Graeme Day

List of Publications by Year in Descending Order

140 papers	9,716 citations	58 h-index	96 g-index
177 ext. papers	10,905 ext. citations	7.2 avg, IF	6.35 L-index

#	Paper	IF	Citations
140	Surprising Chemistry of 6-Azidotetrazolo[5,1-]phthalazine: What a Purported Natural Product Reveals about the Polymorphism of Explosives.. *Journal of Organic Chemistry*, **2022**, 87, 6680-6694	4.2	2
139	Inherent Ethyl Acetate Selectivity in a Trianglimine Molecular Solid. *Chemistry - A European Journal*, **2021**, 27, 10589-10594	4.8	3
138	Digital navigation of energy-structure-function maps for hydrogen-bonded porous molecular crystals. *Nature Communications*, **2021**, 12, 817	17.4	11
137	Exploration and Optimization in Crystal Structure Prediction: Combining Basin Hopping with Quasi-Random Sampling. *Journal of Chemical Theory and Computation*, **2021**, 17, 1988-1999	6.4	5
136	Accelerating computational discovery of porous solids through improved navigation of energy-structure-function maps. *Science Advances*, **2021**, 7,	14.3	2
135	Photocatalytic proton reduction by a computationally identified, molecular hydrogen-bonded framework. *Journal of Materials Chemistry A*, **2020**, 8, 7158-7170	13	26
134	Combining forces: complementary techniques brought together to determine tricky crystal structures. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2020**, 76, 294-295	1.8	0
133	Crystal structure determination of an elusive methanol solvate hydrate of catechin using crystal structure prediction and NMR crystallography. *CrystEngComm*, **2020**, 22, 4969-4981	3.3	7
132	An Expandable Hydrogen-Bonded Organic Framework Characterized by Three-Dimensional Electron Diffraction. *Journal of the American Chemical Society*, **2020**, 142, 12743-12750	16.4	28
131	Evolutionary chemical space exploration for functional materials: computational organic semiconductor discovery. *Chemical Science*, **2020**, 11, 4922-4933	9.4	12
130	Structure prediction of crystals, surfaces and nanoparticles. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2020**, 378, 20190600	3	12
129	Multifidelity Statistical Machine Learning for Molecular Crystal Structure Prediction. *Journal of Physical Chemistry A*, **2020**, 124, 8065-8078	2.8	22
128	Minimizing Polymorphic Risk through Cooperative Computational and Experimental Exploration. *Journal of the American Chemical Society*, **2020**, 142, 16668-16680	16.4	13
127	Mining predicted crystal structure landscapes with high throughput crystallisation: old molecules, new insights. *Chemical Science*, **2019**, 10, 9988-9997	9.4	36
126	Explaining crystallization preferences of two polyphenolic diastereoisomers by crystal structure prediction. *CrystEngComm*, **2019**, 21, 2067-2079	3.3	13
125	Rapid Structure Determination of Molecular Solids Using Chemical Shifts Directed by Unambiguous Prior Constraints. *Journal of the American Chemical Society*, **2019**, 141, 16624-16634	16.4	26
124	Machine-Learned Fragment-Based Energies for Crystal Structure Prediction. *Journal of Chemical Theory and Computation*, **2019**, 15, 2743-2758	6.4	19

123	Exploring the Multi-minima Behavior of Small Molecule Crystal Polymorphs at Finite Temperature. *Crystal Growth and Design*, **2019**, 19, 5568-5580	3.5	16
122	From Concept to Crystals via Prediction: Multi-Component Organic Cage Pots by Social Self-Sorting. *Angewandte Chemie*, **2019**, 131, 16421-16427	3.6	17
121	From Concept to Crystals via Prediction: Multi-Component Organic Cage Pots by Social Self-Sorting. *Angewandte Chemie - International Edition*, **2019**, 58, 16275-16281	16.4	35
120	Understanding the formation of apremilast cocrystals. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2019**, 75, 803-814	1.8	10
119	Pasteur's tartaramide/malamide quasiracemates: new entries and departures from near inversion symmetry. *CrystEngComm*, **2018**, 20, 4213-4220	3.3	2
118	Near-Ideal Xylene Selectivity in Adaptive Molecular Pillar[n]arene Crystals. *Journal of the American Chemical Society*, **2018**, 140, 6921-6930	16.4	130
117	Large-Scale Computational Screening of Molecular Organic Semiconductors Using Crystal Structure Prediction. *Chemistry of Materials*, **2018**, 30, 4361-4371	9.6	53
116	Energy-Structure-Function Maps: Cartography for Materials Discovery. *Advanced Materials*, **2018**, 30, e1704944	24	24
115	Machine learning for the structure-energy-property landscapes of molecular crystals. *Chemical Science*, **2018**, 9, 1289-1300	9.4	98
114	Evaluating the Energetic Driving Force for Cocrystal Formation. *Crystal Growth and Design*, **2018**, 18, 892-904	3.5	102
113	Applications of crystal structure prediction - inorganic and network structures: general discussion. *Faraday Discussions*, **2018**, 211, 613-642	3.6	4
112	Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acid–Base Co-Crystals. *Angewandte Chemie*, **2018**, 130, 15122-15126	3.6	8
111	Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acid-Base Co-Crystals. *Angewandte Chemie - International Edition*, **2018**, 57, 14906-14910	16.4	27
110	Structure searching methods: general discussion. *Faraday Discussions*, **2018**, 211, 133-180	3.6	3
109	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. *Faraday Discussions*, **2018**, 211, 325-381	3.6	6
108	Applications of crystal structure prediction - organic molecular structures: general discussion. *Faraday Discussions*, **2018**, 211, 493-539	3.6	6
107	Computational modelling of solvent effects in a prolific solvatomorphic porous organic cage. *Faraday Discussions*, **2018**, 211, 383-399	3.6	26
106	Clathrate Structure Determination by Combining Crystal Structure Prediction with Computational and Experimental Xe NMR Spectroscopy. *Chemistry - A European Journal*, **2017**, 23, 5258-5269	4.8	14

105	Application of computational methods to the design and characterisation of porous molecular materials. *Chemical Society Reviews*, **2017**, 46, 3286-3301	58.5	50
104	Computationally-Guided Synthetic Control over Pore Size in Isostructural Porous Organic Cages. *ACS Central Science*, **2017**, 3, 734-742	16.8	51
103	Functional materials discovery using energy-structure-function maps. *Nature*, **2017**, 543, 657-664	50.4	238
102	Predicted energy-structure-function maps for the evaluation of small molecule organic semiconductors. *Journal of Materials Chemistry C*, **2017**, 5, 7574-7584	7.1	55
101	The Plot Thickens: Gelation by Phenylalanine in Water and Dimethyl Sulfoxide. *Crystal Growth and Design*, **2017**, 17, 4100-4109	3.5	16
100	Pharmaceutical polymorph control in a drug-mimetic supramolecular gel. *Chemical Science*, **2017**, 8, 78-84	9.4	72
99	Reticular synthesis of porous molecular 1D nanotubes and 3D networks. *Nature Chemistry*, **2017**, 9, 17-25	17.6	90
98	Report on the sixth blind test of organic crystal structure prediction methods. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2016**, 72, 439-59	1.8	338
97	An optimized intermolecular force field for hydrogen-bonded organic molecular crystals using atomic multipole electrostatics. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2016**, 72, 477-87	1.8	19
96	Advances in Crystal Structure Prediction and Applications to Pharmaceutical Materials **2016**, 87-115		2
95	Benchmark fragment-based (1)H, (13)C, (15)N and (17)O chemical shift predictions in molecular crystals. *Physical Chemistry Chemical Physics*, **2016**, 18, 21686-709	3.6	70
94	Modelling temperature-dependent properties of polymorphic organic molecular crystals. *Physical Chemistry Chemical Physics*, **2016**, 18, 31132-31143	3.6	59
93	Convergence Properties of Crystal Structure Prediction by Quasi-Random Sampling. *Journal of Chemical Theory and Computation*, **2016**, 12, 910-24	6.4	51
92	Resorcinol Crystallization from the Melt: A New Ambient Phase and New "Riddles". *Journal of the American Chemical Society*, **2016**, 138, 4881-9	16.4	55
91	Rationalization of the Color Properties of Fluorescein in the Solid State: A Combined Computational and Experimental Study. *Chemistry - A European Journal*, **2016**, 22, 10065-73	4.8	21
90	Correction: Substituent interference on supramolecular assembly in urea gelators: synthesis, structure prediction and NMR. *Soft Matter*, **2016**, 12, 5489	3.6	1
89	Substituent interference on supramolecular assembly in urea gelators: synthesis, structure prediction and NMR. *Soft Matter*, **2016**, 12, 4034-43	3.6	19
88	Accurate force fields and methods for modelling organic molecular crystals at finite temperatures. *Physical Chemistry Chemical Physics*, **2016**, 18, 15828-37	3.6	67

87	Solid-State Chemistry and Polymorphism of the Nucleobase Adenine. *Crystal Growth and Design*, **2016**, 16, 3262-3270	3.5	17
86	Enhanced NMR Discrimination of Pharmaceutically Relevant Molecular Crystal Forms through Fragment-Based Ab Initio Chemical Shift Predictions. *Crystal Growth and Design*, **2016**, 16, 6479-6493	3.5	27
85	Modelling of crystal structure of cis-1,2,3,6 and 3,4,5,6-tetrahydrophthalic anhydrides using lattice energy calculations. *Journal of Molecular Modeling*, **2015**, 21, 211	2	1
84	Static and lattice vibrational energy differences between polymorphs. *CrystEngComm*, **2015**, 17, 5154-5165	3.3	249
83	Co-crystallisation of cytosine with 1,10-phenanthroline: computational screening and experimental realisation. *CrystEngComm*, **2015**, 17, 7130-7141	3.3	11
82	Highly Unusual Triangular Crystals of Theophylline: The Influence of Solvent on the Growth Rates of Polar Crystal Faces. *Crystal Growth and Design*, **2015**, 15, 2514-2523	3.5	14
81	Predicted crystal energy landscapes of porous organic cages. *Chemical Science*, **2014**, 5, 2235-2245	9.4	62
80	Controlling the crystallization of porous organic cages: molecular analogs of isoreticular frameworks using shape-specific directing solvents. *Journal of the American Chemical Society*, **2014**, 136, 1438-48	16.4	94
79	Which conformations make stable crystal structures? Mapping crystalline molecular geometries to the conformational energy landscape. *Chemical Science*, **2014**, 5, 3173-3182	9.4	125
78	Is the equilibrium composition of mechanochemical reactions predictable using computational chemistry?. *Faraday Discussions*, **2014**, 170, 41-57	3.6	17
77	Cocrystallization by Freeze-Drying: Preparation of Novel Multicomponent Crystal Forms. *Crystal Growth and Design*, **2013**, 13, 4599-4606	3.5	65
76	The curious case of (caffeine)(benzoic acid): how heteronuclear seeding allowed the formation of an elusive cocrystal. *Chemical Science*, **2013**, 4, 4417	9.4	97
75	De novo determination of the crystal structure of a large drug molecule by crystal structure prediction-based powder NMR crystallography. *Journal of the American Chemical Society*, **2013**, 135, 17501-7	16.4	142
74	The monolayer structure of 1,2-bis(4-pyridyl)ethylene physisorbed on a graphite surface. *Molecular Physics*, **2013**, 111, 73-79	1.7	12
73	Powder crystallography of pharmaceutical materials by combined crystal structure prediction and solid-state 1H NMR spectroscopy. *Physical Chemistry Chemical Physics*, **2013**, 15, 8069-80	3.6	134
72	Determination of the crystal structure of a new polymorph of theophylline. *Chemistry - A European Journal*, **2013**, 19, 7883-8	4.8	40
71	In silico design of supramolecules from their precursors: odd-even effects in cage-forming reactions. *Journal of the American Chemical Society*, **2013**, 135, 9307-10	16.4	65
70	Polymorph identification and crystal structure determination by a combined crystal structure prediction and transmission electron microscopy approach. *Chemistry - A European Journal*, **2013**, 19, 7874-82	4.8	31

69	Single-crystal investigation of L-tryptophan with ZR= 16. *Acta Crystallographica Section B: Structural Science*, **2012**, 68, 549-57		46
68	Isostructural organic binary-host frameworks with tuneable and diversely decorated inclusion cavities. *CrystEngComm*, **2012**, 14, 7898	3.3	22
67	Crystal Structure Prediction **2012**,		1
66	Computational Methods for the Assignment of Vibrational Modes in Crystalline Materials. *Springer Series in Optical Sciences*, **2012**, 151-190	0.5	3
65	Finally: the crystal structure ofL-tryptophan. *Acta Crystallographica Section A: Foundations and Advances*, **2012**, 68, s114-s114		
64	Modification of luminescent properties of a coumarin derivative by formation of multi-component crystals. *CrystEngComm*, **2012**, 14, 5121	3.3	55
63	Towards the computation-led design of porous molecular crystals. *Acta Crystallographica Section A: Foundations and Advances*, **2012**, 68, s108-s108		
62	Current approaches to predicting molecular organic crystal structures. *Crystallography Reviews*, **2011**, 17, 3-52	1.3	169
61	Effect of Fluorination on Molecular Conformation in the Solid State: Tuning the Conformation of Cocrystal Formers. *Crystal Growth and Design*, **2011**, 11, 972-981	3.5	19
60	Solid-state dynamic combinatorial chemistry: reversibility and thermodynamic product selection in covalent mechanosynthesis. *Chemical Science*, **2011**, 2, 696	9.4	129
59	Successful prediction of a model pharmaceutical in the fifth blind test of crystal structure prediction. *International Journal of Pharmaceutics*, **2011**, 418, 168-78	6.5	105
58	Modular and predictable assembly of porous organic molecular crystals. *Nature*, **2011**, 474, 367-71	50.4	396
57	Towards crystal structure prediction of complex organic compounds--a report on the fifth blind test. *Acta Crystallographica Section B: Structural Science*, **2011**, 67, 535-51		318
56	On□Off Porosity Switching in a Molecular Organic Solid. *Angewandte Chemie*, **2011**, 123, 775-779	3.6	61
55	Titelbild: On□Off Porosity Switching in a Molecular Organic Solid (Angew. Chem. 3/2011). *Angewandte Chemie*, **2011**, 123, 579-579	3.6	
54	A Cocrystal Strategy to Tune the Luminescent Properties of Stilbene-Type Organic Solid-State Materials. *Angewandte Chemie*, **2011**, 123, 12691-12694	3.6	81
53	On-off porosity switching in a molecular organic solid. *Angewandte Chemie - International Edition*, **2011**, 50, 749-53	16.4	153
52	Cover Picture: On□Off Porosity Switching in a Molecular Organic Solid (Angew. Chem. Int. Ed. 3/2011). *Angewandte Chemie - International Edition*, **2011**, 50, 555-555	16.4	

51	A cocrystal strategy to tune the luminescent properties of stilbene-type organic solid-state materials. *Angewandte Chemie - International Edition*, **2011**, 50, 12483-6	16.4	396
50	Structure prediction, disorder and dynamics in a DMSO solvate of carbamazepine. *Physical Chemistry Chemical Physics*, **2011**, 13, 12808-16	3.6	30
49	Pseudoracemic amino acid complexes: blind predictions for flexible two-component crystals. *Physical Chemistry Chemical Physics*, **2010**, 12, 8466-77	3.6	45
48	A study into the effect of subtle structural details and disorder on the terahertz spectrum of crystalline benzoic acid. *Physical Chemistry Chemical Physics*, **2010**, 12, 5329-40	3.6	63
47	Crystal packing predictions of the alpha-amino acids: methods assessment and structural observations. *CrystEngComm*, **2010**, 12, 2443	3.3	31
46	Predicting stoichiometry and structure of solvates. *Chemical Communications*, **2010**, 46, 2224-6	5.8	72
45	The delicate balance between gelation and crystallisation: structural and computational investigations. *Soft Matter*, **2010**, 6, 4144	3.6	108
44	Interaction of charge carriers with lattice vibrations in oligoacene crystals from naphthalene to pentacene. *Journal of the American Chemical Society*, **2010**, 132, 14437-46	16.4	113
43	Modelling organic crystal structures using distributed multipole and polarizability-based model intermolecular potentials. *Physical Chemistry Chemical Physics*, **2010**, 12, 8478-90	3.6	231
42	Powder crystallography by combined crystal structure prediction and high-resolution 1H solid-state NMR spectroscopy. *Journal of the American Chemical Society*, **2010**, 132, 2564-6	16.4	175
41	Experimental and predicted crystal structures of Pigment Red 168 and other dihalogenated anthanthrones. *Acta Crystallographica Section B: Structural Science*, **2010**, 66, 515-26		5
40	Improving Mechanical Properties of Crystalline Solids by Cocrystal Formation: New Compressible Forms of Paracetamol. *Advanced Materials*, **2009**, 21, 3905-3909	24	404
39	Predicting inclusion behaviour and framework structures in organic crystals. *Chemistry - A European Journal*, **2009**, 15, 13033-40	4.8	60
38	Significant progress in predicting the crystal structures of small organic molecules--a report on the fourth blind test. *Acta Crystallographica Section B: Structural Science*, **2009**, 65, 107-25		334
37	Testing the Sensitivity of Terahertz Spectroscopy to Changes in Molecular and Supramolecular Structure: A Study of Structurally Similar Cocrystals. *Crystal Growth and Design*, **2009**, 9, 1452-1460	3.5	83
36	Interaction of Charge Carriers with Lattice Vibrations in Organic Molecular Semiconductors: Naphthalene as a Case Study. *Journal of Physical Chemistry C*, **2009**, 113, 4679-4686	3.8	97
35	Molecular Polarization Effects on the Relative Energies of the Real and Putative Crystal Structures of Valine. *Journal of Chemical Theory and Computation*, **2008**, 4, 1795-805	6.4	74
34	Predicting intrinsic aqueous solubility by a thermodynamic cycle. *Molecular Pharmaceutics*, **2008**, 5, 266-79	5.6	91

33	Structural diversity in imidazolidinone organocatalysts: a synchrotron and computational study. *Acta Crystallographica Section C: Crystal Structure Communications*, **2008**, 64, o10-4		23
32	Towards prediction of stoichiometry in crystalline multicomponent complexes. *Chemistry - A European Journal*, **2008**, 14, 8830-6	4.8	79
31	Structure calculation of an elastic hydrogel from sonication of rigid small molecule components. *Angewandte Chemie - International Edition*, **2008**, 47, 1058-62	16.4	100
30	Modeling the interplay of inter- and intramolecular hydrogen bonding in conformational polymorphs. *Journal of Chemical Physics*, **2008**, 128, 244708	3.9	78
29	Database guided conformation selection in crystal structure prediction of alanine. *CrystEngComm*, **2007**, 9, 595	3.3	28
28	Space group selection for crystal structure prediction of solvates. *CrystEngComm*, **2007**, 9, 556	3.3	30
27	Importance of Molecular Shape for the Overall Stability of Hydrogen Bond Motifs in the Crystal Structures of Various Carbamazepine-Type Drug Molecules. *Crystal Growth and Design*, **2007**, 7, 100-107	3.5	48
26	A strategy for predicting the crystal structures of flexible molecules: the polymorphism of phenobarbital. *Physical Chemistry Chemical Physics*, **2007**, 9, 1693-704	3.6	98
25	Terahertz time-domain spectroscopy and the quantitative monitoring of mechanochemical cocrystal formation. *Nature Materials*, **2007**, 6, 206-9	27	225
24	Solvent inclusion in form II carbamazepine. *Chemical Communications*, **2007**, 1600-2	5.8	56
23	Prediction and observation of isostructurality induced by solvent incorporation in multicomponent crystals. *Journal of the American Chemical Society*, **2006**, 128, 14466-7	16.4	80
22	Investigating the latent polymorphism of maleic acid. *Chemical Communications*, **2006**, 54-6	5.8	72
21	An Experiment in Crystal Structure Prediction by Popular Vote. *Crystal Growth and Design*, **2006**, 6, 1985-1990	3.5	20
20	Polymorphism of Scyllo-Inositol: Joining Crystal Structure Prediction with Experiment to Elucidate the Structures of Two Polymorphs. *Crystal Growth and Design*, **2006**, 6, 2301-2307	3.5	18
19	Amide Pyramidalization in Carbamazepine: A Flexibility Problem in Crystal Structure Prediction?. *Crystal Growth and Design*, **2006**, 6, 1858-1866	3.5	56
18	Understanding the influence of polymorphism on phonon spectra: lattice dynamics calculations and terahertz spectroscopy of carbamazepine. *Journal of Physical Chemistry B*, **2006**, 110, 447-56	3.4	145
17	Realizing Predicted Crystal Structures at Extreme Conditions: The Low-Temperature and High-Pressure Crystal Structures of 2-Chlorophenol and 4-Fluorophenol. *Crystal Growth and Design*, **2005**, 5, 1055-1071	3.5	59
16	Beyond the Isotropic Atom Model in Crystal Structure Prediction of Rigid Molecules: Atomic Multipoles versus Point Charges. *Crystal Growth and Design*, **2005**, 5, 1023-1033	3.5	106

15	A third blind test of crystal structure prediction. *Acta Crystallographica Section B: Structural Science*, **2005**, 61, 511-27		326
14	Dynamics in crystals of rigid organic molecules: contrasting the phonon frequencies calculated by molecular dynamics with harmonic lattice dynamics for imidazole and 5-azauracil. *Molecular Physics*, **2004**, 102, 1067-1083	1.7	31
13	Sensitivity of Morphology Prediction to the Force Field: Paracetamol as an Example. *Crystal Growth and Design*, **2004**, 4, 1341-1349	3.5	14
12	An Assessment of Lattice Energy Minimization for the Prediction of Molecular Organic Crystal Structures. *Crystal Growth and Design*, **2004**, 4, 1327-1340	3.5	84
11	A nonempirical anisotropic atom-atom model potential for chlorobenzene crystals. *Journal of the American Chemical Society*, **2003**, 125, 16434-43	16.4	87
10	A computational and experimental search for polymorphs of parabanic acid a salutary tale leading to the crystal structure of oxo-ureido-acetic acid methyl ester. *CrystEngComm*, **2003**, 5, 3-9	3.3	28
9	Atomistic Calculations of Phonon Frequencies and Thermodynamic Quantities for Crystals of Rigid Organic Molecules. *Journal of Physical Chemistry B*, **2003**, 107, 10919-10933	3.4	82
8	A study of the known and hypothetical crystal structures of pyridine: why are there four molecules in the asymmetric unit cell?. *CrystEngComm*, **2002**, 4, 348-355	3.3	78
7	The prediction, morphology, and mechanical properties of the polymorphs of paracetamol. *Journal of the American Chemical Society*, **2001**, 123, 5086-94	16.4	239
6	Elastic Constant Calculations for Molecular Organic Crystals. *Crystal Growth and Design*, **2001**, 1, 13-27	3.5	95
5	Properties of Crystalline Organic Molecules **2001**, 3-50		2
4	Electronic excitations in homopolyatomic bismuth cations: spectroscopic measurements in molten salts and an ab initio CI-singles study. *Chemistry - A European Journal*, **2000**, 6, 1078-86	4.8	21
3	Synthesis, structure, electrostatic properties and spectroscopy of 3-methyl-4,5,6,7-tetrafluoro-1H-indazole. An experimental and ab initio computational study *Journal of the Chemical Society Perkin Transactions II*, **1998**, 2713-2720		16
2	On the effects of basis set truncation and electron correlation in conformers of 2-hydroxy-acetamide. *Advances in Quantum Chemistry*, **1998**, 32, 93-107	1.4	1
1	Computational Crystal Structure Prediction: Towards In SilicoSolid Form Screening43-66		4