Rui Guo

List of Publications by Year
in descending order

28 papers	1,034 citations	567281 15 h-index	526287 27 g-index
28 all docs	28 docs citations	28 times ranked	1267 citing authors

#	Article	IF	Citations
1	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
2	Isomorphous template induced crystallisation: a robust method for the targeted crystallisation of computationally predicted metastable polymorphs. Chemical Communications, 2016, 52, 7384-7386.	4.1	57
3	Biological and Biomedical Applications of Two-Dimensional Vibrational Spectroscopy: Proteomics, Imaging, and Structural Analysis. Accounts of Chemical Research, 2009, 42, 1322-1331.	15.6	53
4	Successful Computationally Directed Templating of Metastable Pharmaceutical Polymorphs. Crystal Growth and Design, 2018, 18, 5322-5331.	3.0	52
5	Protein identification and quantification by two-dimensional infrared spectroscopy: Implications for an all-optical proteomic platform. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 15352-15357.	7.1	50
6	Direct Observation of Templated Two-Step Nucleation Mechanism during Olanzapine Hydrate Formation. Crystal Growth and Design, 2017, 17, 6382-6393.	3.0	41
7	Are Oxygen and Sulfur Atoms Structurally Equivalent in Organic Crystals?. Crystal Growth and Design, 2017, 17, 827-833.	3.0	35
8	Direct identification and decongestion of Fermi resonances by control of pulse time ordering in two-dimensional IR spectroscopy. Journal of Chemical Physics, 2007, 127, 114513.	3.0	33
9	Unraveling Complexity in the Solid Form Screening of a Pharmaceutical Salt: Why so Many Forms? Why so Few?. Crystal Growth and Design, 2017, 17, 5349-5365.	3.0	33
10	Optical fingerprinting of peptides using two-dimensional infrared spectroscopy: Proof of principle. Analytical Biochemistry, 2008, 374, 358-365.	2.4	31
11	Detection of complex formation and determination of intermolecular geometry through electrical anharmonic coupling of molecular vibrations using electron-vibrationâ€“vibration two-dimensional infrared spectroscopy. Physical Chemistry Chemical Physics, 2009, 11, 8417.	2.8	27
12	Decongestion of methylene spectra in biological and non-biological systems using picosecond 2DIR spectroscopy measuring electron-vibrationâ€“vibration coupling. Chemical Physics, 2008, 350, 201-211.	1.9	23
13	Reversible, Two-Step Single-Crystal to Single-Crystal Phase Transitions between Desloratadine Forms I, II, and III. Crystal Growth and Design, 2020, 20, 1800-1810.	3.0	20
14	Serendipitous isolation of a disappearing conformational polymorph of succinic acid challenges computational polymorph prediction. CrystEngComm, 2018, 20, 3971-3977.	2.6	19
15	Identification and Relative Quantification of Tyrosine Nitration in a Model Peptide Using Two-Dimensional Infrared Spectroscopy. Journal of Physical Chemistry B, 2014, 118, 12855-12864.	2.6	16
16	The (Current) Acridine Solid Form Landscape: Eight Polymorphs and a Hydrate. Crystal Growth and Design, 2019, 19, 4884-4893.	3.0	16
17	Toward Physics-Based Solubility Computation for Pharmaceuticals to Rival Informatics. Journal of Chemical Theory and Computation, 2021, 17, 3700-3709.	5.3	15
18	Geometry determination of complexes in a molecular liquid mixture using electronâ€“vibrationâ€“vibration two-dimensional infrared spectroscopy with a vibrational transition density cube method. Physical Chemistry Chemical Physics, 2012, 14, 14023.	2.8	13

#	Article	IF	Citations
19	Concomitant conformational dimorphism in 1,2-bis(9-anthryl)acetylene. CrystEngComm, 2015, 17, 4877-4882.	2.6	10
20	Detection of Drug Binding to a Target Protein Using EVV 2DIR Spectroscopy. Journal of Physical Chemistry B, 2019, 123, 3598-3606.	2.6	9
21	Color Differences Highlight Concomitant Polymorphism of Chalcones. Crystal Growth and Design, 2020, 20, 6346-6355.	3.0	9
22	Calculation of Diamagnetic Susceptibility Tensors of Organic Crystals: From Coronene to Pharmaceutical Polymorphs. Journal of Physical Chemistry A, 2020, 124, 1409-1420.	2.5	8
23	Potential for the detection of molecular complexes and determination of interaction geometry by 2DIR: Application to protein sciences. Faraday Discussions, 2011, 150, 161.	3.2	7
24	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. Faraday Discussions, 2018, 211, 325-381.	3.2	7
25	On the Application of Strong Magnetic Fields during Organic Crystal Growth. Crystal Growth and Design, 2021, 21, 6254-6265.	3.0	2
26	Crystal Structure and Twisted Aggregates of Oxcarbazepine Form III. Crystal Growth and Design, 2022, 22, 4146-4156.	3.0	2
27	Diabat method for polymorph free energies: Extension to molecular crystals. Journal of Chemical Physics, 2020, 153, 244105.	3.0	1
28	Detection of Molecular Complex Formation and Direct Determination of Intermolecular Interaction Geometries by a Hybrid Raman-Infrared Multidimensional Coherent Spectroscopy: Implications for High Throughput Biology. , 2010, , .		0