Kevin J Roberts

List of Publications by Citations

135 papers	3,343 citations	35 h-index	52 g-index
147 ext. papers	3,715 ext. citations	3.4 avg, IF	5.07 L-index

#	Paper	IF	Citations
135	Application of Bravais-Friedel-Donnay-Harker, attachment energy and Ising models to predicting and understanding the morphology of molecular crystals. *Journal Physics D: Applied Physics*, **1991**, 24, 89-99	3	303
134	In-Process ATR-FTIR Spectroscopy for Closed-Loop Supersaturation Control of a Batch Crystallizer Producing Monosodium Glutamate Crystals of Defined Size. *Industrial & Engineering Chemistry Research*, **2003**, 42, 198-206	3.9	119
133	A fluorescence EXAFS study of the structure of copper-rich precipitates in Fe□u and Fe□u□i alloys. *Philosophical Magazine Letters*, **1990**, 61, 223-229	1	115
132	Nucleation, Growth, and Pseudo-Polymorphic Behavior of Citric Acid As Monitored in Situ by Attenuated Total Reflection Fourier Transform Infrared Spectroscopy. *Journal of Physical Chemistry B*, **2001**, 105, 10723-10730	3.4	103
131	Investigation into the structures of some normal alkanes within the homologous series C13H28 to C60H122 using high-resolution synchrotron X-ray powder diffraction. *Journal of Materials Chemistry* , **1994**, 4, 977		102
130	In Situ Small Angle X-ray Scattering (SAXS) Studies of Polymorphism with the Associated Crystallization of Cocoa Butter Fat Using Shearing Conditions. *Crystal Growth and Design*, **2002**, 2, 221-226	3.5	88
129	Scalable solution cocrystallization: case of carbamazepine-nicotinamide I. *CrystEngComm*, **2009**, 11, 501-509	3.9	84
128	Effect of cooling rate on the critical undercooling for crystallization. *Journal of Crystal Growth*, **2010** , 312, 698-704	1.6	83
127	Real-time product morphology monitoring in crystallization using imaging technique. *AICHE Journal* , **2005**, 51, 1406-1414	3.6	80
126	Morphological population balance for modeling crystal growth in face directions. *AICHE Journal*, **2008**, 54, 209-222	3.6	63
125	In Situ Measurement of Solution Concentration during the Batch Cooling Crystallization of l-Glutamic Acid using ATR-FTIR Spectroscopy Coupled with Chemometrics. *Crystal Growth and Design*, **2009**, 9, 692-706	3.5	62
124	Application of Grid-Based Molecular Methods for Modeling Solvent-Dependent Crystal Growth Morphology:□Aspirin Crystallized from Aqueous Ethanolic Solution. *Crystal Growth and Design*, **2007** , 7, 1571-1574	3.5	54
123	An Examination of the Nucleation Kinetics of n-Alkanes in the Homologous Series C13H28 to C32H66, and Their Relationship to Structural Type, Associated with Crystallization from Stagnant Melts. *Langmuir*, **1996**, 12, 5722-5728	4	52
122	A Structural□Kinetic Approach to Model Face-Specific Solution/Crystal Surface Energy Associated with the Crystallization of Acetyl Salicylic Acid from Supersaturated Aqueous/Ethanol Solution. *Crystal Growth and Design*, **2006**, 6, 1324-1334	3.5	51
121	Precision measurement of the growth rate and mechanism of ibuprofen {001} and {011} as a function of crystallization environment. *CrystEngComm*, **2014**, 16, 4568-4586	3.3	49
120	Measurements and modelling of free-surface turbulent flows induced by a magnetic stirrer in an unbaffled stirred tank reactor. *Chemical Engineering Science*, **2009**, 64, 4197-4209	4.4	49
119	Influence of Solvent Composition on the Crystal Morphology and Structure of p-Aminobenzoic Acid Crystallized from Mixed Ethanol and Nitromethane Solutions. *Crystal Growth and Design*, **2017**, 17, 4151-4161	3.5	48

118	The breakage behaviour of Aspirin under quasi-static indentation and single particle impact loading: effect of crystallographic anisotropy. *International Journal of Pharmaceutics*, **2011**, 411, 49-63	6.5	46
117	Investigation into the structures of binary-, tertiary- and quinternary-mixtures of n-alkanes and real diesel waxes using high-resolution synchrotron X-ray powder diffraction. *Journal of Materials Chemistry*, **1998**, 8, 859-869		46
116	Modeling Turbulent Flows with Free-Surface in Unbaffled Agitated Vessels. *Industrial & Engineering Chemistry Research*, **2006**, 45, 2881-2891	3.9	45
115	An Examination into the Effect of Stirrer Material and Agitation Rate on the Nucleation of l-Glutamic Acid Batch Crystallized from Supersaturated Aqueous Solutions. *Crystal Growth and Design*, **2004**, 4, 1039-1044	3.5	44
114	Integration of crystal morphology modeling and on-line shape measurement. *AICHE Journal*, **2006**, 52, 2297-2305	3.6	43
113	Examination of the Process Scale Dependence of l-Glutamic Acid Batch Crystallized from Supersaturated Aqueous Solutions in Relation to Reactor Hydrodynamics. *Industrial & Engineering Chemistry Research*, **2004**, 43, 1227-1234	3.9	43
112	Modeling the crystal morphology of alpha-lactose monohydrate. *Journal of Pharmaceutical Sciences* , **1997**, 86, 135-41	3.9	41
111	Polymorphic transformation of l-glutamic acid monitored using combined on-line video microscopy and X-ray diffraction. *Journal of Crystal Growth*, **2006**, 294, 35-40	1.6	41
110	Scale up study of retreat curve impeller stirred tanks using LDA measurements and CFD simulation. *Chemical Engineering Journal*, **2005**, 108, 81-90	14.7	41
109	The importance of considering growth-induced conformational change in predicting the morphology of benzophenone. *Journal Physics D: Applied Physics*, **1993**, 26, B7-B21	3	41
108	Examination of the Semi-Batch Crystallization of Benzophenone from Saturated Methanol Solution via Aqueous Antisolvent Drowning-Out as Monitored In-Process Using ATR FTIR Spectroscopy. *Crystal Growth and Design*, **2004**, 4, 1053-1060	3.5	40
107	Simulation of energetic stability of facetted l-glutamic acid nanocrystalline clusters in relation to their polymorphic phase stability as a function of crystal size. *Journal of Physical Chemistry B*, **2005**, 109, 19550-2	3.4	39
106	On-line monitoring of a crystallization process. *AICHE Journal*, **2003**, 49, 373-378	3.6	39
105	X-ray powder diffraction studies of alkanes: unit-cell parameters of the homologous series C18H38 to C28H58. *Acta Crystallographica Section B: Structural Science*, **1991**, 47, 280-284		39
104	Solid-state NMR and computational studies of 4-methyl-2-nitroacetanilide. *Magnetic Resonance in Chemistry*, **2006**, 44, 325-33	2.1	38
103	In Situ Measurement of Particle Size during the Crystallization of l-Glutamic Acid under Two Polymorphic Forms: Influence of Crystal Habit on Ultrasonic Attenuation Measurements. *Crystal Growth and Design*, **2002**, 2, 227-234	3.5	38
102	The solid state, surface and morphological properties of p-aminobenzoic acid in terms of the strength and directionality of its intermolecular synthons. *CrystEngComm*, **2015**, 17, 5768-5788	3.3	37
101	Dependence of the critical undercooling for crystallization on the cooling rate. *Journal of Physical Chemistry B*, **2010**, 114, 5441-6	3.4	35

100	Towards an understanding of the nucleation of alpha-para amino benzoic acid from ethanolic solutions: a multi-scale approach. *Faraday Discussions*, **2015**, 179, 79-114	3.6	34
99	Nucleation mechanism and kinetics from the analysis of polythermal crystallisation data: methyl stearate from kerosene solutions. *CrystEngComm*, **2014**, 16, 974-991	3.3	33
98	An Examination of the Kinetics of the Solution-Mediated Polymorphic Phase Transformation between □and □Forms of l-Glutamic Acid as Determined Using Online Powder X-ray Diffraction. *Crystal Growth and Design*, **2008**, 8, 2205-2216	3.5	32
97	Crystal Morphology and Interfacial Stability of□RS-Ibuprofen in Relation to Its Molecular and Synthonic Structure. *Crystal Growth and Design*, **2017**, 17, 3088-3099	3.5	31
96	Formulation pre-screening of inhalation powders using computational atom-atom systematic search method. *Molecular Pharmaceutics*, **2015**, 12, 18-33	5.6	31
95	Deriving empirical potentials for molecular ionic materials. *Mineralogical Magazine*, **1995**, 59, 617-622	1.7	31
94	Application of Systematic Search Methods to Studies of the Structures of Urea□Dihydroxy Benzene Cocrystals. *Journal of Physical Chemistry B*, **2003**, 107, 11820-11826	3.4	30
93	LDA Measurements and CFD Modeling of a Stirred Vessel with a Retreat Curve Impeller. *Industrial & Engineering Chemistry Research*, **2004**, 43, 6534-6547	3.9	28
92	On the Crystal Polymorphic Forms of l-Glutamic Acid Following Temperature Programmed Crystallization in a Batch Oscillatory Baffled Crystallizer. *Crystal Growth and Design*, **2004**, 4, 1129-1135	3.5	26
91	Molecular Modeling of Crystal□Crystal Interactions between the □and □Polymorphic Forms of l-Glutamic Acid Using Grid-Based Methods. *Crystal Growth and Design*, **2007**, 7, 875-884	3.5	25
90	Dislocations in energetic materials Dislocation characterization and post-growth motion in single crystals of cyclotrimethylene trinitramine. *Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties*, **1986**, 53, 531-542		25
89	Particle Shape Characterisation via Image Analysis: from Laboratory Studies to In-process Measurements Using an in Situ Particle Viewer System. *Organic Process Research and Development*, **2008**, 12, 837-849	3.9	24
88	The influence of solution environment on the nucleation kinetics and crystallisability of para-aminobenzoic acid. *Physical Chemistry Chemical Physics*, **2016**, 18, 27507-27520	3.6	23
87	Habit Modification of the Active Pharmaceutical Ingredient Lovastatin Through a Predictive Solvent Selection Approach. *Journal of Pharmaceutical Sciences*, **2019**, 108, 1779-1787	3.9	22
86	Grid-based molecular modeling for pharmaceutical salt screening: Case example of 3,4,6,7,8,9-hexahydro-2H-pyrimido (1,2-a) pyrimidinium acetate. *Journal of Pharmaceutical Sciences*, **2006**, 95, 2361-72	3.9	22
85	A comparative assessment of the influence of different crystallization screening methodologies on the solid forms of carbamazepine co-crystals. *CrystEngComm*, **2013**, 15, 3862	3.3	21
84	An In-Situ Synchrotron X-ray Diffraction Tomography Study of Crystallization and Preferred Crystal Orientation in a Stirred Reactor. *Crystal Growth and Design*, **2005**, 5, 395-397	3.5	21
83	Molecular Modeling of Bulk Impurity Segregation and Impurity-Mediated Crystal Habit Modification of Naphthalene and Phenanthrene in the Presence of Heteroimpurity Species. *Journal of Physical Chemistry B*, **2003**, 107, 4826-4833	3.4	21

82	In-Process Monitoring and Control of Supersaturation in Seeded Batch Cooling Crystallisation of l-Glutamic Acid: From Laboratory to Industrial Pilot Plant. *Organic Process Research and Development*, **2011**, 15, 540-555	3.9	20
81	Morphology and Associated Surface Chemistry of l-Isoleucine Crystals Modeled under the Influence of l-Leucine Additive Molecules. *Crystal Growth and Design*, **2012**, 12, 2195-2203	3.5	19
80	Prediction of the Polar Morphology of Sodium Chlorate Using a Surface-Specific Attachment Energy Model. *Journal of Physical Chemistry B*, **1998**, 102, 7044-7049	3.4	19
79	An examination of binding motifs associated with inter-particle interactions between facetted nano-crystals of acetylsalicylic acid and ascorbic acid through the application of molecular grid-based search methods. *Journal of Pharmaceutical Sciences*, **2009**, 98, 4589-602	3.9	18
78	Application of a Computational Systematic Search Strategy to Study Polymorphism in Phenazine and Perylene. *Journal of Physical Chemistry B*, **1999**, 103, 7762-7770	3.4	18
77	Understanding the Solvent-Induced Habit Modification of Benzophenone in Terms of Molecular Recognition at the Crystal/Solution Interface.. *Chemistry of Materials*, **1994**, 6, 1099-1102	9.6	18
76	Structural variability within, and polymorphic stability of, nano-crystalline molecular clusters of L-glutamic acid and D-mannitol, modelled with respect to their size, shape and crystallisability *CrystEngComm*, **2012**, 14, 1069-1082	3.3	17
75	In Situ Ultrasonic Attenuation Spectroscopic Study of the Dynamic Evolution of Particle Size during Solution-Phase Crystallization of Urea. *Crystal Growth and Design*, **2003**, 3, 67-72	3.5	17
74	Free-surface turbulent flow induced by a Rushton turbine in an unbaffled dish-bottom stirred tank reactor: LDV measurements and CFD simulations. *Canadian Journal of Chemical Engineering*, **2011**, 89, 745-753	2.3	16
73	Investigation of inter- and intra-molecular packing in the solid state for crystals of normal alkanes and homologous mixtures using FT-IR spectroscopy. *Journal of Materials Science*, **1994**, 29, 1915-1919	4.3	16
72	Examination of inequivalent wetting on the crystal habit surfaces of RS-ibuprofen using grid-based molecular modelling. *Physical Chemistry Chemical Physics*, **2018**, 20, 11622-11633	3.6	14
71	Molecular and Solid-State Modeling of the Crystal Purity and Morphology of Caprolactam in the Presence of Synthesis Impurities and the Imino-Tautomeric Species Caprolactim. *Journal of Physical Chemistry B*, **2003**, 107, 13262-13272	3.4	14
70	The crystal morphology and growth rates of triclinic N-docosane crystallising from N-dodecane solutions. *Journal of Crystal Growth*, **2015**, 416, 47-56	1.6	13
69	Molecular Characterization of Strongly and Weakly Interfacially Active Asphaltenes by High-Resolution Mass Spectrometry. *Energy & Fuels*, **2020**, 34, 13966-13976	4.1	13
68	Morphology and Growth of Methyl Stearate as a Function of Crystallization Environment. *Crystal Growth and Design*, **2017**, 17, 563-575	3.5	12
67	Aggregation Behavior of E-SARA Asphaltene Fractions Studied by Small-Angle Neutron Scattering. *Energy & Fuels*, **2020**, 34, 6894-6903	4.1	12
66	In-situ study of the solid solid phase transitions occurring in real diesel wax crystalline systems using differential scanning calorimetry and high-resolution synchrotron X-ray powder diffraction. *Journal of Materials Chemistry*, **1999**, 9, 2385-2392		12
65	Conformational and structural stability of the single molecule and hydrogen bonded clusters of para aminobenzoic acid in the gas and solution phases. *CrystEngComm*, **2018**, 20, 7543-7555	3.3	12

64	Evaluation of Force-Field Calculations of Lattice Energies on a Large Public Dataset, Assessment of Pharmaceutical Relevance, and Comparison to Density Functional Theory. *Journal of Chemical Information and Modeling*, **2019**, 59, 4778-4792	6.1	11
63	Molecular modelling of the incorporation of habit modifying additives: glycine in the presence of L-alanine. *CrystEngComm*, **2011**, 13, 4935	3.3	11
62	A structural study of polymorphism in phenyl salicylate: determination of the crystal structure of a meta-stable phase from X-ray powder diffraction data using a direct space systematic search method. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2002**, 217,	1	11
61	In-situ X-ray diffraction studies of lead dioxide in sulphuric acid during potential cycling. *Phase Transitions*, **1992**, 39, 135-144	1.3	11
60	Synthonic Engineering Modelling Tools for Product and Process Design. *NATO Science for Peace and Security Series A: Chemistry and Biology*, **2017**, 155-176	0.1	11
59	Kinetics of the Aqueous-Ethanol Solution Mediated Transformation between the Beta and Alpha Polymorphs of p-Aminobenzoic Acid. *Crystal Growth and Design*, **2018**, 18, 1117-1125	3.5	10
58	Measuring the Particle Packing of l-Glutamic Acid Crystals through X-ray Computed Tomography for Understanding Powder Flow and Consolidation Behavior. *Crystal Growth and Design*, **2020**, 20, 4252-4263	3.5	9
57	Direction of the polymorphic form of entacapone using an electrochemical tuneable surface template. *CrystEngComm*, **2014**, 16, 3487-3493	3.3	9
56	Computational Modelling Study of the Growth Morphology of the Normal Alkane Docosane and Its Mediation by Tailor-Made Additives. *Molecular Crystals and Liquid Crystals*, **1994**, 248, 243-276		9
55	Combining Morphological Population Balances with Face-Specific Growth Kinetics Data to Model and Predict the Crystallization Processes for Ibuprofen. *Industrial & Engineering Chemistry Research*, **2018**, 57, 16379-16394	3.9	9
54	Synthonic Engineering **2016**, 175-210		8
53	Particle Informatics Advancing Our Understanding of Particle Properties through Digital Design. *Crystal Growth and Design*, **2019**, 19, 5258-5266	3.5	8
52	Isothermal by Design: An Accelerated Approach to the Prediction of the Crystallizability of Slowly Nucleating Systems. *Organic Process Research and Development*, **2019**, 23, 1948-1959	3.9	8
51	Crystallographic Structure, Intermolecular Packing Energetics, Crystal Morphology and Surface Chemistry of Salmeterol Xinafoate (Form I). *Journal of Pharmaceutical Sciences*, **2017**, 106, 882-891	3.9	8
50	Molecular Modelling of the Morphology of Organic Crystals in the Presence of Impurity Species: Recent Applications to Naphthalene, Phenanthrene, and Caprolactam Crystals. *Molecular Crystals and Liquid Crystals*, **2005**, 440, 235-257	0.5	8
49	Chain length dependent polymorphism in even number n-alkanes: line profile analysis of synchrotron powder X-ray diffraction data. *Journal of Materials Science Letters*, **1996**, 15, 1193-1196		8
48	Synchrotron radiation damage in sodium bromate. *Journal of Materials Science Letters*, **1982**, 1, 300-302		8
47	The perfection of polybis (p-toluene sulphonate) diacetylene crystals. *Journal of Materials Science Letters*, **1982**, 1, 150-152		8

46	Crystal Growth and Morphology of Molecular Crystals. *NATO Science for Peace and Security Series A: Chemistry and Biology*, **2017**, 109-131	0.1	8
45	The influence of solid state information and descriptor selection on statistical models of temperature dependent aqueous solubility. *Journal of Cheminformatics*, **2018**, 10, 44	8.6	8
44	A Digital Workflow Supporting the Selection of Solvents for Optimizing the Crystallizability of p-Aminobenzoic Acid. *Organic Process Research and Development*, **2020**, 24, 500-507	3.9	7
43	On-Line Analytical Techniques for Monitoring Crystallisation Processes of Organic Speciality Chemicals. *Molecular Crystals and Liquid Crystals*, **2001**, 356, 273-287		7
42	An examination of the 140°C phase transition in triammonium hydrogen sulphate (NH4)3H(SO4)2 using synchrotron radiation white-beam topography. *Phase Transitions*, **1992**, 39, 171-185	1.3	7
41	Understanding and Designing Tailor-Made Additives for Controlling Nucleation: Case Study of p-Aminobenzoic Acid Crystallizing from Ethanolic Solutions. *Crystal Growth and Design*, **2021**, 21, 1946-1958	3.5	7
40	The Role of Solvent Composition and Polymorph Surface Chemistry in the Solution-Mediated Phase Transformation Process of Cefaclor. *Industrial & Engineering Chemistry Research*, **2018**, 57, 16925-16933	3.9	7
39	Using Soft X-ray Absorption Spectroscopy to Examine the Structural Changes Taking Place around Si and Al Atoms in Kaolinite Following Flash Calcination. *Japanese Journal of Applied Physics*, **1993**, 32, 652	1.4	6
38	Crystallisation Route Map. *NATO Science for Peace and Security Series A: Chemistry and Biology*, **2017** , 179-213	0.1	6
37	Molecular, Solid-State and Surface Structures of the Conformational Polymorphic Forms of Ritonavir in Relation to their Physicochemical Properties. *Pharmaceutical Research*, **2021**, 38, 971-990	4.5	6
36	Assessment of the Thermal Degradation of Sodium Lauroyl Isethionate Using Predictive Isoconversional Kinetics and a Temperature-Resolved Analysis of Evolved Gases. *Industrial & Engineering Chemistry Research*, **2019**, 58, 8112-8122	3.9	5
35	Solubility and Nucleation of Methyl Stearate as a Function of Crystallization Environment. *Energy & Fuels*, **2018**, 32, 3447-3459	4.1	5
34	Process-Focused Synthesis, Crystallization, and Physicochemical Characterization of Sodium Lauroyl Isethionate. *ACS Sustainable Chemistry and Engineering*, **2018**, 6, 2667-2675	8.3	5
33	Off-the-shelf DFT-DISPersion methods: Are they now "on-trend" for organic molecular crystals?. *Journal of Chemical Physics*, **2019**, 151, 044106	3.9	5
32	X-ray Topographic and Polarized Optical Microscopy Studies of Inversion Twinning in Sodium Chlorate Single Crystals Grown in the Presence of Sodium Dithionate Impurities. *Crystal Growth and Design*, **2014**, 14, 6084-6092	3.5	5
31	A novel technique combining high-resolution synchrotron x-ray microtomography and x-ray diffraction for characterization of micro particulates. *Measurement Science and Technology*, **2011**, 22, 115703	2	5
30	Potential fitting to molecular ionic materials. *The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties*, **1996**, 73, 147-152		5
29	Environmental facility for synchrotron radiation topography. *Review of Scientific Instruments*, **1989**, 60, 2498-2501	1.7	5

28	Surface and bulk growth-induced strains in flux grown yttrium aluminium garnet. *Journal of Materials Science Letters*, **1982**, 1, 1-3		5
27	Solubility and crystallisability of the ternary system: Hexadecane and octadecane representative in fuel solvents. *Fuel*, **2018**, 226, 665-674	7.1	5
26	Molecular aggregation of L-isoleucine in aqueous solution and its impact on the determination of solubility and nucleation kinetics. *Journal of Crystal Growth*, **2019**, 519, 91-99	1.6	4
25	The Effect of Surface Molecular Conformational Change on Morphology: A Study of Benzil (0001). *Molecular Crystals and Liquid Crystals*, **1996**, 277, 29-37		4
24	Investigating the Orientations of Langmuir Blodgett Films of Copper Tetra-t-Butyl Phthalocyanine Using Polarised, Ultra-Soft Xanes Spectroscopy. *Molecular Crystals and Liquid Crystals*, **1996**, 278, 157-164		4
23	Using X-ray Absorption Spectroscopy to Probe Structural Change in the Chemical Solid-State. *Molecular Crystals and Liquid Crystals*, **1994**, 248, 207-242		4
22	X-ray powder diffraction studies of n-alkanes: a re-examination of the unit-cell parameters of C24H50 and C26H54. *Acta Crystallographica Section B: Structural Science*, **1992**, 48, 746-746		4
21	The application of an automated crystallization cell used to study the nucleation kinetics of potash alum. *Journal of Materials Science Letters*, **1993**, 12, 1741-1744		4
20	Characterization of the Structural Environment of Dithionate Ions Associated with Their Role in the Crystal Habit Modification of Sodium Chlorate. *Crystal Growth and Design*, **2018**, 18, 3328-3338	3.5	4
19	Determining the Crystal Structures of Organic Solids using X-Ray Powder Diffraction Together with Molecular and Solid State Modeling Techniques. *Molecular Crystals and Liquid Crystals*, **2001**, 356, 389-405		3
18	Using Polarised, Ultra-Soft X-Ray Absorption Spectroscopy to Probe Molecular Orientation in Benzotriazole Films Adsorbed on Partly Oxidised Copper. *Molecular Crystals and Liquid Crystals*, **1996**, 278, 27-36		3
17	The Crystal Structure of Triphendioxazine as Solved by a New Ab Initio Method Utilising High Resolution Powder Diffraction and Computational Chemistry Techniques. *Molecular Crystals and Liquid Crystals*, **1994**, 248, 277-289		3
16	Pharmaceutical Solid-State Characterisation Techniques. *NATO Science for Peace and Security Series A: Chemistry and Biology*, **2017**, 367-393	0.1	3
15	Influence of solution chemistry on the solubility, crystallisability and nucleation behaviour of eicosane in toluene : acetone mixed-solvents. *CrystEngComm*, **2021**, 23, 3109-3125	3.3	3
14	A digital workflow from crystallographic structure to single crystal particle attributes for predicting the formulation properties of terbutaline sulfate. *CrystEngComm*, **2020**, 22, 3347-3360	3.3	2
13	The integrated DL_POLY/DL_FIELD/DL_ANALYSER software platform for molecular dynamics simulations for exploration of the synthonic interactions in saturated benzoic acid/hexane solutions. *Molecular Simulation*, **2021**, 47, 257-272	2	2
12	Crystallographic tomography and molecular modelling of structured organic polycrystalline powders. *CrystEngComm*, **2021**, 23, 2520-2531	3.3	2
11	Isothermal by Design: Comparison with an Established Isothermal Nucleation Kinetics Analysis Method. *Chemical Engineering and Technology*, **2020**, 43, 1971-1980	2	1

10	The thermal expansion coefficients of the alpha and beta polymorphic forms of p-aminobenzoic acid in relation to their bulk crystal chemistry. *CrystEngComm*, **2018**, 20, 4099-4102	3.3	1
9	A NEXAFS Spectroscopic Examination of the Supramolecular Organization of a Red Reactive Azo Dye Adsorbed onto Cellulose Substrates. *Journal of Materials Science Letters*, **1998**, 17, 1223-1225		1
8	Comparison of the Crystal Chemistry, the Process Conditions for Crystallization and the Relative Structural Stability of Two Polymorphic Forms of NG-monomethyl-l-arginine Hydrochloride. *Organic Process Research and Development*, **2008**, 12, 860-868	3.9	1
7	Structural Characterisation of Condensed Molecular Materials using Polarised NEXAFS Spectroscopy. *Molecular Crystals and Liquid Crystals*, **1998**, 313, 39-53		1
6	Digital Design of Batch Cooling Crystallization Processes: Computational Fluid Dynamics Methodology for Modeling Free-Surface Hydrodynamics in Agitated Crystallizers. *Organic Process Research and Development*, **2020**, 24, 2565-2582	3.9	1
5	Influence of a polymeric additive on the crystallisability and nucleation mechanism for the model fuel system of eicosane crystallising from supersaturated toluene solutions. *Journal of Crystal Growth*, **2022**, 581, 126470	1.6	0
4	A Digital Mechanistic Workflow for Predicting Solvent-Mediated Crystal Morphology: The and Forms of l-Glutamic Acid.. *Crystal Growth and Design*, **2022**, 22, 3042-3059	3.5	0
3	A NEXAFS Spectroscopic Examination of the Supramolecular Organization of a Red Reactive Azo Dye Adsorbed onto Cellulose Substrates. *Journal of Materials Science Letters*, **1998**, 17, 1871-1874		
2	Measured Growth Rates of Ibuprofen: Comparing Single Crystal and Bulk Suspensions Data. *Chemical Engineering and Technology*, **2021**, 44, 1287-1293	2	
1	Data for crystallisation, dissolution and saturation temperatures of the ternary system: Hexadecane and octadecane representative in fuel solvents. *Data in Brief*, **2018**, 19, 1382-1392	1.2	