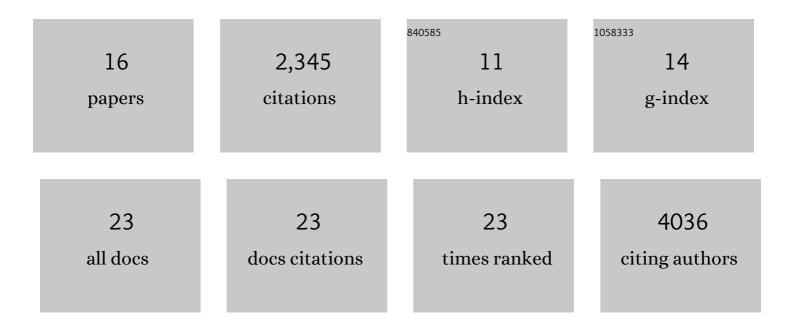
Steen Lysgaard

List of Publications by Year in descending order

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| # | Article | IF | CITATIONS |
|----|--|-----|-----------|
| 1 | The atomic simulation environment—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 CO ₂ 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/SiO ₂ multilayer 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 Zinc–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 Al ₂ S ₃ and Its Relevance in Secondary Al–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 |