Milica Feldt

List of Publications by Year
in descending order

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29	1,047	516710 16	454955 30
papers	citations	h-index	g-index

31	31	31	1223
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Mild Câ^'H/Câ^'C Activation by Zâ€Selective Cobalt Catalysis. Angewandte Chemie - International Edition, 2016, 55, 7408-7412.	13.8	166
2	Cobalt(III)-Catalyzed Hydroarylation of Allenes via Câ€“H Activation. ACS Catalysis, 2017, 7, 2511-2515.	11.2	107
3	Manganese(I)â€Catalyzed Dispersionâ€Enabled Câ^'H/Câ^'C Activation. Chemistry - A European Journal, 2017, 23, 5443-5447.	3.3	98
4	Toward Highly Accurate Spin State Energetics in First-Row Transition Metal Complexes: A Combined CASPT2/CC Approach. Journal of Chemical Theory and Computation, 2018, 14, 2446-2455.	5.3	95
5	Synergistic Heterobimetallic Manifold for Expedient Manganese(I)â€Catalyzed Câ^'H Cyanation. Chemistry - A European Journal, 2016, 22, 17958-17961.	3.3	75
6	Free-energy perturbation and quantum mechanical study of SAMPL4 octa-acid hostâ€“guest binding energies. Journal of Computer-Aided Molecular Design, 2014, 28, 375-400.	2.9	70
7	Mild Câ^'H/Câ^'C Activation by Zâ€Selective Cobalt Catalysis. Angewandte Chemie, 2016, 128, 7534-7538.	2.0	52
8	Limits of Coupled-Cluster Calculations for Non-Heme Iron Complexes. Journal of Chemical Theory and Computation, 2019, 15, 922-937.	5.3	51
9	Online conferences â€“ Towards a new (virtual) reality. Computational and Theoretical Chemistry, 2020, 1189, 112975.	2.5	42
10	Study of ligand effects in aurophilic interactions using local correlation methods. Physical Chemistry Chemical Physics, 2013, 15, 18115.	2.8	37
11	Ab Initio Calculations for Spin-Gaps of Non-Heme Iron Complexes. Journal of Chemical Theory and Computation, 2019, 15, 4297-4304.	5.3	31
12	All That Binds Is Not Goldâ€”The Relative Weight of Aurophilic Interactions in Complex Formation. Journal of Physical Chemistry A, 2018, 122, 6918-6925.	2.5	26
13	A quantum-mechanical study of the reaction mechanism of sulfite oxidase. Journal of Biological Inorganic Chemistry, 2014, 19, 1165-1179.	2.6	23
14	A Computational Comparison of Oxygen Atom Transfer Catalyzed by Dimethyl SulfÂoxide Reductase with Mo and W. European Journal of Inorganic Chemistry, 2015, 2015, 3580-3589.	2.0	23
15	QM/MM study of the reaction mechanism of sulfite oxidase. Scientific Reports, 2018, 8, 4684.	3.3	22
16	Coupledâ€Cluster Interaction Energies for 200â€Atom Hostâ€“Guest Systems. ChemPhysChem, 2014, 15, 3270-3281.	2.1	18
17	Energetics of non-heme iron reactivity: can ab initio calculations provide the right answer?. Physical Chemistry Chemical Physics, 2020, 22, 23908-23919.	2.8	16
18	Ab Initio Methods in Firstâ€Row Transition Metal Chemistry. European Journal of Inorganic Chemistry, 2022, 2022, .	2.0	14

#	Article	IF	Citations
19	Modelling absorption and emission of a meso-anilineâ€“BODIPY based dye with molecular mechanics. Physical Chemistry Chemical Physics, 2018, 20, 14537-14544.	2.8	11
20	Cycloadditions with a Stable Chargeâ€Separated Cyclobutadieneâ€Type Amidoâ€Substituted Silicon Ring Compound. Angewandte Chemie - International Edition, 2021, 60, 21761-21766.	13.8	11
21	Local Hybrid QM/QM Calculations of Reaction Pathways in Metallobiosites. Journal of Chemical Theory and Computation, 2014, 10, 5397-5404.	5.3	10
22	Reactivity of the Bicyclic Amidoâ€Substituted Silicon(I) Ring Compound Si₄{N(SiMe₃)Mes}₄ with FLPâ€Type Character. Chemistry - A European Journal, 2021, 27, 17361-17368.	3.3	10
23	Assessment of local coupled cluster methods for excited states of <scp>BODIPY</scp>/<scp>Azaâ€BODIPY</scp> families. Journal of Computational Chemistry, 2021, 42, 144-155.	3.3	9
24	Oxophosphonium-alkyne cycloaddition reactions: reversible formation of 1,2-oxaphosphetes and six-membered phosphorus heterocycles. Journal of the American Chemical Society, 2020, 142, 9818-9826.	13.7	8
25	Hybrid Local Molecular Orbital: Molecular Orbital Calculations for Open Shell Systems. Journal of Chemical Theory and Computation, 2018, 14, 5192-5202.	5.3	6
26	Reactivity of an NHC-Coordinated Trisilacyclopropylidene with Transition Metal Carbonyl Compounds. Organometallics, 2020, 39, 4387-4394.	2.3	6
27	Cycloadditionen mit einer stabilen ladungsseparierten cyclobutadienartigen Siliciumringverbindung. Angewandte Chemie, 2021, 133, 21929-21934.	2.0	3
28	Thiophosphoniumâ€“Alkyne Cycloaddition Reactions: A Heavy Congener of the Carbonylâ€“Alkyne Metathesis. Inorganic Chemistry, 2021, 60, 14509-14514.	4.0	3
29	CHAPTER 7. Computational Studies of Molybdenum and Tungsten Enzymes. 2-Oxoglutarate-Dependent Oxygenases, 2016, , 275-321.	0.8	3