SarahÂ L Price

List of Publications by Year
in descending order

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189 papers	13,039 citations	19657 61 h-index	25787 108 g-index
196 all docs	196 docs citations	196 times ranked	7505 citing authors

#	Article	IF	Citations
1	Packing Preferences of Chalcones: A Model Conjugated Pharmaceutical Scaffold. Crystal Growth and Design, 2022, 22, 1801-1816.	3.0	6
2	Progress in understanding crystallisation: a personal perspective. Faraday Discussions, 2022, 235, 569-581.	3.2	2
3	Crystal Structure and Twisted Aggregates of Oxcarbazepine Form III. Crystal Growth and Design, 2022, 22, 4146-4156.	3.0	2
4	A non-empirical intermolecular force-field for trinitrobenzene and its application in crystal structure prediction. Journal of Chemical Physics, 2021, 154, 094123.	3.0	6
5	Toward Physics-Based Solubility Computation for Pharmaceuticals to Rival Informatics. Journal of Chemical Theory and Computation, 2021, 17, 3700-3709.	5.3	15
6	The Crystal Structure of 5â€Aminouracil and the Ambiguity of Alternative Polymorphs #. Israel Journal of Chemistry, 2021, 61, 590.	2.3	1
7	On the Application of Strong Magnetic Fields during Organic Crystal Growth. Crystal Growth and Design, 2021, 21, 6254-6265.	3.0	2
8	Color Differences Highlight Concomitant Polymorphism of Chalcones. Crystal Growth and Design, 2020, 20, 6346-6355.	3.0	9
9	Systematic Finite-Temperature Reduction of Crystal Energy Landscapes. Crystal Growth and Design, 2020, 20, 6847-6862.	3.0	21
10	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
11	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
12	Diabat method for polymorph free energies: Extension to molecular crystals. Journal of Chemical Physics, 2020, 153, 244105.	3.0	1
13	A Prolific Solvate Former, Galunisertib, under the Pressure of Crystal Structure Prediction, Produces Ten Diverse Polymorphs. Journal of the American Chemical Society, 2019, 141, 13887-13897.	13.7	109
14	The (Current) Acridine Solid Form Landscape: Eight Polymorphs and a Hydrate. Crystal Growth and Design, 2019, 19, 4884-4893.	3.0	16
15	The solid state forms of the sex hormone 17-Î²-estradiol. CrystEngComm, 2019, 21, 2154-2163.	2.6	13
16	Charge Distributions of Nitro Groups Within Organic Explosive Crystals: Effects on Sensitivity and Modeling. ACS Omega, 2019, 4, 8614-8625.	3.5	13
17	Crystal structure prediction of flexible pharmaceutical-like molecules: density functional tight-binding as an intermediate optimisation method and for free energy estimation. Faraday Discussions, 2018, 211, 275-296.	3.2	29
18	Applications of crystal structure prediction â€“ inorganic and network structures: general discussion. Faraday Discussions, 2018, 211, 613-642.	3.2	6

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19	Control and prediction of the organic solid state: a challenge to theory and experiment <sup />. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2018, 474, 20180351.	2.1	46
20	Structure searching methods: general discussion. Faraday Discussions, 2018, 211, 133-180.	3.2	3
21	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. Faraday Discussions, 2018, 211, 325-381.	3.2	7
22	Applications of crystal structure prediction â€“ organic molecular structures: general discussion. Faraday Discussions, 2018, 211, 493-539.	3.2	8
23	Serendipitous isolation of a disappearing conformational polymorph of succinic acid challenges computational polymorph prediction. CrystEngComm, 2018, 20, 3971-3977.	2.6	19
24	Successful Computationally Directed Templating of Metastable Pharmaceutical Polymorphs. Crystal Growth and Design, 2018, 18, 5322-5331.	3.0	52
25	Is zeroth order crystal structure prediction (CSP_0) coming to maturity? What should we aim for in an ideal crystal structure prediction code?. Faraday Discussions, 2018, 211, 9-30.	3.2	78
26	Are Oxygen and Sulfur Atoms Structurally Equivalent in Organic Crystals?. Crystal Growth and Design, 2017, 17, 827-833.	3.0	35
27	Direct Observation of Templated Two-Step Nucleation Mechanism during Olanzapine Hydrate Formation. Crystal Growth and Design, 2017, 17, 6382-6393.	3.0	41
28	Correction to Thermochemistry of Racemic and Enantiopure Organic Crystals for Predicting Enantiomer Separation. Crystal Growth and Design, 2017, 17, 6149-6149.	3.0	0
29	Thermal Expansion of Carbamazepine: Systematic Crystallographic Measurements Challenge Quantum Chemical Calculations. Journal of Physical Chemistry Letters, 2017, 8, 4319-4324.	4.6	50
30	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
31	Use of Crystal Structure Informatics for Defining the Conformational Space Needed for Predicting Crystal Structures of Pharmaceutical Molecules. Journal of Chemical Theory and Computation, 2017, 13, 5163-5171.	5.3	19
32	Thermochemistry of Racemic and Enantiopure Organic Crystals for Predicting Enantiomer Separation. Crystal Growth and Design, 2017, 17, 4676-4686.	3.0	33
33	From dimers to the solid-state: Distributed intermolecular force-fields for pyridine. Journal of Chemical Physics, 2017, 147, 161722.	3.0	16
34	Molecular Crystal Structure Prediction. , 2017, , 333-363.		16
35	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
36	Can computed crystal energy landscapes help understand pharmaceutical solids?. Chemical Communications, 2016, 52, 7065-7077.	4.1	146

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37	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
38	The potential of computed crystal energy landscapes to aid solid-form development. Drug Discovery Today, 2016, 21, 912-923.	6.4	91
39	Concomitant conformational dimorphism in 1,2-bis(9-anthryl)acetylene. CrystEngComm, 2015, 17, 4877-4882.	2.6	10
40	Molecular self-assembly and clustering in nucleation processes: general discussion. Faraday Discussions, 2015, 179, 155-197.	3.2	10
41	Are the Crystal Structures of Enantiopure and Racemic Mandelic Acids Determined by Kinetics or Thermodynamics?. Journal of the American Chemical Society, 2015, 137, 11095-11104.	13.7	57
42	Navigating the Waters of Unconventional Crystalline Hydrates. Molecular Pharmaceutics, 2015, 12, 3069-3088.	4.6	62
43	Nucleation in complex multi-component and multi-phase systems: general discussion. Faraday Discussions, 2015, 179, 503-542.	3.2	6
44	Analysis of the conformational profiles of fenamates shows route towards novel, higher accuracy, force-fields for pharmaceuticals. Physical Chemistry Chemical Physics, 2015, 17, 7936-7948.	2.8	23
45	A molecular picture of the problems in ensuring structural purity of tazofelone. Journal of Molecular Structure, 2014, 1078, 26-42.	3.6	37
46	Contrasting Polymorphism of Related Small Molecule Drugs Correlated and Guided by the Computed Crystal Energy Landscape. Crystal Growth and Design, 2014, 14, 2056-2072.	3.0	72
47	Lattice energy, nailed?. Science, 2014, 345, 619-620.	12.6	10
48	Predicting crystal structures of organic compounds. Chemical Society Reviews, 2014, 43, 2098-2111.	38.1	421
49	Absorbing a Little Water: The Structural, Thermodynamic, and Kinetic Relationship between Pyrogallol and Its Tetarto-Hydrate. Crystal Growth and Design, 2013, 13, 4071-4083.	3.0	39
50	Exploring the Experimental and Computed Crystal Energy Landscape of Olanzapine. Crystal Growth and Design, 2013, 13, 1602-1617.	3.0	123
51	Complex Polymorphic System of Gallic Acidâ€"Five Monohydrates, Three Anhydrates, and over 20 Solvates. Crystal Growth and Design, 2013, 13, 19-23.	3.0	97
52	Evaluating a Crystal Energy Landscape in the Context of Industrial Polymorph Screening. Crystal Growth and Design, 2013, 13, 2396-2406.	3.0	58
53	Why don't we find more polymorphs?. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2013, 69, 313-328.	1.1	179
54	Screening for cocrystals of succinic acid and 4-aminobenzoic acid. CrystEngComm, 2012, 14, 2454.	2.6	41

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55	The unexpected but predictable tetrazole packing in flexible 1-benzyl-1H-tetrazole. CrystEngComm, 2012, 14, 6441.	2.6	9
56	Is the Fenamate Group a Polymorphophore? Contrasting the Crystal Energy Landscapes of Fenamic and Tolfenamic Acids. Crystal Growth and Design, 2012, 12, 4230-4239.	3.0	56
57	The Complexity of Hydration of Phloroglucinol: A Comprehensive Structural and Thermodynamic Characterization. Journal of Physical Chemistry B, 2012, 116, 3961-3972.	2.6	60
58	Which, if any, hydrates will crystallise? Predicting hydrate formation of two dihydroxybenzoic acids. Chemical Communications, 2011, 47, 5443-5445.	4.1	92
59	Solid-State Forms of Î²-Resorcylic Acid: How Exhaustive Should a Polymorph Screen Be?. Crystal Growth and Design, 2011, 11, 210-220.	3.0	55
60	A strategy for producing predicted polymorphs: catemeric carbamazepine form V. Chemical Communications, 2011, 47, 7074.	4.1	176
61	Substitutional and orientational disorder in organic crystals: a symmetry-adapted ensemble model. Physical Chemistry Chemical Physics, 2011, 13, 9590.	2.8	49
62	Experimental and Predicted Crystal Energy Landscapes of Chlorothiazide. Crystal Growth and Design, 2011, 11, 405-413.	3.0	9
63	Testing a Variety of Electronic-Structure-Based Methods for the Relative Energies of 5-Formyluracil Crystals. Journal of Chemical Theory and Computation, 2011, 7, 2685-2688.	5.3	23
64	Racemic Naproxen: A Multidisciplinary Structural and Thermodynamic Comparison with the Enantiopure Form. Crystal Growth and Design, 2011, 11, 5659-5669.	3.0	53
65	Successful prediction of a model pharmaceutical in the fifth blind test of crystal structure prediction. International Journal of Pharmaceutics, 2011, 418, 168-178.	5.2	110
66	Computational prediction of salt and cocrystal structuresâ€”Does a proton position matter?. International Journal of Pharmaceutics, 2011, 418, 187-198.	5.2	60
67	Towards crystal structure prediction of complex organic compounds â€“ a report on the fifth blind test. Acta Crystallographica Section B: Structural Science, 2011, 67, 535-551.	1.8	358
68	A computationally inspired investigation of the solid forms of (R)â€1â€phenylethylammoniumâ€(S)â€2â€phenylbutyrate. Chirality, 2010, 22, 447-455.	2.6	6
69	Modelling organic crystal structures using distributed multipole and polarizability-based model intermolecular potentials. Physical Chemistry Chemical Physics, 2010, 12, 8478.	2.8	268
70	Spontaneous Resolution of Enantiomers by Crystallization: Insights from Computed Crystal Energy Landscapes. Crystal Growth and Design, 2010, 10, 1749-1756.	3.0	40
71	Isomers, Conformers, and Cocrystal Stoichiometry: Insights from the Crystal Energy Landscapes of Caffeine with the Hydroxybenzoic Acids. Crystal Growth and Design, 2010, 10, 3263-3272.	3.0	40
72	Carbamazepine Co-crystallization with Pyridine Carboxamides: Rationalization by Complementary Phase Diagrams and Crystal Energy Landscapes. Crystal Growth and Design, 2010, 10, 903-912.	3.0	75

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73	A predicted dimer-based polymorph of 10,11-dihydrocarbamazepine (Form IV). CrystEngComm, 2010, 12, 64-66.	2.6	21
74	Significant progress in predicting the crystal structures of small organic molecules â€“ a report on the fourth blind test. Acta Crystallographica Section B: Structural Science, 2009, 65, 107-125.	1.8	371
75	Salt or Cocrystal? A New Series of Crystal Structures Formed from Simple Pyridines and Carboxylic Acids. Crystal Growth and Design, 2009, 9, 2881-2889.	3.0	183
76	Computed Crystal Energy Landscapes for Understanding and Predicting Organic Crystal Structures and Polymorphism. Accounts of Chemical Research, 2009, 42, 117-126.	15.6	333
77	Can the Formation of Pharmaceutical Cocrystals Be Computationally Predicted? 2. Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2009, 5, 1432-1448.	5.3	118
78	Can the Formation of Pharmaceutical Cocrystals Be Computationally Predicted? I. Comparison of Lattice Energies. Crystal Growth and Design, 2009, 9, 442-453.	3.0	141
79	A first principles prediction of the crystal structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si4.gif" display="inline" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mspace width="0.35em" height="0.8ex" /><mml:mtext>C</mml:mtext></mml:mrow><mml:mrow><mml:mn>6</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mrow> Chemical Physics Letters, 2008, 456, 105-109.	2.6	79
80	Modeling the interplay of inter- and intramolecular hydrogen bonding in conformational polymorphs. Journal of Chemical Physics, 2008, 128, 244708.	3.0	83
81	Computational prediction of organic crystal structures and polymorphism. International Reviews in Physical Chemistry, 2008, 27, 541-568.	2.3	103
82	From crystal structure prediction to polymorph prediction: interpreting the crystal energy landscape. Physical Chemistry Chemical Physics, 2008, 10, 1996.	2.8	159
83	Is the Induction Energy Important for Modeling Organic Crystals?. Journal of Chemical Theory and Computation, 2008, 4, 522-532.	5.3	55
84	A Systematic Experimental and Theoretical Study of the Crystalline State of Six Chloronitrobenzenes. Crystal Growth and Design, 2008, 8, 24-36.	3.0	24
85	Predictable Disorder versus Polymorphism in the Rationalization of Structural Diversity: A Multidisciplinary Study of Eniluracil. Crystal Growth and Design, 2008, 8, 3474-3481.	3.0	49
86	Accurate Induction Energies for Small Organic Molecules. 2. Development and Testing of Distributed Polarizability Models against SAPT(DFT) Energies. Journal of Chemical Theory and Computation, 2008, 4, 19-32.	5.3	77
87	Discovery of three polymorphs of 7-fluoroisatin reveals challenges in using computational crystal structure prediction as a complement to experimental screening. CrystEngComm, 2008, , .	2.6	3
88	The crystal structures of chloro and methyl ortho-benzoic acids and their co-crystal: rationalizing similarities and differences. CrystEngComm, 2008, 10, 1848.	2.6	48
89	Solid Phases of Cyclopentane:â€‰ Combined Experimental and Simulation Study. Journal of Physical Chemistry B, 2008, 112, 3746-3758.	2.6	39
90	Colored Polymorphs: Thermochemical and Structural Features of N-Picryl- p-toluidine Polymorphs and Solvates. Crystal Growth and Design, 2008, 8, 1977-1989.	3.0	38

#	Article	IF	Citations
91	The observed and energetically feasible crystal structures of 5-substituted uracils. New Journal of Chemistry, 2008, 32, 1761.	2.8	39
92	The Thermal Stability of Lattice-Energy Minima of 5-Fluorouracil:Â Metadynamics as an Aid to Polymorph Prediction. Journal of Physical Chemistry B, 2008, 112, 4298-4308.	2.6	64
93	On the Calculation and Interpretation of Crystal Energy Landscapes. NATO Science for Peace and Security Series B: Physics and Biophysics, 2008, , 333-349.	0.3	0
94	Toward the Prediction of Organic Hydrate Crystal Structures. Journal of Chemical Theory and Computation, 2007, 3, 1597-1608.	5.3	52
95	Search for a Predicted Hydrogen Bonding Motif â^' A Multidisciplinary Investigation into the Polymorphism of 3-Azabicyclo[3.3.1]nonane-2,4-dione. Journal of the American Chemical Society, 2007, 129, 3649-3657.	13.7	61
96	Crystallization and Crystal Energy Landscape of Hydrochlorothiazide. Crystal Growth and Design, 2007, 7, 705-712.	3.0	41
97	Toward More Accurate Model Intermolecular Potentials for Organic Molecules. Reviews in Computational Chemistry, 2007, , 225-289.	1.5	16
98	Toward the Computational Design of Diastereomeric Resolving Agents:Â An Experimental and Computational Study of 1-Phenylethylammonium-2-phenylacetate Derivatives. Journal of Physical Chemistry B, 2007, 111, 5326-5336.	2.6	47
99	Carbonic Acid:â€‰ From Polyamorphism to Polymorphism. Journal of the American Chemical Society, 2007, 129, 13863-13871.	13.7	61
100	The polymorphism of progesterone: Stabilization of a â€˜disappearingâ€™ polymorph by coâ€crystallization. Journal of Pharmaceutical Sciences, 2007, 96, 3419-3431.	3.3	72
101	Racemic progesterone: predicted in silico and produced in the solid state. Chemical Communications, 2006, , 4921-3.	4.1	10
102	Kinetic Insights into the Role of the Solvent in the Polymorphism of 5-Fluorouracil from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 3323-3329.	2.6	107
103	Applications Of Dl_poly And Dl_multi To Organic Molecular Crystals. Molecular Simulation, 2006, 32, 985-997.	2.0	27
104	Energy Minimization of Crystal Structures Containing Flexible Molecules. Journal of Chemical Theory and Computation, 2006, 2, 1184-1199.	5.3	83
105	Blind crystal structure prediction of a novel second polymorph of 1-hydroxy-7-azabenzotriazole. Acta Crystallographica Section B: Structural Science, 2006, 62, 642-650.	1.8	9
106	Molecular Conformations and Relative Stabilities Can Be as Demanding of the Electronic Structure Method as Intermolecular Calculations. Journal of Physical Chemistry A, 2006, 110, 8-12.	2.5	115
107	An Automated Parallel Crystallisation Search for Predicted Crystal Structures and Packing Motifs of Carbamazepine. Journal of Pharmaceutical Sciences, 2006, 95, 1918-1930.	3.3	114
108	Modelling Intermolecular Forces for Organic Crystal Structure Prediction. Structure and Bonding, 2005, , 81-123.	1.0	13

#	Article	IF	Citations
109	Calculation of Attachment Energies and Relative Volume Growth Rates As an Aid to Polymorph Prediction. Crystal Growth and Design, 2005, 5, 879-885.	3.0	52
110	Grid Service Orchestration Using the Business Process Execution Language (BPEL). Journal of Grid Computing, 2005, 3, 283-304.	3.9	123
111	Validation of a search technique for crystal structure prediction of flexible molecules by application to piracetam. Acta Crystallographica Section B: Structural Science, 2005, 61, 558-568.	1.8	54
112	Computational prediction and X-ray determination of the crystal structures of 3-oxauracil and 5-hydroxyuracilâ€"an informal blind test. CrystEngComm, 2005, 7, 421.	2.6	11
113	Challenges of Crystal Structure Prediction of Diastereomeric Salt Pairs. Journal of Physical Chemistry B, 2005, 109, 17134-17150.	2.6	50
114	Investigating Unused Hydrogen Bond Acceptors Using Known and Hypothetical Crystal Polymorphism. Crystal Growth and Design, 2005, 5, 983-993.	3.0	49
115	A New Polymorph of 5-Fluorouracil Found Following Computational Crystal Structure Predictions. Journal of the American Chemical Society, 2005, 127, 1116-1117.	13.7	164
116	Groth's Original Concomitant Polymorphs Revisited. Crystal Growth and Design, 2005, 5, 2197-2209.	3.0	40
117	Toward a Molecular Understanding of Crystal Agglomeration. Crystal Growth and Design, 2005, 5, 3-16.	3.0	75
118	Crystal Structure Prediction. , 2004, , 371-379.		4
119	The computational prediction of pharmaceutical crystal structures and polymorphism. Advanced Drug Delivery Reviews, 2004, 56, 301-319.	13.7	215
120	Towards a Fundamental Understanding of the Mechanics of Crystal Agglomeration: A Microscopic and Molecular Approach. Particle and Particle Systems Characterization, 2004, 21, 276-283.	2.3	5
121	Surface Structure of a Complex Inorganic Crystal in Aqueous Solution from Classical Molecular Simulation. Journal of Physical Chemistry B, 2004, 108, 12537-12546.	2.6	8
122	Characterization of Complicated New Polymorphs of Chlorothalonil by X-ray Diffraction and Computer Crystal Structure Prediction. Journal of the American Chemical Society, 2004, 126, 7071-7081.	13.7	52
123	An Experimental and Theoretical Search for Polymorphs of Barbituric Acid:â€‰ The Challenges of Even Limited Conformational Flexibility. Crystal Growth and Design, 2004, 4, 979-987.	3.0	70
124	Toward Crystal Structure Prediction for Conformationally Flexible Molecules:â€‰ The Headaches Illustrated by Aspirin. Crystal Growth and Design, 2004, 4, 1119-1127.	3.0	154
125	Quantifying intermolecular interactions and their use in computational crystal structure prediction. CrystEngComm, 2004, 6, 344.	2.6	59
126	Interference between the Hydrogen Bonds to the Two Rings of Nicotine. Journal of the American Chemical Society, 2003, 125, 5988-5997.	13.7	23

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127	A Nonempirical Anisotropic Atomâ˘Atom Model Potential for Chlorobenzene Crystals. Journal of the American Chemical Society, 2003, 125, 16434-16443.	13.7	98
128	Atomistic Calculations of Phonon Frequencies and Thermodynamic Quantities for Crystals of Rigid Organic Molecules. Journal of Physical Chemistry B, 2003, 107, 10919-10933.	2.6	88
129	Innovation in crystal engineeringÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂ. CrystEngComm, 2002, 4, 500-509.	2.6	235
130	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.	2.6	86
131	Crystal structure prediction of small organic molecules: a second blind test. Acta Crystallographica Section B: Structural Science, 2002, 58, 647-661.	1.8	334
132	Morphologies of Organic Crystals:â€‰ Sensitivity of Attachment Energy Predictions to the Model Intermolecular Potential. Crystal Growth and Design, 2001, 1, 447-453.	3.0	46
133	The Determination of the Crystal Structure of Anhydrous Theophylline by X-ray Powder Diffraction with a Systematic Search Algorithm, Lattice Energy Calculations, and13C and15N Solid-State NMR:Â A Question of Polymorphism in a Given Unit Cell. Journal of Physical Chemistry B, 2001, 105, 5818-5826.	2.6	92
134	Which organic crystal structures are predictable by lattice energy minimisation?. CrystEngComm, 2001, 3, 178-212.	2.6	61
135	The Prediction, Morphology, and Mechanical Properties of the Polymorphs of Paracetamol. Journal of the American Chemical Society, 2001, 123, 5086-5094.	13.7	283
136	Diffusion Monte Carlo simulations on uracilâ€“water using an anisotropic atomâ€“atom potential model. Faraday Discussions, 2001, 118, 95-108.	3.2	20
137	Elastic Constant Calculations for Molecular Organic Crystals. Crystal Growth and Design, 2001, 1, 13-27.	3.0	110
138	Anisotropic Repulsion Potentials for Cyanuric Chloride (C3N3Cl3) and Their Application to Modeling the Crystal Structures of Azaaromatic Chlorides. Journal of Physical Chemistry A, 2001, 105, 9961-9971.	2.5	22
139	Ab initio calculations on indoleâ€“water, 1-methylindoleâ€“water and indoleâ€“(water)2. Chemical Physics Letters, 2000, 331, 253-261.	2.6	40
140	A test of crystal structure prediction of small organic molecules. Acta Crystallographica Section B: Structural Science, 2000, 56, 697-714.	1.8	376
141	Dimer or Catemer? Low-Energy Crystal Packings for Small Carboxylic Acids. Journal of Physical Chemistry B, 2000, 104, 2647-2655.	2.6	140
142	Ab initio and diffusion Monte Carlo study of uracilâ€“water, thymineâ€“water, cytosineâ€“water, and cytosineâ€“(water)2. Physical Chemistry Chemical Physics, 2000, 2, 1281-1290.	2.8	88
143	Developments in computational studies of crystallization and morphology applied to urea. Physical Chemistry Chemical Physics, 2000, 2, 3017-3027.	2.8	29
144	A Systematic Nonempirical Method of Deriving Model Intermolecular Potentials for Organic Molecules:Â Application To Amides. Journal of Physical Chemistry A, 2000, 104, 10958-10971.	2.5	38

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145	The errors in lattice energy minimisation studies: sensitivity to experimental variations in the molecular structure of paracetamol. CrystEngComm, 2000, 2, 183.	2.6	30
146	Aza analogues of nucleic acid bases: experimental determination and computational prediction of the crystal structure of anhydrous 5-azauracil. Journal of Molecular Structure, 1999, 485-486, 349-361.	3.6	15
147	Electrostatic factors in DNA intercalation. Biopolymers, 1999, 52, 84-93.	2.4	53
148	A non-empirical method of determining atom?atom repulsion parameters: application to the crystal structure prediction of an oxyboryl derivative. CrystEngComm, 1999, 1, 24-32.	2.6	6
149	Ab Initio Calculations on Uracilâ˜Water. Journal of Physical Chemistry A, 1999, 103, 1611-1618.	2.5	119
150	A Non-Empirical Intermolecular Potential for Oxalic Acid Crystal Structures. Journal of Physical Chemistry A, 1999, 103, 6448-6457.	2.5	38
151	Three Polymorphs of 2-Amino-5-nitropyrimidine:Â Experimental Structures and Theoretical Predictions. Journal of the American Chemical Society, 1998, 120, 8986-8993.	13.7	61
152	Crystal structure predictions for acetic acid. Journal of Computational Chemistry, 1998, 19, 459-474.	3.3	85
153	Crystal structure predictions for acetic acid. Journal of Computational Chemistry, 1998, 19, 459.	3.3	2
154	Predictions of Crystal Packings for Uracil, 6-Azauracil, and Allopurinol:Â The Interplay between Hydrogen Bonding and Close Packing. Journal of Physical Chemistry A, 1997, 101, 2198-2206.	2.5	61
155	The orientation of N-H...O=C and N-H...N hydrogen bonds in biological systems: how good is a point charge as a model for a hydrogen bonding atom?. Journal of Computer-Aided Molecular Design, 1997, 11, 479-490.	2.9	18
156	Hydrogen bonding of carbonyl, ether, and ester oxygen atoms with alkanol hydroxyl groups. Journal of Computational Chemistry, 1997, 18, 757-774.	3.3	195
157	On the lack of hydrogen bonds in the crystal structure of alloxan. Chemical Physics Letters, 1997, 265, 532-537.	2.6	42
158	Anisotropic atom-atom potentials. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1996, 73, 95-106.	0.6	12
159	Role of Electrostatic Interactions in Determining the Crystal Structures of Polar Organic Molecules. A Distributed Multipole Study. The Journal of Physical Chemistry, 1996, 100, 7352-7360.	2.9	280
160	Applications of realistic electrostatic modelling to molecules in complexes, solids and proteins. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 2997.	1.7	97
161	A Computational Investigation of the Dynamics of Urea Molecules in Solids. Molecular Simulation, 1996, 18, 303-323.	2.0	1
162	Modelling the interactions of protein side-chains. Molecular Engineering, 1995, 5, 89-105.	0.2	2

#	Article	IF	Citations
163	The matching of electrostatic extrema: A useful method in drug design? A study of phosphodiesterase III inhibitors. Journal of Computer-Aided Molecular Design, 1995, 9, 33-43.	2.9	33
164	Relative binding orientations of adenosine A1 receptor ligands â€" A test case for Distributed Multipole Analysis in medicinal chemistry. Journal of Computer-Aided Molecular Design, 1995, 9, 44-54.	2.9	19
165	Solvent interactions with n ring systems in proteins. Protein Engineering, Design and Selection, 1995, 8, 109-116.	2.1	24
166	Modelling the Interactions of Protein Side-Chains. Jerusalem Symposia on Quantum Chemistry and Biochemistry, 1995, , 119-135.	0.2	1
167	Structural and dynamic properties of hydrogen bonding in a tetrahedral arrangement of methanol molecules. A theoretical investigation. Chemical Physics Letters, 1994, 225, 273-279.	2.6	5
168	Amino/Aromatic Interactions in Proteins: Is the Evidence Stacked Against Hydrogen Bonding?. Journal of Molecular Biology, 1994, 239, 315-331.	4.2	319
169	Amino/aromatic interactions. Nature, 1993, 366, 413-413.	27.8	50
170	What base pairings can occur in DNA? A distributed multipole study of the electrostatic interactions between normal and alkylated nucleic acid bases. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 3407.	1.7	26
171	A comparison of three theoretical approaches to the study of side-chain interactions in proteins. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 2619.	1.7	25
172	Electrostatic models for polypeptides: can we assume transferability?. Journal of the Chemical Society, Faraday Transactions, 1992, 88, 1755.	1.7	61
173	The effect of basis set and electron correlation on the predicted electrostatic interactions of peptides. Journal of the American Chemical Society, 1992, 114, 8268-8276.	13.7	46
174	Towards an understanding of the arginine-aspartate interaction. Journal of Molecular Biology, 1992, 226, 251-262.	4.2	103
175	On the relative strengths of amideâ€¦amide and amideâ€¦water hydrogen bonds. Chemical Physics Letters, 1991, 180, 517-523.	2.6	64
176	The nature of the N ? H?O?C hydrogen bond: An intermolecular perturbation theory study of the formamide/formaldehyde complex. Journal of Computational Chemistry, 1990, 11, 1217-1233.	3.3	104
177	A systematic intermolecular potential method applied to chlorine. Molecular Physics, 1990, 71, 1381-1404.	1.7	56
178	An overlap model for estimating the anisotropy of repulsion. Molecular Physics, 1990, 69, 507-533.	1.7	103
179	Towards Realistic Model Intermolecular Potentials. , 1990, , 29-54.		5
180	The representation of molecular electrostatics using interactive graphics. International Journal of Quantum Chemistry, 1989, 36, 73-85.	2.0	1

#	Article	IF	Citations
181	Is the Isotropic Atomâ€"Atom Model Potential Adequate?. Molecular Simulation, 1988, 1, 135-156.	2.0	33
182	Application of Woodward-Hoffmann ideas to solid-state polymorphic phase transitions with specific reference to polymerization ofS2N2and the black phosphorus toA7(arsenic) structural transformation. Physical Review B, 1982, 25, 5778-5789.	3.2	15
183	Role of the crystal-field theory in determining the structures of spinels. Journal of the American Chemical Society, 1982, 104, 92-95.	13.7	181
184	An interpretation of structural sorting diagrams for AB type compounds using molecular orbital ideas. Journal of Physics and Chemistry of Solids, 1982, 43, 521-531.	4.0	7
185	The factors influencing cation site-preferences in spinels a new mendelyevian approach. Physics and Chemistry of Minerals, 1982, 8, 69-76.	0.8	37
186	Factors influencing solid-state structureâ€"an analysis using pseudopotential radii structural maps. Physical Review B, 1981, 24, 2903-2912.	3.2	69
187	Heats of reaction in the solid state and their relationship to Bloch-Zunger structural diagrams. Physical Review B, 1981, 23, 5642-5644.	3.2	5
188	On the inversion of thermophysical properties generated from anisotropic potential energy functions. Chemical Physics Letters, 1980, 74, 193-195.	2.6	7
189	The Nature and Geometry of Intermolecular Interactions: Combination of 3D-Database Information with Theoretical Tools. , 0, , 241-252.		0