

Ian Bush

List of Publications by Year in descending order

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9
papers

586
citations

1307594

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1474206

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docs citations

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times ranked

825
citing authors

#	ARTICLE	IF	CITATIONS
1	Realistic Models of Hydroxylated Amorphous Silica Surfaces and MCM-41 Mesoporous Material Simulated by Large-scale Periodic B3LYP Calculations. <i>Advanced Materials</i> , 2008, 20, 4579-4583.	21.0	199
2	QuEST and High Performance Simulation of Quantum Computers. <i>Scientific Reports</i> , 2019, 9, 10736.	3.3	136
3	The CRYSTAL code, 1976–2020 and beyond, a long story. <i>Journal of Chemical Physics</i> , 2020, 152, 204111.	3.0	133
4	A new massively parallel version of CRYSTAL for large systems on high performance computing architectures. <i>Journal of Computational Chemistry</i> , 2012, 33, 2276-2284.	3.3	43
5	Parallel implementation of the ab initio CRYSTAL program: electronic structure calculations for periodic systems. <i>Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences</i> , 2011, 467, 2112-2126.	2.1	35
6	Elucidating the Interaction of CO ₂ in the Giant Metal-Organic Framework MIL-100 through Large-Scale Periodic Ab Initio Modeling. <i>Journal of Physical Chemistry C</i> , 2019, 123, 28677-28687.	3.1	15
7	Cost-effective composite methods for large-scale solid-state calculations. <i>Faraday Discussions</i> , 2020, 224, 292-308.	3.2	13
8	Materials and Molecular Modeling at the Exascale. <i>Computing in Science and Engineering</i> , 2022, 24, 36-45.	1.2	7
9	Barely sufficient practices in scientific computing. <i>Patterns</i> , 2021, 2, 100206.	5.9	5