Katharina Boguslawski

List of Publications by Year
in descending order

38	1,497	331642 21	315719 38
papers	citations	h-index	g-index

43	43	43	882
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Assessing the Accuracy of Tailored Coupled Cluster Methods Corrected by Electronic Wave Functions of Polynomial Cost. Journal of Chemical Theory and Computation, 2022, 18, 96-117.	5.3	15
2	Orbital entanglement and correlation from pCCD-tailored coupled cluster wave functions. Journal of Chemical Physics, 2021, 154, 084111.	3.0	13
3	Pythonic Black-box Electronic Structure Tool (PyBEST). An open-source Python platform for electronic structure calculations at the interface between chemistry and physics. Computer Physics Communications, 2021, 264, 107933.	7.5	16
4	Open-shell extensions to closed-shell pCCD. Chemical Communications, 2021, 57, 12277-12280.	4.1	9
5	Mixed uranyl and neptunyl cationâ€“cation interaction-driven clusters: structures, energetic stability, and nuclear quadrupole interactions. Physical Chemistry Chemical Physics, 2020, 22, 10845-10852.	2.8	7
6	Assessing the accuracy of simplified coupled cluster methods for electronic excited states in f0 actinide compounds. Physical Chemistry Chemical Physics, 2019, 21, 19039-19053.	2.8	19
7	Elucidating cationâ€“cation interactions in neptunyl dications using multi-referenceab initiotheory. Physical Chemistry Chemical Physics, 2019, 21, 744-759.	2.8	12
8	Modeling the electronic structures of the ground and excited states of the ytterbium atom and the ytterbium dimer: A modern quantum chemistry perspective. International Journal of Quantum Chemistry, 2019, 119, e25983.	2.0	21
9	Benchmarking the Accuracy of Seniority-Zero Wave Function Methods for Noncovalent Interactions. Journal of Chemical Theory and Computation, 2019, 15, 4021-4035.	5.3	15
10	New Strategies in Modeling Electronic Structures and Properties with Applications to Actinides. Challenges and Advances in Computational Chemistry and Physics, 2019, , 121-160.	0.6	5
11	Targeting Doubly Excited States with Equation of Motion Coupled Cluster Theory Restricted to Double Excitations. Journal of Chemical Theory and Computation, 2019, 15, 18-24.	5.3	29
12	Relativistic Methods in Computational Quantum Chemistry. , 2017, , 885-926.		4
13	On the multi-reference nature of plutonium oxides: PuO22+, PuO2, PuO3 and PuO2(OH)2. Physical Chemistry Chemical Physics, 2017, 19, 4317-4329.	2.8	27
14	Benchmark of Dynamic Electron Correlation Models for Seniority-Zero Wave Functions and Their Application to Thermochemistry. Journal of Chemical Theory and Computation, 2017, 13, 5966-5983.	5.3	22
15	Targeting excited states in all-trans polyenes with electron-pair states. Journal of Chemical Physics, 2016, 145, 234105.	3.0	35
16	Analysis of two-orbital correlations in wave functions restricted to electron-pair states. Physical Review B, 2016, 94, .	3.2	27
17	Dissecting the cationâ€“cation interaction between two uranyl units. Physical Chemistry Chemical Physics, 2016, 18, 18305-18311.	2.8	14
18	Relativistic Methods in Computational Quantum Chemistry. , 2016, , 1-43.		2

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19	Dissecting the bond-formation process of d 10-metalâ€“ethene complexes with multireference approaches. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	14
20	A quantum informational approach for dissecting chemical reactions. Chemical Physics Letters, 2015, 621, 160-164.	2.6	28
21	Singlet ground state actinide chemistry with geminals. Physical Chemistry Chemical Physics, 2015, 17, 14427-14436.	2.8	35
22	The effect of nitrido, azide, and nitrosyl ligands on magnetization densities and magnetic properties of iridium PNP pincer-type complexes. RSC Advances, 2015, 5, 84311-84320.	3.6	1
23	Linearized Coupled Cluster Correction on the Antisymmetric Product of 1-Reference Orbital Geminals. Journal of Chemical Theory and Computation, 2015, 11, 5252-5261.	5.3	48
24	Selection of active spaces for multiconfigurational wavefunctions. Journal of Chemical Physics, 2015, 142, 244104.	3.0	84
25	Orbital entanglement in quantum chemistry. International Journal of Quantum Chemistry, 2015, 115, 1289-1295.	2.0	71
26	Projected seniority-two orbital optimization of the antisymmetric product of one-reference orbital geminal. Journal of Chemical Physics, 2014, 140, 214114.	3.0	68
27	Efficient description of strongly correlated electrons with mean-field cost. Physical Review B, 2014, 89, .	3.2	95
28	Unravelling the quantum-entanglement effect of noble gas coordination on the spin ground state of CUO. Physical Chemistry Chemical Physics, 2014, 16, 719-727.	2.8	46
29	Nonvariational Orbital Optimization Techniques for the AP1roG Wave Function. Journal of Chemical Theory and Computation, 2014, 10, 4873-4882.	5.3	59
30	Quantum entanglement in carbonâ€“carbon, carbonâ€“phosphorus and siliconâ€“silicon bonds. Physical Chemistry Chemical Physics, 2014, 16, 8872-8880.	2.8	39
31	Assessing the Accuracy of New Geminal-Based Approaches. Journal of Physical Chemistry A, 2014, 118, 9058-9068.	2.5	77
32	Optimized unrestricted Kohnâ€“Sham potentials from ab initio spin densities. Journal of Chemical Physics, 2013, 138, 044111.	3.0	25
33	Orbital Entanglement in Bond-Formation Processes. Journal of Chemical Theory and Computation, 2013, 9, 2959-2973.	5.3	98
34	Entanglement Measures for Single- and Multireference Correlation Effects. Journal of Physical Chemistry Letters, 2012, 3, 3129-3135.	4.6	143
35	Accurate ab Initio Spin Densities. Journal of Chemical Theory and Computation, 2012, 8, 1970-1982.	5.3	79
36	A Refined, Efficient Mean Solvation Force Model that Includes the Interior Volume Contribution. Journal of Physical Chemistry B, 2011, 115, 4547-4557.	2.6	14

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37	Can DFT Accurately Predict Spin Densities? Analysis of Discrepancies in Iron Nitrosyl Complexes. Journal of Chemical Theory and Computation, 2011, 7, 2740-2752.	5.3	96
38	Construction of CASCI-type wave functions for very large active spaces. Journal of Chemical Physics, 2011, 134, 224101.	3.0	46