Kurt R Glaesemann

List of Publications by Year
in descending order

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22	863	759233 12	752698 20
papers	citations	h-index	g-index

27	27	27	930
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Further developments in the local-orbital density-functional-theory tight-binding method. Physical Review B, 2001, 64, .	3.2	232
2	A transient semimetallic layer in detonating nitromethane. Nature Physics, 2008, 4, 72-76.	16.7	139
3	A natural orbital diagnostic for multiconfigurational character in correlated wave functions. Journal of Chemical Physics, 1999, 110, 4199-4207.	3.0	90
4	Ab Initio Calculations of Reactive Pathways for Î±-Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (Î±-HMX). Journal of Physical Chemistry A, 2000, 104, 11384-11389.	2.5	82
5	On the Ordering of Orbital Energies in High-Spin ROHF^{â€}. Journal of Physical Chemistry A, 2010, 114, 8772-8777.	2.5	40
6	A study of FeCO+ with correlated wavefunctions. Physical Chemistry Chemical Physics, 1999, 1, 967-975.	2.8	31
7	An improved thermodynamic energy estimator for path integral simulations. Journal of Chemical Physics, 2002, 116, 5951-5955.	3.0	31
8	Improved heat capacity estimator for path integral simulations. Journal of Chemical Physics, 2002, 117, 3020-3026.	3.0	31
9	A path integral approach to molecular thermochemistry. Journal of Chemical Physics, 2003, 118, 1596-1603.	3.0	23
10	Investigation of a grid-free density functional theory (DFT) approach. Journal of Chemical Physics, 1998, 108, 9959-9969.	3.0	20
11	EOMCC, MRPT, and TDDFT Studies of Charge Transfer Processes in Mixed-Valence Compounds: Application to the Spiro Molecule^{â€}. Journal of Physical Chemistry A, 2010, 114, 8764-8771.	2.5	20
12	Massively parallel linear-scaling algorithm in an ab initio local-orbital total-energy method. Journal of Computational Physics, 2003, 188, 1-15.	3.8	12
13	Quantitative molecular thermochemistry based on path integrals. Journal of Chemical Physics, 2005, 123, 034103.	3.0	12
14	Auxiliary basis sets for grid-free density functional theory. Journal of Chemical Physics, 2000, 112, 10738-10745.	3.0	11
15	Free Energies for Degradation Reactions of 1,2,3-Trichloropropane from ab Initio Electronic Structure Theory. Journal of Physical Chemistry A, 2010, 114, 12269-12282.	2.5	10
16	Sub-second state estimation implementation and its evaluation with real data. , 2015, , .		9
17	Integrated State Estimation and Contingency Analysis Software Implementation using High Performance Computing Techniques. IFAC-PapersOnLine, 2015, 48, 227-232.	0.9	7
18	Evaluation of gradient corrections in grid-free density functional theory. Journal of Chemical Physics, 1999, 110, 6580-6582.	3.0	6

#	Article	IF	Citations
19	Improved woodâ€“kirkwood detonation chemical kinetics. Theoretical Chemistry Accounts, 2008, 120, 37-43.	1.4	4
20	Contingency Analysis Post-Processing With Advanced Computing and Visualization. IFAC-PapersOnLine, 2017, 50, 55-60.	0.9	3
21	A TRANSIENT SEMI-METALLIC LAYER IN DETONATING NITROMETHANE. , 2008, , .		1
22	Aiding Cascading Analysis Modelling with High-performance-computing Technology. IFAC-PapersOnLine, 2018, 51, 639-644.	0.9	1