Shyam S Dwaraknath

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7318967/publications.pdf

Version: 2024-02-01

36 papers	1,704 citations	361413 20 h-index	377865 34 g-index
37 all docs	37 docs citations	37 times ranked	2850 citing authors

#	Article	IF	Citations
1	Accelerating the discovery of materials for clean energy in the era of smart automation. Nature Reviews Materials, 2018, 3, 5-20.	48.7	489
2	Thermodynamic limit for synthesis of metastable inorganic materials. Science Advances, 2018, 4, eaaq0148.	10.3	212
3	High-throughput density-functional perturbation theory phonons for inorganic materials. Scientific Data, 2018, 5, 180065.	5.3	122
4	Computational Approach for Epitaxial Polymorph Stabilization through Substrate Selection. ACS Applied Materials & Interfaces, 2016, 8, 13086-13093.	8.0	78
5	The existence and impact of persistent ferroelectric domains in MAPbI ₃. Science Advances, 2019, 5, eaas9311.	10.3	77
6	Assessing High-Throughput Descriptors for Prediction of Transparent Conductors. Chemistry of Materials, 2018, 30, 8375-8389.	6.7	60
7	OPTIMADE, an API for exchanging materials data. Scientific Data, 2021, 8, 217.	5.3	49
8	Toward a Mechanistic Model of Solidâ€“Electrolyte Interphase Formation and Evolution in Lithium-Ion Batteries. ACS Energy Letters, 2022, 7, 1446-1453.	17.4	46
9	A graph-based network for predicting chemical reaction pathways in solid-state materials synthesis. Nature Communications, 2021, 12, 3097.	12.8	44
10	BonDNet: a graph neural network for the prediction of bond dissociation energies for charged molecules. Chemical Science, 2021, 12, 1858-1868.	7.4	44
11	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
12	A chemically consistent graph architecture for massive reaction networks applied to solid-electrolyte interphase formation. Chemical Science, 2021, 12, 4931-4939.	7.4	36
13	propnet: A Knowledge Graph for Materials Science. Matter, 2020, 2, 464-480.	10.0	34
14	An improved symmetry-based approach to reciprocal space path selection in band structure calculations. Npj Computational Materials, 2020, 6, .	8.7	33
15	Evaluation of thermodynamic equations of state across chemistry and structure in the materials project. Npj Computational Materials, 2018, 4, .	8.7	32
16	Performance comparison of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi>r</mml:mi></mml:mrow><mml:mn>2</mml	2.4	31
	and SCAN metaGGA density functionals for solid materials via an automated, high-throughput computational workflow. Physical Review Materials, 2022, 6, .		
17	Rapid generation of optimal generalized Monkhorst-Pack grids. Computational Materials Science, 2021, 187, 110100.	3.0	25
18	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

#	Article	IF	Citations
19	Defect-Accommodating Intermediates Yield Selective Low-Temperature Synthesis of YMnO₃ Polymorphs. Inorganic Chemistry, 2020, 59, 13639-13650.	4.0	22
20	Database of ab initio L-edge X-ray absorption near edge structure. Scientific Data, 2021, 8, 153.	5.3	21
21	Harnessing the Materials Project for machine-learning and accelerated discovery. MRS Bulletin, 2018, 43, 664-669.	3.5	20
22	The diffusion of cesium, strontium, and europium in silicon carbide. Journal of Nuclear Materials, 2016, 476, 155-167.	2.7	19
23	Quantum chemical calculations of lithium-ion battery electrolyte and interphase species. Scientific Data, 2021, 8, 203.	5.3	19
24	Convergence acceleration in machine learning potentials for atomistic simulations. , 2022, 1, 61-69.		18
25	Improving machine learning performance on small chemical reaction data with unsupervised contrastive pretraining. Chemical Science, 2022, 13, 1446-1458.	7.4	17
26	Development of a multi-layer diffusion couple to study fission product transport in Î²-SiC. Journal of Nuclear Materials, 2014, 444, 170-174.	2.7	15
27	Radiation enhanced diffusion of cesium, strontium, and europium in silicon carbide. Journal of Nuclear Materials, 2016, 474, 76-87.	2.7	15
28	Lowering Ternary Oxide Synthesis Temperatures by Solid-State Cometathesis Reactions. Chemistry of Materials, 2021, 33, 3692-3701.	6.7	14
29	The Materials Project: Accelerating Materials Design Through Theory-Driven Data and Tools. , 2018, , 1-34.		11
30	Enabling materials informatics for 29Si solid-state NMR of crystalline materials. Npj Computational Materials, 2020, 6, .	8.7	11
31	Theoryâ€Guided Synthesis of a Metastable Leadâ€Free Piezoelectric Polymorph. Advanced Materials, 2018, 30, 1800559.	21.0	6
32	Origin of Disorder Tolerance in Piezoelectric Materials and Design of Polar Systems. Chemistry of Materials, 2020, 32, 2836-2842.	6.7	4
33	Reaction Selectivity in Cometathesis: Yttrium Manganese Oxides. Chemistry of Materials, 2022, 34, 4694-4702.	6.7	4
34	Effective Local Geometry Descriptor for 29Si NMR Q4 Anisotropy. Journal of Physical Chemistry C, 2021, 125, 19481-19488.	3.1	3
35	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
36	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