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	Ab Initio Methods in Firstâ€Row Transition Metal Chemistry. European Journal of Inorganic Chemistry, 2022, 2022, .	2.0	14
2	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
3	Cycloadditions with a Stable Chargeâ€Separated Cyclobutadieneâ€Type Amidoâ€Substituted Silicon Ring Compound. Angewandte Chemie - International Edition, 2021, 60, 21761-21766.	13.8	11
4	Cycloadditionen mit einer stabilen ladungsseparierten cyclobutadienartigen Siliciumringverbindung. Angewandte Chemie, 2021, 133, 21929-21934.	2.0	3
5	Thiophosphoniumâ€“Alkyne Cycloaddition Reactions: A Heavy Congener of the Carbonylâ€“Alkyne Metathesis. Inorganic Chemistry, 2021, 60, 14509-14514.	4.0	3
6	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
7	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
8	Reactivity of an NHC-Coordinated Trisilacyclopropylidene with Transition Metal Carbonyl Compounds. Organometallics, 2020, 39, 4387-4394.	2.3	6
9	Online conferences â€“ Towards a new (virtual) reality. Computational and Theoretical Chemistry, 2020, 1189, 112975.	2.5	42
10	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
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	Limits of Coupled-Cluster Calculations for Non-Heme Iron Complexes. Journal of Chemical Theory and Computation, 2019, 15, 922-937.	5.3	51
13	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
14	QM/MM study of the reaction mechanism of sulfite oxidase. Scientific Reports, 2018, 8, 4684.	3.3	22
15	Hybrid Local Molecular Orbital: Molecular Orbital Calculations for Open Shell Systems. Journal of Chemical Theory and Computation, 2018, 14, 5192-5202.	5.3	6
16	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
17	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
18	Cobalt(III)-Catalyzed Hydroarylation of Allenes via Câ€“H Activation. ACS Catalysis, 2017, 7, 2511-2515.	11.2	107

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19	Manganese(I)â€Catalyzed Dispersionâ€Enabled Câ^'H/Câ^'C Activation. Chemistry - A European Journal, 2017, 23, 5443-5447.	3.3	98
20	Mild Câ^'H/Câ^'C Activation by Zâ€Selective Cobalt Catalysis. Angewandte Chemie - International Edition, 2016, 55, 7408-7412.	13.8	166
21	Mild Câ^'H/Câ^'C Activation by Zâ€Selective Cobalt Catalysis. Angewandte Chemie, 2016, 128, 7534-7538.	2.0	52
22	Synergistic Heterobimetallic Manifold for Expedient Manganese(I)â€Catalyzed Câ^'H Cyanation. Chemistry - A European Journal, 2016, 22, 17958-17961.	3.3	75
23	CHAPTER 7. Computational Studies of Molybdenum and Tungsten Enzymes. 2-Oxoglutarate-Dependent Oxygenases, 2016, , 275-321.	0.8	3
24	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
25	Local Hybrid QM/QM Calculations of Reaction Pathways in Metallobiosites. Journal of Chemical Theory and Computation, 2014, 10, 5397-5404.	5.3	10
26	Coupledâ€Cluster Interaction Energies for 200â€Atom Hostâ€“Guest Systems. ChemPhysChem, 2014, 15, 3270-3281.	2.1	18
27	A quantum-mechanical study of the reaction mechanism of sulfite oxidase. Journal of Biological Inorganic Chemistry, 2014, 19, 1165-1179.	2.6	23
28	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
29	Study of ligand effects in aurophilic interactions using local correlation methods. Physical Chemistry Chemical Physics, 2013, 15, 18115.	2.8	37