Leopold Talirz

List of Publications by Year
in descending order

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26	3,970	430442	642321
papers	citations	18	23
		h-index	g-index

28	28	28	4602
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Data-Driven Matching of Experimental Crystal Structures and Gas Adsorption Isotherms of Metalâ€“Organic Frameworks. Journal of Chemical & Engineering Data, 2022, 67, 1743-1756.	1.0	6
2	AiiDAlab â€“ an ecosystem for developing, executing, and sharing scientific workflows. Computational Materials Science, 2021, 188, 110165.	1.4	40
3	OPTIMADE, an API for exchanging materials data. Scientific Data, 2021, 8, 217.	2.4	49
4	Virtual Computational Chemistry Teaching Laboratoriesâ€”Hands-On at a Distance. Journal of Chemical Education, 2021, 98, 3163-3171.	1.1	15
5	Trends in atomistic simulation software usage [Article v1.0]. Living Journal of Computational Molecular Science, 2021, 3, .	2.2	7
6	Too Many Materials and Too Many Applications: An Experimental Problem Waiting for a Computational Solution. ACS Central Science, 2020, 6, 1890-1900.	5.3	63
7	AiiDA 1.0, a scalable computational infrastructure for automated reproducible workflows and data provenance. Scientific Data, 2020, 7, 300.	2.4	142
8	Materials Cloud, a platform for open computational science. Scientific Data, 2020, 7, 299.	2.4	189
9	In Silico Discovery of Covalent Organic Frameworks for Carbon Capture. ACS Applied Materials & Interfaces, 2020, 12, 21559-21568.	4.0	43
10	Electronic Structure of Atomically Precise Graphene Nanoribbons. , 2020, , 685-719.		0
11	Band Gap of Atomically Precise Graphene Nanoribbons as a Function of Ribbon Length and Termination. ChemPhysChem, 2019, 20, 2348-2353.	1.0	17
12	Building a Consistent and Reproducible Database for Adsorption Evaluation in Covalentâ€“Organic Frameworks. ACS Central Science, 2019, 5, 1663-1675.	5.3	89
13	Capturing chemical intuition in synthesis of metal-organic frameworks. Nature Communications, 2019, 10, 539.	5.8	153
14	Electronic Structure of Atomically Precise Graphene Nanoribbons. , 2019, , 1-35.		0
15	Toward GW Calculations on Thousands of Atoms. Journal of Physical Chemistry Letters, 2018, 9, 306-312.	2.1	104
16	Electronic Structure of Atomically Precise Graphene Nanoribbons. , 2018, , 1-35.		1
17	In Silico Design of 2D and 3D Covalent Organic Frameworks for Methane Storage Applications. Chemistry of Materials, 2018, 30, 5069-5086.	3.2	101
18	On-Surface Synthesis and Characterization of 9-Atom Wide Armchair Graphene Nanoribbons. ACS Nano, 2017, 11, 1380-1388.	7.3	270

#	Article	IF	Citations
19	Giant edge state splitting at atomically precise graphene zigzag edges. Nature Communications, 2016, 7, 11507.	5.8	207
20	Onâ€Surface Synthesis of Atomically Precise Graphene Nanoribbons. Advanced Materials, 2016, 28, 6222-6231.	11.1	410
21	On-surface synthesis of graphene nanoribbons with zigzag edge topology. Nature, 2016, 531, 489-492.	13.7	1,154
22	Synthesis of Atomically Precise Graphene-Based Nanostructures: A Simulation Point of View. Advances in Atom and Single Molecule Machines, 2016, , 237-268.	0.0	5
23	Electronic band dispersion of graphene nanoribbons via Fourier-transformed scanning tunneling spectroscopy. Physical Review B, 2015, 91, .	1.1	85
24	On-Surface Synthesis of BN-Substituted Heteroaromatic Networks. ACS Nano, 2015, 9, 9228-9235.	7.3	78
25	Graphene nanoribbon heterojunctions. Nature Nanotechnology, 2014, 9, 896-900.	15.6	528
26	Termini of Bottom-Up Fabricated Graphene Nanoribbons. Journal of the American Chemical Society, 2013, 135, 2060-2063.	6.6	214