# Daniel Schwalbe-Koda

List of Publications by Year
in descending order



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

| # | Article | IF | Citations |
|---|---|---|---|
| 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 |