations. *Journal of Chemical Physics*, **2010**, 133, 134106	3.9	29
22	Quantum computing applied to calculations of molecular energies: CH2 benchmark. *Journal of Chemical Physics*, **2010**, 133, 194106	3.9	41
21	Multireference Mukherjee's coupled cluster method with triexcitations in the linked formulation: Efficient implementation and applications. *Journal of Chemical Physics*, **2010**, 132, 154105	3.9	48
20	Non-adiabatic dynamics of pyrrole: Dependence of deactivation mechanisms on the excitation energy. *Chemical Physics*, **2010**, 375, 26-34	2.3	115
19	Multireference R12 Coupled Cluster Theory. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 251-266	0.7	9
18	Method of moments for the continuous transition between the Brillouin□Wigner-type and Rayleigh□Schr□dinger-type multireference coupled cluster theories. *Molecular Physics*, **2009**, 107, 1209-1221	1.7	34
17	Optimization of mixed quantum-classical dynamics: Time-derivative coupling terms and selected couplings. *Chemical Physics*, **2009**, 356, 147-152	2.3	90
16	Multireference state-specific Mukherjee's coupled cluster method with noniterative triexcitations. *Journal of Chemical Physics*, **2008**, 129, 184105	3.9	98
15	Multireference Brillouin-Wigner coupled cluster method with singles, doubles, and triples: efficient implementation and comparison with approximate approaches. *Journal of Chemical Physics*, **2008**, 128, 104108	3.9	59
14	Coupled Cluster Study of Polycyclopentanes: Structure and Properties of C5H2n, n = 0-4. *Collection of Czechoslovak Chemical Communications*, **2008**, 73, 1525-1551		15

13	Analytic gradient for the multireference Brillouin-Wigner coupled cluster method and for the state-universal multireference coupled cluster method. *Journal of Chemical Physics*, **2007**, 127, 114103	3.9	42
12	Multireference Brillouin-Wigner coupled clusters method with noniterative perturbative connected triples. *Journal of Chemical Physics*, **2006**, 124, 144112	3.9	71
11	Ab initio nonadiabatic dynamics study of ultrafast radiationless decay over conical intersections illustrated on the Na3F cluster. *Journal of Chemical Physics*, **2006**, 125, 24303	3.9	38
10	The singlet-triplet gap in trimethylenmethane and the ring-opening of methylenecyclopropane: a multireference Brillouin-Wigner coupled cluster study. *Journal of Physical Chemistry A*, **2006**, 110, 11765-9	2.8	48
9	Multiple pathways in the photodynamics of a polar bond: A case study of silaethylene. *Chemical Physics Letters*, **2006**, 418, 377-382	2.5	30
8	Multireference coupled cluster method based on the Brillouin-Wigner perturbation theory **2005**, 465-481		5
7	Multireference configuration interaction and coupled-cluster calculations on the X3a1and b1 states of the NF molecule. *International Journal of Quantum Chemistry*, **2005**, 104, 458-467	2.1	22
6	Towards the multireference Brillouin-Wigner coupled-clusters method with iterative connected triples: MR BWCCSDT-alpha approximation. *Journal of Chemical Physics*, **2005**, 122, 181101	3.9	50
5	Multireference BrillouinWigner Coupled Cluster Singles and Doubles Study of the SingletTriplet Separation in Alkylcarbenes*Journal of Physical Chemistry A*, **2004**, 108, 3125-3128	2.8	29
4	Multireference Brillouin-Wigner Coupled Cluster Singles and Doubles (MRBWCCSD) and Multireference Doubles Configuration Interaction (MRD-CI) Calculations for the Bergman Cyclization Reaction. *Collection of Czechoslovak Chemical Communications*, **2003**, 68, 2309-2321		24
3	Four- and 8-reference state-specific BrillouinWigner coupled-cluster method: Study of the singlet oxygen. *International Journal of Quantum Chemistry*, **2002**, 90, 1031-1037	2.1	38
2	State-Specific BrillouinWigner Multireference Coupled Cluster Study of the SingletTriplet Separation in the Tetramethyleneethane Diradical. *Journal of Physical Chemistry A*, **2001**, 105, 1354-1356	2.8	66
1	Four-Reference State-Specific Brillouin-Wigner Coupled-Cluster Method: Study of the IBr Molecule. *International Journal of Molecular Sciences*, **2001**, 2, 281-290	6.3	25