Aurora Cruz-Cabeza

List of Publications by Year
in descending order

82 papers	4,548 citations	147801 31 h-index	102487 66 g-index
88 all docs	88 docs citations	88 times ranked	4132 citing authors

#	Article	IF	Citations
1	Conformational Polymorphism. Chemical Reviews, 2014, 114, 2170-2191.	47.7	590
2	Facts and fictions about polymorphism. Chemical Society Reviews, 2015, 44, 8619-8635.	38.1	499
3	Acidâ€“base crystalline complexes and the pKa rule. CrystEngComm, 2012, 14, 6362.	2.6	464
4	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
5	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
6	Solvation and surface effects on polymorph stabilities at the nanoscale. Chemical Science, 2016, 7, 6617-6627.	7.4	128
7	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
8	Towards Prediction of Stoichiometry in Crystalline Multicomponent Complexes. Chemistry - A European Journal, 2008, 14, 8830-8836.	3.3	92
9	Prediction and Observation of Isostructurality Induced by Solvent Incorporation in Multicomponent Crystals. Journal of the American Chemical Society, 2006, 128, 14466-14467.	13.7	91
10	Can the study of self-assembly in solution lead to a good model for the nucleation pathway? The case of tolfenamic acid.. Chemical Science, 2015, 6, 3515-3524.	7.4	85
11	Predicting stoichiometry and structure of solvates. Chemical Communications, 2010, 46, 2224.	4.1	78
12	Open questions in organic crystal polymorphism. Communications Chemistry, 2020, 3, .	4.5	77
13	â€œGuanigmaâ€• The Revised Structure of Biogenic Anhydrous Guanine. Chemistry of Materials, 2015, 27, 8289-8297.	6.7	74
14	Aromatic stacking â€“ a key step in nucleation. Chemical Communications, 2017, 53, 7905-7908.	4.1	70
15	Solvent inclusion in form II carbamazepine. Chemical Communications, 2007, , 1600.	4.1	62
16	Predicting Inclusion Behaviour and Framework Structures in Organic Crystals. Chemistry - A European Journal, 2009, 15, 13033-13040.	3.3	61
17	Amide Pyramidalization in Carbamazepine:â€‰ A Flexibility Problem in Crystal Structure Prediction?. Crystal Growth and Design, 2006, 6, 1858-1866.	3.0	60
18	Identification, classification and relative stability of tautomers in the cambridge structural database. CrystEngComm, 2011, 13, 93-98.	2.6	58

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19	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
20	Concerning Elusive Crystal Forms: The Case of Paracetamol. Journal of the American Chemical Society, 2020, 142, 6682-6689.	13.7	54
21	Pharmaceutical hydrates under ambient conditions from high-pressure seeds: a case study of GABA monohydrate. Chemical Communications, 2014, 50, 1817-1819.	4.1	53
22	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.	3.0	52
23	Metal-Exchanged Î² Zeolites as Catalysts for the Conversion of Acetone to Hydrocarbons. Materials, 2012, 5, 121-134.	2.9	46
24	Space group selection for crystal structure prediction of solvates. CrystEngComm, 2007, 9, 556.	2.6	45
25	Crystal nucleation and growth in a polymorphic system: Ostwald's rule,p-aminobenzoic acid and nucleation transition states. CrystEngComm, 2018, 20, 768-776.	2.6	42
26	Controlling molecular tautomerism through supramolecular selectivity. Chemical Communications, 2013, 49, 7929.	4.1	38
27	Structure prediction, disorder and dynamics in a DMSO solvate of carbamazepine. Physical Chemistry Chemical Physics, 2011, 13, 12808.	2.8	36
28	Transition metal exchanged Î² zeolites: Characterization of the metal state and catalytic application in the methanol conversion to hydrocarbons. Microporous and Mesoporous Materials, 2013, 179, 30-39.	4.4	36
29	Systematic conformational bias in small-molecule crystal structures is rare and explicable. CrystEngComm, 2012, 14, 6797.	2.6	34
30	Synthon preferences in cocrystals of cis-carboxamides:carboxylic acids. CrystEngComm, 2012, 14, 2552.	2.6	33
31	Local environment and acidity in alkaline and alkaline-earth exchanged Î² zeolite: Structural analysis and catalytic properties. Microporous and Mesoporous Materials, 2011, 142, 672-679.	4.4	32
32	Salts, Cocrystals, and Ionic Cocrystals of a â€œSimpleâ€•Tautomeric Compound. Crystal Growth and Design, 2018, 18, 6973-6983.	3.0	32
33	The Kinetic Story of Tailor-made Additives in Polymorphic Systems: New Data and Molecular Insights for p-Aminobenzoic Acid. Crystal Growth and Design, 2018, 18, 7518-7525.	3.0	31
34	Nanoindentation of Molecular Crystals: Lessons Learned from Aspirin. Crystal Growth and Design, 2020, 20, 5956-5966.	3.0	31
35	Crystal structure prediction: are we there yet?. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 437-438.	1.1	30
36	Polymorphism in p-aminobenzoic acid. CrystEngComm, 2019, 21, 2034-2042.	2.6	30

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37	Cocrystals Help Break the â€œRulesâ€•of Isostructurality: Solid Solutions and Polymorphism in the Malic/Tartaric Acid System. Crystal Growth and Design, 2018, 18, 855-863.	3.0	27
38	The unexpected discovery of the ninth polymorph of tolfenamic acid. CrystEngComm, 2021, 23, 3636-3647.	2.6	25
39	Switching polymorph stabilities with impurities provides a thermodynamic route to benzamide form III. Communications Chemistry, 2021, 4, .	4.5	25
40	When Crystals Do Not Grow: The Growth Dead Zone. Crystal Growth and Design, 2019, 19, 4579-4587.	3.0	23
41	Observed and predicted hydrogen bond motifs in crystal structures of hydantoins, dihydrouracils and uracils. New Journal of Chemistry, 2012, 36, 1347.	2.8	22
42	A 2:1 sulfamethazineâ€“theophylline cocrystal exhibiting two tautomers of sulfamethazine. Acta Crystallographica Section C: Crystal Structure Communications, 2011, 67, o306-o309.	0.4	21
43	Same or different â€“ that is the question: identification of crystal forms from crystal structure data. CrystEngComm, 2020, 22, 7170-7185.	2.6	21
44	Transforming Computed Energy Landscapes into Experimental Realities: The Role of Structural Rugosity. Angewandte Chemie - International Edition, 2020, 59, 20357-20360.	13.8	21
45	On the entropy cost of making solvates. Chemical Communications, 2020, 56, 5127-5130.	4.1	21
46	On the prevalence of smooth polymorphs at the nanoscale: implications for pharmaceuticals. CrystEngComm, 2019, 21, 2203-2211.	2.6	20
47	The role of solvation in proton transfer reactions: implications for predicting salt/co-crystal formation using the Î”pK_a rule. Faraday Discussions, 2022, 235, 446-466.	3.2	20
48	Annular tautomerism: experimental observations and quantum mechanics calculations. Journal of Computer-Aided Molecular Design, 2010, 24, 575-586.	2.9	18
49	Impact of Crystal Structure and Molecular Conformation on the Hydration Kinetics of Fluconazole. Crystal Growth and Design, 2019, 19, 7193-7205.	3.0	17
50	The Curious Case of 2-Propyl-1H-benzimidazole in the Solid State: An Experimental and Theoretical Study. Journal of Physical Chemistry A, 2017, 121, 5665-5674.	2.5	14
51	On the kinetics of solvate formation through mechanochemistry. CrystEngComm, 2019, 21, 2097-2104.	2.6	14
52	The interplay of intra- and intermolecular errors in modeling conformational polymorphs. Journal of Chemical Physics, 2022, 156, 104112.	3.0	14
53	Isolation and evolution of labile sulfur allotropesviakinetic encapsulation in interactive porous networks. IUCrJ, 2016, 3, 232-236.	2.2	13
54	Can molecular flexibility control crystallization? The case ofparasubstituted benzoic acids. Chemical Science, 2021, 12, 993-1000.	7.4	12

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55	Can solvated intermediates inform us about nucleation pathways? The case of Î²-pABA. CrystEngComm, 2020, 22, 7447-7459.	2.6	11
56	Discovery and recovery of delta p-aminobenzoic acid. CrystEngComm, 2019, 21, 2058-2066.	2.6	10
57	Transforming Computed Energy Landscapes into Experimental Realities: The Role of Structural Rugosity. Angewandte Chemie, 2020, 132, 20537-20540.	2.0	10
58	Is it usual to be unusual? An investigation into molecular conformations in organic crystals. CrystEngComm, 2020, 22, 7217-7228.	2.6	10
59	Conformation and geometry of cyclopropane rings having Ï€-acceptor substituents: a theoretical and database study. Acta Crystallographica Section B: Structural Science, 2011, 67, 94-102.	1.8	9
60	A novel image analysis technique for 2D characterization of overlapping needle-like crystals. Powder Technology, 2022, 399, 116827.	4.2	9
61	Conformational Change in Molecular Crystals: Impact of Solvate Formation and Importance of Conformational Free Energies. Crystal Growth and Design, 2021, 21, 6924-6936.	3.0	9
62	Applications of crystal structure prediction â€“ organic molecular structures: general discussion. Faraday Discussions, 2018, 211, 493-539.	3.2	8
63	Conformational Change Initiates Dehydration in Fluconazole Monohydrate. Crystal Growth and Design, 2020, 20, 6044-6056.	3.0	8
64	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. Faraday Discussions, 2018, 211, 325-381.	3.2	7
65	Impact of polymorphism on mechanical properties of molecular crystals: a study of p-amino and p-nitro benzoic acid with nanoindentation. CrystEngComm, 2021, 23, 2027-2033.	2.6	7
66	Conformational aspects of polymorphs and phases of 2-propyl-1H-benzimidazole. IUCrJ, 2018, 5, 706-715.	2.2	7
67	Enhanced Concentration of Medium Strength BrÃ¶nsted Acid Sites in Aluminium-Modified Î² Zeolite. Catalysis Letters, 2012, 142, 112-117.	2.6	6
68	Hydrogen-bond landscapes, geometry and energetics of squaric acid and its mono- and dianions: a Cambridge Structural Database, IsoStar and computational study. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2013, 69, 514-523.	1.1	6
69	Crystal Growth Cell Incorporating Automated Image Analysis Enabling Measurement of Facet Specific Crystal Growth Rates. Crystal Growth and Design, 2022, 22, 2837-2848.	3.0	6
70	Isomechanical Groups in Molecular Crystals and Role of Aromatic Interactions. Crystal Growth and Design, 2020, 20, 7516-7525.	3.0	5
71	Geometry and conformation of cyclopropane derivatives having Ïƒ-acceptor and Ïƒ-donor substituents: a theoretical and crystal structure database study. Acta Crystallographica Section B: Structural Science, 2012, 68, 182-188.	1.8	4
72	Probing anisotropic mechanical behaviour in carbamazepine form III. CrystEngComm, 2021, 23, 5826-5838.	2.6	4

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73	Brittle Behavior in Aspirin Crystals: Evidence of Spalling Fracture. Crystal Growth and Design, 2021, 21, 1786-1790.	3.0	4
74	The Impact of Ionic Surfactants on the Crystallisation of Glycine Polymorphs. Israel Journal of Chemistry, 2021, 61, 573-582.	2.3	3
75	Controlling desolvation through polymer-assisted grinding. CrystEngComm, 2022, 24, 2305-2313.	2.6	3
76	Validation of the Existence of Tetrameric Species of Potassium Trimethylsilanolate in the Gas Phase with a Theoretical Cluster Model:Â Role of the Counterion as Charge Localizer in the Structure. Journal of Physical Chemistry A, 2007, 111, 2629-2633.	2.5	2
77	A Truly Polymorphic Issue in Honor of Prof Joel Bernstein. Crystal Growth and Design, 2020, 20, 2819-2823.	3.0	2
78	Multicomponent Crystals of Chlorpropamide: Multiple Conformers, Multiple Zâ€², and Proton Transfer at Play. Crystal Growth and Design, 2021, 21, 3158-3167.	3.0	2
79	The solid state of pharmaceuticals. CrystEngComm, 2019, 21, 2031-2033.	2.6	1
80	Does the Age of Pharmaceuticals Matter? Undetectable Hydrate Seeds Impact Hydration Behavior. Crystal Growth and Design, 2021, 21, 1912-1916.	3.0	1
81	Joel Bernstein (1941â€“2019). Crystal Growth and Design, 2019, 19, 521-522.	3.0	0
82	Professor Roger Davey: Master of All Crystal Trades. Crystal Growth and Design, 0, , .	3.0	0