

Andrius Merkys

List of Publications by Year in descending order

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Version: 2024-02-01

19
papers

3,266
citations

759055

12
h-index

996849

15
g-index

20
all docs

20
docs citations

20
times ranked

5734
citing authors

#	ARTICLE	IF	CITATIONS
1	Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds. <i>Nature Nanotechnology</i> , 2018, 13, 246-252.	15.6	1,317
2	Crystallography Open Database (COD): an open-access collection of crystal structures and platform for world-wide collaboration. <i>Nucleic Acids Research</i> , 2012, 40, D420-D427.	6.5	826
3	<i>AceDRG</i>: a stereochemical description generator for ligands. <i>Acta Crystallographica Section D: Structural Biology</i> , 2017, 73, 112-122.	1.1	254
4	Validation of the Crystallography Open Database using the Crystallographic Information Framework. <i>Journal of Applied Crystallography</i> , 2021, 54, 661-672.	1.9	179
5	AiiDA 1.0, a scalable computational infrastructure for automated reproducible workflows and data provenance. <i>Scientific Data</i> , 2020, 7, 300.	2.4	142
6	<i>COD::CIF::Parser</i>: an error-correcting CIF parser for the Perl language. <i>Journal of Applied Crystallography</i> , 2016, 49, 292-301.	1.9	139
7	Computing stoichiometric molecular composition from crystal structures. <i>Journal of Applied Crystallography</i> , 2015, 48, 85-91.	1.9	133
8	Using SMILES strings for the description of chemical connectivity in the Crystallography Open Database. <i>Journal of Cheminformatics</i> , 2018, 10, 23.	2.8	126
9	OPTIMADE, an API for exchanging materials data. <i>Scientific Data</i> , 2021, 8, 217.	2.4	49
10	Raman Open Database: first interconnected Raman X-ray diffraction open-access resource for material identification. <i>Journal of Applied Crystallography</i> , 2019, 52, 618-625.	1.9	34
11	A posteriori metadata from automated provenance tracking: integration of AiiDA and TCOD. <i>Journal of Cheminformatics</i> , 2017, 9, 56.	2.8	24
12	Validation and extraction of molecular-geometry information from small-molecule databases. <i>Acta Crystallographica Section D: Structural Biology</i> , 2017, 73, 103-111.	1.1	19
13	Crystallography Open Database (COD)., 2020, , 1863-1881.		8
14	Launching the Theoretical Crystallography Open Database. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2014, 70, C1736-C1736.	0.0	6
15	Crystallography Open Database (COD)., 2018, , 1-19.		3
16	A new generation of CCP4 monomer library based on Crystallography Open Database. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2014, 70, C338-C338.	0.0	1
17	Proving the correctness of the algorithm for building a crystallographic space group. <i>Journal of Applied Crystallography</i> , 2022, 55, 515-525.	1.9	1
18	Stereochemical statistics in Crystallography Open Database. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2013, 69, s388-s389.	0.3	0

#	ARTICLE	IF	CITATIONS
19	Chemical information presentation in the Crystallography Open Database. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1710-C1710.	0.0	0