Steen Lysgaard

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/3369000/publications.pdf

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16	2,345	840585 11	1058333 14
papers	citations	h-index	g-index

23	23	23	4036
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The atomic simulation environmentâ€”a Python library for working with atoms. Journal of Physics Condensed Matter, 2017, 29, 273002.	0.7	1,933
2	Genetic algorithms for computational materials discovery accelerated by machine learning. Npj Computational Materials, 2019, 5, .	3.5	136
3	A DFT-based genetic algorithm search for AuCu nanoalloy electrocatalysts for CO₂ reduction. Physical Chemistry Chemical Physics, 2015, 17, 28270-28276.	1.3	65
4	Resolving the stability and structure of strontium chloride amines from equilibrium pressures, XRD and DFT. International Journal of Hydrogen Energy, 2012, 37, 18927-18936.	3.8	37
5	Genetic Algorithm Procreation Operators for Alloy Nanoparticle Catalysts. Topics in Catalysis, 2014, 57, 33-39.	1.3	27
6	Decoupling strain and ligand effects in ternary nanoparticles for improved ORR electrocatalysis. Physical Chemistry Chemical Physics, 2016, 18, 24737-24745.	1.3	26
7	Vertical charge-carrier transport in Si nanocrystal/SiO₂multilayer structures. Nanotechnology, 2009, 20, 195201.	1.3	24
8	Designing mixed metal halide ammines for ammonia storage using density functional theory and genetic algorithms. Physical Chemistry Chemical Physics, 2014, 16, 19732-19740.	1.3	24
9	Combined DFT and Differential Electrochemical Mass Spectrometry Investigation of the Effect of Dopants in Secondary Zincâ€“Air Batteries. ChemSusChem, 2018, 11, 1933-1941.	3.6	23
10	Accelerated DFT-Based Design of Materials for Ammonia Storage. Chemistry of Materials, 2015, 27, 4552-4561.	3.2	18
11	Surface adsorption in strontium chloride ammines. Journal of Chemical Physics, 2013, 138, 164701.	1.2	15
12	Unfolding the structural stability of nanoalloys via symmetry-constrained genetic algorithm and neural network potential. Npj Computational Materials, 2022, 8, .	3.5	9
13	Ab initio Molecular Dynamics Investigations of the Speciation and Reactivity of Deep Eutectic Electrolytes in Aluminum Batteries. ChemSusChem, 2021, 14, 2034-2041.	3.6	6
14	Charge Transport in Al₂S₃ and Its Relevance in Secondary Alâ€“S Batteries. Journal of Physical Chemistry C, 2021, 125, 16444-16450.	1.5	2
15	Computational Design of Catalysts, Electrolytes, and Materials for Energy Storage. , 2013, , 499-521.		0
16	Ab initio Molecular Dynamics Investigations of the Speciation and Reactivity of Deep Eutectic Electrolytes in Aluminum Batteries. ChemSusChem, 2021, 14, 1973-1973.	3.6	0