

Steen Lysgaard

List of Publications by Year in descending order

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Version: 2024-02-01

16
papers

2,345
citations

840585

11
h-index

1058333

14
g-index

23
all docs

23
docs citations

23
times ranked

4036
citing authors

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