Jiri Brabec

List of Publications by Year
in descending order

33	768	516681 16	526264 27
papers	citations	h-index	g-index

36	36	36	978
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The Effect of Geometry, Spin, and Orbital Optimization in Achieving Accurate, Correlated Results for Ironâ€“Sulfur Cubanes. Journal of Chemical Theory and Computation, 2022, 18, 687-702.	5.3	10
2	Interplay between Ï€-Conjugation and Exchange Magnetism in One-Dimensional Porphyrinoid Polymers. Journal of the American Chemical Society, 2022, 144, 12725-12731.	13.7	15
3	On-Surface Synthesis and Characterization of [7]Triangulene Quantum Ring. Nano Letters, 2021, 21, 861-867.	9.1	59
4	Unravelling the Open-Shell Character of Peripentacene on Au(111). Journal of Physical Chemistry Letters, 2021, 12, 330-336.	4.6	36
5	On-Surface Strain-Driven Synthesis of Nonalternant Non-Benzenoid Aromatic Compounds Containing Four- to Eight-Membered Rings. Journal of the American Chemical Society, 2021, 143, 14694-14702.	13.7	31
6	Machine Learning-Assisted Selection of Active Spaces for Strongly Correlated Transition Metal Systems. Journal of Chemical Theory and Computation, 2021, 17, 6053-6072.	5.3	17
7	Massively parallel quantum chemical density matrix renormalization group method. Journal of Computational Chemistry, 2021, 42, 534-544.	3.3	34
8	On-Surface Hydrogenation of Buckybowls: From Curved Aromatic Molecules to Planar Non-KekulÃ© Aromatic Hydrocarbons. ACS Nano, 2020, 14, 16735-16742.	14.6	15
9	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.	5.3	11
10	Solving Coupled Cluster Equations by the Newton Krylov Method. Frontiers in Chemistry, 2020, 8, 590184.	3.6	6
11	Toward the efficient local tailored coupled cluster approximation and the peculiar case of oxo-Mn(Salen). Journal of Chemical Physics, 2019, 151, 084112.	3.0	12
12	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.	2.8	12
13	Numerical and Theoretical Aspects of the DMRG-TCC Method Exemplified by the Nitrogen Dimer. Journal of Chemical Theory and Computation, 2019, 15, 2206-2220.	5.3	36
14	Domain-Based Local Pair Natural Orbital Version of Mukherjeeâ€™s State-Specific Coupled Cluster Method. Journal of Chemical Theory and Computation, 2018, 14, 1370-1382.	5.3	29
15	Regularized and Renormalized Many-Body Techniques for Describing Correlated Molecular Systems: A Coupled-Cluster Perspective. Annual Reports in Computational Chemistry, 2018, 14, 3-45.	1.7	4
16	Chelation and stabilization of berkelium in oxidation state +IV. Nature Chemistry, 2017, 9, 843-849.	13.6	74
17	A MRCC study of the isomerisation of cyclopropane. Molecular Physics, 2017, 115, 2743-2754.	1.7	7
18	Efficient block preconditioned eigensolvers for linear response time-dependent density functional theory. Computer Physics Communications, 2017, 221, 42-52.	7.5	11

#	Article	IF	Citations
19	Reducedâ€cost sparsityâ€exploiting algorithm for solving coupledâ€cluster equations. Journal of Computational Chemistry, 2016, 37, 1059-1067.	3.3	5
20	Perturbative universal state-selective correction for state-specific multi-reference coupled cluster methods. Journal of Chemical Physics, 2016, 145, 164106.	3.0	6
21	Coupled Cluster Method with Single and Double Excitations Tailored by Matrix Product State Wave Functions. Journal of Physical Chemistry Letters, 2016, 7, 4072-4078.	4.6	74
22	Iterative universal state selective correction for the Brillouin-Wigner multireference coupled-cluster theory. Journal of Chemical Physics, 2015, 142, 114106.	3.0	6
23	Nonlinear Optical Properties of Fluorescent Dyes Allow for Accurate Determination of Their Molecular Orientations in Phospholipid Membranes. Journal of Physical Chemistry B, 2015, 119, 9706-9716.	2.6	10
24	Efficient Algorithms for Estimating the Absorption Spectrum within Linear Response TDDFT. Journal of Chemical Theory and Computation, 2015, 11, 5197-5208.	5.3	35
25	Fluorescence of PRODAN in water: A computational QM/MM MD study. Chemical Physics Letters, 2014, 597, 57-62.	2.6	14
26	Coupled Cluster Theories for Strongly Correlated Molecular Systems. Springer Series in Solid-state Sciences, 2013, , 237-271.	0.3	2
27	Universal state-selective corrections to multi-reference coupled-cluster theories with single and double excitations. Journal of Chemical Physics, 2012, 136, 124102.	3.0	21
28	Communication: Application of state-specific multireference coupled cluster methods to core-level excitations. Journal of Chemical Physics, 2012, 137, 171101.	3.0	42
29	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.	3.0	19
30	Parallel Implementation of Multireference Coupled-Cluster Theories Based on the Reference-Level Parallelism. Journal of Chemical Theory and Computation, 2012, 8, 487-497.	5.3	25
31	Towards large-scale calculations with State-Specific Multireference Coupled Cluster methods: Studies on dodecane, naphthynes, and polycarbenes. Chemical Physics Letters, 2012, 542, 128-133.	2.6	13
32	Massively parallel implementation of the multireference Brillouinâ€“Wigner CCSD method. Chemical Physics Letters, 2011, 514, 347-351.	2.6	22
33	The Singletâ^'Triplet Gap in Trimethylenmethane and the Ring-Opening of Methylenecyclopropane:â€‰ A Multireference Brillouinâ^'Wigner Coupled Cluster Study. Journal of Physical Chemistry A, 2006, 110, 11765-11769.	2.5	50