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List of Publications by Year in descending order

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1039406 1199166 12 495 9 12 citations h-index g-index papers 12 12 12 779 docs citations times ranked citing authors all docs

#	Article	IF	CITATIONS
1	Materials Cloud, a platform for open computational science. Scientific Data, 2020, 7, 299.	2.4	189
2	AiiDA 1.0, a scalable computational infrastructure for automated reproducible workflows and data provenance. Scientific Data, 2020, 7, 300.	2.4	142
3	Workflows in AiiDA: Engineering a high-throughput, event-based engine for robust and modular computational workflows. Computational Materials Science, 2021, 187, 110086.	1.4	63
4	Oxygen-stabilized triangular defects in hexagonal boron nitride. Physical Review B, 2015, 92, .	1.1	24
5	Workflow Engineering in Materials Design within the BATTERY 2030 + Project. Advanced Energy Materials, 2022, 12, .	10.2	18
6	Virtual Computational Chemistry Teaching Laboratories—Hands-On at a Distance. Journal of Chemical Education, 2021, 98, 3163-3171.	1.1	15
7	Exploiting the P L_2,3 absorption edge for optics: spectroscopic and structural characterization of cubic boron phosphide thin films. Optical Materials Express, 2016, 6, 3946.	1.6	10
8	Common workflows for computing material properties using different quantum engines. Npj Computational Materials, 2021, 7, .	3.5	10
9	Self-healing in B ₁₂ P ₂ through Mediated Defect Recombination. Chemistry of Materials, 2016, 28, 8415-8428.	3.2	9
10	Determining crystal phase purity in c-BP through X-ray absorption spectroscopy. Physical Chemistry Chemical Physics, 2017, 19, 8174-8187.	1.3	7
11	Detection of defect populations in superhard semiconductor boron subphosphide B ₁₂ P ₂ through X-ray absorption spectroscopy. Journal of Materials Chemistry A, 2017, 5, 5737-5749.	5.2	7
12	kiwiPy: Robust, high-volume, messaging for big-data and computational science workflows. Journal of Open Source Software, 2020, 5, 2351.	2.0	1