Daniel Schwalbe-Koda

List of Publications by Year
in descending order

19 papers	638 citations	687363 13 h-index	839539 18 g-index
24 all docs	24 docs citations	24 times ranked	691 citing authors

#	Article	IF	Citations
1	Learning Matter: Materials Design with Machine Learning and Atomistic Simulations. Accounts of Materials Research, 2022, 3, 343-357.	11.7	31
2	Sampling lattices in semi-grand canonical ensemble with autoregressive machine learning. Npj Computational Materials, 2022, 8, .	8.7	3
3	Tunable CHA/AEI Zeolite Intergrowths with A Priori Biselective Organic Structureâ€Directing Agents: Controlling Enrichment and Implications for Selective Catalytic Reduction of NOx. Angewandte Chemie - International Edition, 2022, 61, .	13.8	18
4	Repurposing Templates for Zeolite Synthesis from Simulations and Data Mining. Chemistry of Materials, 2022, 34, 5366-5376.	6.7	5
5	Supramolecular Recognition in Crystalline Nanocavities through Monte Carlo and Voronoi Network Algorithms. Journal of Physical Chemistry C, 2021, 125, 3009-3017.	3.1	15
6	Active learning accelerates ab initio molecular dynamics on reactive energy surfaces. CheM, 2021, 7, 738-751.	11.7	42
7	Discovering Relationships between OSDAs and Zeolites through Data Mining and Generative Neural Networks. ACS Central Science, 2021, 7, 858-867.	11.3	57
8	Benchmarking binding energy calculations for organic structure-directing agents in pure-silica zeolites. Journal of Chemical Physics, 2021, 154, 174109.	3.0	26
9	Differentiable sampling of molecular geometries with uncertainty-based adversarial attacks. Nature Communications, 2021, 12, 5104.	12.8	34
10	A priori control of zeolite phase competition and intergrowth with high-throughput simulations. Science, 2021, 374, 308-315.	12.6	90
11	Data-Driven Design of Biselective Templates for Intergrowth Zeolites. Journal of Physical Chemistry Letters, 2021, 12, 10689-10694.	4.6	12
12	Temperature-transferable coarse-graining of ionic liquids with dual graph convolutional neural networks. Journal of Chemical Physics, 2020, 153, 164501.	3.0	35
13	Generative Models for Automatic Chemical Design. Lecture Notes in Physics, 2020, , 445-467.	0.7	42
14	Graph similarity drives zeolite diffusionless transformations and intergrowth. Nature Materials, 2019, 18, 1177-1181.	27.5	54
15	Tuning Electronic Properties and Band Alignments of Phosphorene Combined With MoSe₂ and WSe₂. Journal of Physical Chemistry C, 2017, 121, 3862-3869.	3.1	55
16	Deposition of topological silicene, germanene and stanene on graphene-covered SiC substrates. Scientific Reports, 2017, 7, 15700.	3.3	36
17	Coincidence Lattices and Interlayer Twist in van der Waals Heterostructures: Application of the Coincidence Lattice Method on $$hbox {hBN/MoSe}_2$$ hBN/MoSe 2 Heterobilayer Systems. Journal of Electronic Materials, 2017, 46, 3910-3916.	2.2	9
18	Coincidence Lattices of 2D Crystals: Heterostructure Predictions and Applications. Journal of Physical Chemistry C, 2016, 120, 10895-10908.	3.1	68

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19	Tunable CHA/AEI Zeolite Intergrowths with A Priori Biselective Organic Structureâ€Directing Agents: Controlling Enrichment and Implications for Selective Catalytic Reduction of NOx. Angewandte Chemie, 0, , .	2.0	1