Isaac J Sugden

List of Publications by Year
in descending order

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20 papers	724 citations	933447 10 h-index	996975 15 g-index
20 all docs	20 docs citations	20 times ranked	958 citing authors

#	Article	IF	Citations
1	How many more polymorphs of ROY remain undiscovered. Chemical Science, 2022, 13, 1288-1297.	7.4	41
2	Efficient Screening of Coformers for Active Pharmaceutical Ingredient Cocrystallization. Crystal Growth and Design, 2022, 22, 4513-4527.	3.0	14
3	Crystal Structure Prediction Methods for Organic Molecules: State of the Art. Annual Review of Chemical and Biomolecular Engineering, 2021, 12, 593-623.	6.8	28
4	Computational Screening of Chiral Organic Semiconductors: Exploring Side-Group Functionalization and Assembly to Optimize Charge Transport. Crystal Growth and Design, 2021, 21, 5036-5049.	3.0	11
5	Three new polymorphs of 1,8-diacetylpyrene: a material with packing-dependent luminescence properties and a testbed for crystal structure prediction. Journal of Materials Chemistry C, 2021, 9, 2491-2503.	5.5	6
6	Efficient Screening for Ternary Molecular Ionic Cocrystals Using a Complementary Mechanosynthesis and Computational Structure Prediction Approach. Chemistry - A European Journal, 2020, 26, 4752-4765.	3.3	27
7	Efficient Parameterization of a Surrogate Model of Molecular Interactions in Crystals. Computer Aided Chemical Engineering, 2020, , 493-498.	0.5	2
8	Can solvated intermediates inform us about nucleation pathways? The case of Î²-pABA. CrystEngComm, 2020, 22, 7447-7459.	2.6	11
9	Accurate and efficient representation of intramolecular energy in ab initio generation of crystal structures. II. Smoothed intramolecular potentials. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 423-433.	1.1	9
10	Polymorphism in p-aminobenzoic acid. CrystEngComm, 2019, 21, 2034-2042.	2.6	30
11	Development of accurate and efficient ab initio potentials for effective crystal structure prediction. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, e549-e549.	0.1	0
12	A combined theoretical and experimental investigation into the high-throughput screening of cocrystal coformers. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, e548-e548.	0.1	0
13	Accurate and efficient representation of intramolecular energy in ab initio generation of crystal structures. Part II. Smoothed intramolecular potentials. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e120-e120.	0.1	0
14	New potentials for accurate and efficient ab initio crystal structure prediction methods. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e363-e363.	0.1	0
15	Accurate and efficient representation of intramolecular energy inab initiogeneration of crystal structures. I. Adaptive local approximate models. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 864-874.	1.1	18
16	Impact scenarios in boron carbide: A computational study. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650055.	1.8	4
17	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	1.1	445
18	Accurate and efficient representation of intramolecular energy in ab initio generation of crystal structures. Acta Crystallographica Section A: Foundations and Advances, 2016, 72, s349-s349.	0.1	0

#	Article	IF	Citations
19	Efficient Handling of Molecular Flexibility in Ab Initio Generation of Crystal Structures. Journal of Chemical Theory and Computation, 2015, 11, 1957-1969.	5.3	58
20	Thermal rearrangement mechanisms in icosahedral carboranes and metallocarboranes. Chemical Communications, 2013, 49, 975-977.	4.1	20