Andrius Merkys

List of Publications by Year
in descending order

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		759233	996975
19	3,266	12	15
papers	citations	h-index	g-index

20	20	20	5734
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Proving the correctness of the algorithm for building a crystallographic space group. Journal of Applied Crystallography, 2022, 55, 515-525.	4.5	1
2	Validation of the Crystallography Open Database using the Crystallographic Information Framework. Journal of Applied Crystallography, 2021, 54, 661-672.	4.5	179
3	OPTIMADE, an API for exchanging materials data. Scientific Data, 2021, 8, 217.	5.3	49
4	AiiDA 1.0, a scalable computational infrastructure for automated reproducible workflows and data provenance. Scientific Data, 2020, 7, 300.	5.3	142
5	Crystallography Open Database (COD). , 2020, , 1863-1881.		8
6	Raman Open Database: first interconnected Ramanâ€“X-ray diffraction open-access resource for material identification. Journal of Applied Crystallography, 2019, 52, 618-625.	4.5	34
7	Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds. Nature Nanotechnology, 2018, 13, 246-252.	31.5	1,317
8	Crystallography Open Database (COD). , 2018, , 1-19.		3
9	Using SMILES strings for the description of chemical connectivity in the Crystallography Open Database. Journal of Cheminformatics, 2018, 10, 23.	6.1	126
10	A posteriori metadata from automated provenance tracking: integration of AiiDA and TCOD. Journal of Cheminformatics, 2017, 9, 56.	6.1	24
11	AceDRG: a stereochemical description generator for ligands. Acta Crystallographica Section D: Structural Biology, 2017, 73, 112-122.	2.3	254
12	Validation and extraction of molecular-geometry information from small-molecule databases. Acta Crystallographica Section D: Structural Biology, 2017, 73, 103-111.	2.3	19
13	COD::CIF::Parser: an error-correcting CIF parser for the Perl language. Journal of Applied Crystallography, 2016, 49, 292-301.	4.5	139
14	Computing stoichiometric molecular composition from crystal structures. Journal of Applied Crystallography, 2015, 48, 85-91.	4.5	133
15	Launching the Theoretical Crystallography Open Database. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1736-C1736.	0.1	6
16	A new generation of CCP4 monomer library based on Crystallography Open Database. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C338-C338.	0.1	1
17	Chemical information presentation in the Crystallography Open Database. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1710-C1710.	0.1	0
18	Stereochemical statistics in Crystallography Open Database. Acta Crystallographica Section A: Foundations and Advances, 2013, 69, s388-s389.	0.3	0

#	Article	IF	Citations
19	Crystallography Open Database (COD): an open-access collection of crystal structures and platform for world-wide collaboration. Nucleic Acids Research, 2012, 40, D420-D427.	14.5	826