Nils Edvin Richard Zimmermann

List of Publications by Year
in descending order

21 papers	1,501 citations	516710 16 h-index	752698 20 g-index
29 all docs	29 docs citations	29 times ranked	2015 citing authors

#	Article	IF	Citations
1	Matminer: An open source toolkit for materials data mining. Computational Materials Science, 2018, 152, 60-69.	3.0	446
2	Nucleation of NaCl from Aqueous Solution: Critical Sizes, Ion-Attachment Kinetics, and Rates. Journal of the American Chemical Society, 2015, 137, 13352-13361.	13.7	151
3	PyCDT: A Python toolkit for modeling point defects in semiconductors and insulators. Computer Physics Communications, 2018, 226, 165-179.	7.5	142
4	Path Sampling Calculation of Methane Diffusivity in Natural Gas Hydrates from a Water-Vacancy Assisted Mechanism. Journal of the American Chemical Society, 2008, 130, 17342-17350.	13.7	124
5	Transport in Nanoporous Materials Including MOFs: The Applicability of Fickâ€™s Laws. Angewandte Chemie - International Edition, 2015, 54, 14580-14583.	13.8	90
6	NaCl nucleation from brine in seeded simulations: Sources of uncertainty in rate estimates. Journal of Chemical Physics, 2018, 148, 222838.	3.0	62
7	In-Depth Study of the Influence of Hostâ^'Framework Flexibility on the Diffusion of Small Gas Molecules in One-Dimensional Zeolitic Pore Systems. Journal of Physical Chemistry C, 2007, 111, 17370-17381.	3.1	59
8	Local structure order parameters and site fingerprints for quantification of coordination environment and crystal structure similarity. RSC Advances, 2020, 10, 6063-6081.	3.6	57
9	Assessing Local Structure Motifs Using Order Parameters for Motif Recognition, Interstitial Identification, and Diffusion Path Characterization. Frontiers in Materials, 2017, 4, .	2.4	54
10	Surface Barriers of Hydrocarbon Transport Triggered by Ideal Zeolite Structures. Journal of Physical Chemistry C, 2012, 116, 3677-3683.	3.1	46
11	Transport into Nanosheets: Diffusion Equations Put to Test. Journal of Physical Chemistry C, 2013, 117, 7384-7390.	3.1	43
12	On the Effects of the External Surface on the Equilibrium Transport in Zeolite Crystals. Journal of Physical Chemistry C, 2010, 114, 300-310.	3.1	42
13	History and Utility of Zeolite Framework-Type Discovery from a Data-Science Perspective. Crystal Growth and Design, 2016, 16, 3043-3048.	3.0	41
14	Predicting Local Transport Coefficients at Solidâ€“Gas Interfaces. Journal of Physical Chemistry C, 2012, 116, 18878-18883.	3.1	37
15	Benchmarking Coordination Number Prediction Algorithms on Inorganic Crystal Structures. Inorganic Chemistry, 2021, 60, 1590-1603.	4.0	31
16	Electrostatic Estimation of Intercalant Jump-Diffusion Barriers Using Finite-Size Ion Models. Journal of Physical Chemistry Letters, 2018, 9, 628-634.	4.6	16
17	The Materials Project: Accelerating Materials Design Through Theory-Driven Data and Tools. , 2020, , 1751-1784.		14
18	Adsorption and diffusion in zeolites: the pitfall of isotypic crystal structures. Molecular Simulation, 2011, 37, 986-989.	2.0	13

#	Article	IF	Citations
19	High-throughput assessment of hypothetical zeolite materials for their synthesizeability and industrial deployability. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 437-450.	0.8	12
20	The Materials Project: Accelerating Materials Design Through Theory-Driven Data and Tools. , 2018, , 1-34.		11
21	Quantifying local coordination environment and structural similarity through order parameter-based site fingerprints and their application to machine learning. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, a209-a209.	0.1	0