Shyam S Dwaraknath

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Improving machine learning performance on small chemical reaction data with unsupervised contrastive pretraining. Chemical Science, 2022, 13, 1446-1458.	7.4	17
2	Performance comparison of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"> <mml:msup> <mml:mrow> <mml:mi>r</mml:mi> and SCAN metaGGA density functionals for solid materials via an automated, high-throughput computational workflow. Physical Review Materials, 2022, 6, .</mml:mrow></mml:msup></mml:math 	mrow> <mn 2.4</mn 	nl:mŋ>2
3	Convergence acceleration in machine learning potentials for atomistic simulations. , 2022, 1, 61-69.		18
4	Toward a Mechanistic Model of Solid–Electrolyte Interphase Formation and Evolution in Lithium-Ion Batteries. ACS Energy Letters, 2022, 7, 1446-1453.	17.4	46
5	Reaction Selectivity in Cometathesis: Yttrium Manganese Oxides. Chemistry of Materials, 2022, 34, 4694-4702.	6.7	4
6	Rapid generation of optimal generalized Monkhorst-Pack grids. Computational Materials Science, 2021, 187, 110100.	3.0	25
7	A chemically consistent graph architecture for massive reaction networks applied to solid-electrolyte interphase formation. Chemical Science, 2021, 12, 4931-4939.	7.4	36
8	Lowering Ternary Oxide Synthesis Temperatures by Solid-State Cometathesis Reactions. Chemistry of Materials, 2021, 33, 3692-3701.	6.7	14
9	A graph-based network for predicting chemical reaction pathways in solid-state materials synthesis. Nature Communications, 2021, 12, 3097.	12.8	44
10	Database of ab initio L-edge X-ray absorption near edge structure. Scientific Data, 2021, 8, 153.	5.3	21
11	Quantum chemical calculations of lithium-ion battery electrolyte and interphase species. Scientific Data, 2021, 8, 203.	5.3	19
12	Effective Local Geometry Descriptor for 29Si NMR Q4 Anisotropy. Journal of Physical Chemistry C, 2021, 125, 19481-19488.	3.1	3
13	OPTIMADE, an API for exchanging materials data. Scientific Data, 2021, 8, 217.	5.3	49
14	optimade-python-tools: a Python library for serving and consuming materials data via OPTIMADE APIs. Journal of Open Source Software, 2021, 6, 3458.	4.6	3
15	Selectivity in Yttrium Manganese Oxide Synthesis via Local Chemical Potentials in Hyperdimensional Phase Space. Journal of the American Chemical Society, 2021, 143, 15185-15194.	13.7	25
16	BonDNet: a graph neural network for the prediction of bond dissociation energies for charged molecules. Chemical Science, 2021, 12, 1858-1868.	7.4	44
17	An improved symmetry-based approach to reciprocal space path selection in band structure calculations. Npj Computational Materials, 2020, 6, .	8.7	33
18	Defect-Accommodating Intermediates Yield Selective Low-Temperature Synthesis of YMnO ₃ Polymorphs. Inorganic Chemistry, 2020, 59, 13639-13650.	4.0	22

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19	Enabling materials informatics for 29Si solid-state NMR of crystalline materials. Npj Computational Materials, 2020, 6, .	8.7	11
20	Origin of Disorder Tolerance in Piezoelectric Materials and Design of Polar Systems. Chemistry of Materials, 2020, 32, 2836-2842.	6.7	4
21	propnet: A Knowledge Graph for Materials Science. Matter, 2020, 2, 464-480.	10.0	34
22	The existence and impact of persistent ferroelectric domains in MAPbI ₃ . Science Advances, 2019, 5, eaas9311.	10.3	77
23	High-throughput density-functional perturbation theory phonons for inorganic materials. Scientific Data, 2018, 5, 180065.	5.3	122
24	Accelerating the discovery of materials for clean energy in the era of smart automation. Nature Reviews Materials, 2018, 3, 5-20.	48.7	489
25	Thermodynamic limit for synthesis of metastable inorganic materials. Science Advances, 2018, 4, eaaq0148.	10.3	212
26	The Materials Project: Accelerating Materials Design Through Theory-Driven Data and Tools. , 2018, , 1-34.		11
27	Assessing High-Throughput Descriptors for Prediction of Transparent Conductors. Chemistry of Materials, 2018, 30, 8375-8389.	6.7	60
28	Harnessing the Materials Project for machine-learning and accelerated discovery. MRS Bulletin, 2018, 43, 664-669.	3.5	20
29	Evaluation of thermodynamic equations of state across chemistry and structure in the materials project. Npj Computational Materials, 2018, 4, .	8.7	32
30	Theoryâ€Guided Synthesis of a Metastable Leadâ€Free Piezoelectric Polymorph. Advanced Materials, 2018, 30, 1800559.	21.0	6
31	Multiple ion beam irradiation for the study of radiation damage in materials. Nuclear Instruments & Methods in Physics Research B, 2017, 412, 1-10.	1.4	39
32	Computational Approach for Epitaxial Polymorph Stabilization through Substrate Selection. ACS Applied Materials & Interfaces, 2016, 8, 13086-13093.	8.0	78
33	The diffusion of cesium, strontium, and europium in silicon carbide. Journal of Nuclear Materials, 2016, 476, 155-167.	2.7	19
34	Radiation enhanced diffusion of cesium, strontium, and europium in silicon carbide. Journal of Nuclear Materials, 2016, 474, 76-87.	2.7	15
35	A Multi-Pinhole Faraday Cup Device for Measurement of Discrete Charge Distribution of Heavy and Light Ions. IEEE Transactions on Nuclear Science, 2016, 63, 854-860.	2.0	2
36	Development of a multi-layer diffusion couple to study fission product transport in β-SiC. Journal of Nuclear Materials, 2014, 444, 170-174.	2.7	15