Christoph Scheurer

List of Publications by Year
in descending order

31	614	623734	610901
papers	citations	14 h-index	24 g-index

34	34	34	1024
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A model-free sparse approximation approach to robust formal reaction kinetics. Chemical Engineering Journal, 2022, 433, 134121.	12.7	1
2	Epitaxial Coreâ€Shell Oxide Nanoparticles: Firstâ€Principles Evidence for Increased Activity and Stability of Rutile Catalysts for Acidic Oxygen Evolution. ChemSusChem, 2022, 15, .	6.8	7
3	DFTB Modeling of Lithium-Intercalated Graphite with Machine-Learned Repulsive Potential. Journal of Physical Chemistry A, 2021, 125, 691-699.	2.5	11
4	Revised Atomic Charges for OPLS Force Field Model of Poly(Ethylene Oxide): Benchmarks and Applications in Polymer Electrolyte. Polymers, 2021, 13, 1131.	4.5	18
5	True Nature of the Transition-Metal Carbide/Liquid Interface Determines Its Reactivity. ACS Catalysis, 2021, 11, 4920-4928.	11.2	25
6	Nanoâ€Scale Complexions Facilitate Li Dendriteâ€Free Operation in LATP Solidâ€State Electrolyte. Advanced Energy Materials, 2021, 11, 2100707.	19.5	36
7	Complexions at the Electrolyte/Electrode Interface in Solid Oxide Cells. Advanced Materials Interfaces, 2021, 8, 2100967.	3.7	8
8	Polaron-Assisted Charge Transport in Li-Ion Battery Anode Materials. ACS Applied Energy Materials, 2021, 4, 8583-8591.	5.1	4
9	Accessing Structural, Electronic, Transport and Mesoscale Properties of Li-GICs via a Complete DFTB Model with Machine-Learned Repulsion Potential. Materials, 2021, 14, 6633.	2.9	4
10	On the Role of Long-Range Electrostatics in Machine-Learned Interatomic Potentials for Complex Battery Materials. ACS Applied Energy Materials, 2021, 4, 12562-12569.	5.1	22
11	Data-efficient iterative training of Gaussian approximation potentials: Application to surface structure determination of rutile IrO2 and RuO2. Journal of Chemical Physics, 2021, 155, 244107.	3.0	16
12	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>IrO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Surface Complexions Identified through Machine Learning and Surface Investigations. Physical Review Letters, 2020, 125, 206101.	7.8	32
13	Formation and stability of small polarons at the lithium-terminated Li4Ti5O12 (LTO) (111) surface. Journal of Chemical Physics, 2020, 153, 144701.	3.0	7
14	Interface between graphene and liquid Cu from molecular dynamics simulations. Journal of Chemical Physics, 2020, 153, 074702.	3.0	8
15	Mobile Small Polarons Qualitatively Explain Conductivity in Lithium Titanium Oxide Battery Electrodes. Journal of Physical Chemistry Letters, 2020, 11, 2535-2540.	4.6	11
16	Benefits from using mixed precision computations in the ELPA-AEO and ESSEX-II eigensolver projects. Japan Journal of Industrial and Applied Mathematics, 2019, 36, 699-717.	0.9	10
17	Ab Initio Thermodynamics Insight into the Structural Evolution of Working IrO₂ Catalysts in Proton-Exchange Membrane Electrolyzers. ACS Catalysis, 2019, 9, 4944-4950.	11.2	43
18	Oxygen Evolution Catalysis: Ruthenium Oxide Nanosheets for Enhanced Oxygen Evolution Catalysis in Acidic Medium (Adv. Energy Mater. 15/2019). Advanced Energy Materials, 2019, 9, 1970048.	19.5	4

#	Article	IF	Citations
19	Multi-ion Conduction in Li₃OCl Glass Electrolytes. Journal of Physical Chemistry Letters, 2019, 10, 2264-2269.	4.6	38
20	Ruthenium Oxide Nanosheets for Enhanced Oxygen Evolution Catalysis in Acidic Medium. Advanced Energy Materials, 2019, 9, 1803795.	19.5	147
21	Addressing global uncertainty and sensitivity in first-principles based microkinetic models by an adaptive sparse grid approach. Journal of Chemical Physics, 2018, 148, 034102.	3.0	23
22	Benchmarks and Dielectric Constants for Reparametrized OPLS and Polarizable Force Field Models of Chlorinated Hydrocarbons. Journal of Physical Chemistry B, 2018, 122, 770-779.	2.6	12
23	Ab InitioSimulation of pH-Sensitive Biomarkers in Magnetic Resonance Imaging. Journal of Physical Chemistry A, 2018, 122, 7983-7990.	2.5	0
24	Response properties at the dynamic water/dichloroethane liquidâ€“liquid interface. Molecular Physics, 2018, 116, 3409-3416.	1.7	6
25	Implications of Occupational Disorder on Ion Mobility in Li₄Ti₅O₁₂ Battery Materials. Nano Letters, 2017, 17, 3884-3888.	9.1	35
26	Deuteration of Hyperpolarized 13 C-Labeled Zymonic Acid Enables Sensitivity-Enhanced Dynamic MRI of pH. ChemPhysChem, 2017, 18, 2421-2421.	2.1	1
27	Efficient Implicit Solvation Method for Full Potential DFT. Journal of Chemical Theory and Computation, 2017, 13, 5582-5603.	5.3	30
28	Deuteration of Hyperpolarized ¹³Câ€Labeled Zymonic Acid Enables Sensitivityâ€Enhanced Dynamic MRI of pH. ChemPhysChem, 2017, 18, 2422-2425.	2.1	20
29	The adaptive hierarchical expansion of the kinetic energy operator. Journal of Computational Chemistry, 2013, 34, 1210-1217.	3.3	4
30	Configuration space partitioning and matrix buildup scaling for the vibrational configuration interaction method. Journal of Computational Chemistry, 2013, 34, 27-37.	3.3	16
31	2D Infrared Chemical Exchange Spectroscopy of Ultrafast Isomerizations. ChemPhysChem, 2007, 8, 503-505.	2.1	15