

Kevin J Roberts

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Influence of a polymeric additive on the crystallisability and nucleation mechanism for the model fuel system of eicosane crystallising from supersaturated toluene solutions. <i>Journal of Crystal Growth</i> , 2022 , 581, 126470	1.6	0
134	A Digital Mechanistic Workflow for Predicting Solvent-Mediated Crystal Morphology: The Fundamentals of I-Glutamic Acid. <i>Crystal Growth and Design</i> , 2022 , 22, 3042-3059	3.5	0
133	Measured Growth Rates of Ibuprofen: Comparing Single Crystal and Bulk Suspensions Data. <i>Chemical Engineering and Technology</i> , 2021 , 44, 1287-1293	2	
132	Molecular, Solid-State and Surface Structures of the Conformational Polymorphic Forms of Ritonavir in Relation to their Physicochemical Properties. <i>Pharmaceutical Research</i> , 2021 , 38, 971-990	4.5	6
131	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. <i>Molecular Simulation</i> , 2021 , 47, 257-272	2	2
130	Influence of solution chemistry on the solubility, crystallisability and nucleation behaviour of eicosane in toluene : acetone mixed-solvents. <i>CrystEngComm</i> , 2021 , 23, 3109-3125	3.3	3
129	Crystallographic tomography and molecular modelling of structured organic polycrystalline powders. <i>CrystEngComm</i> , 2021 , 23, 2520-2531	3.3	2
128	Understanding and Designing Tailor-Made Additives for Controlling Nucleation: Case Study of p-Aminobenzoic Acid Crystallizing from Ethanolic Solutions. <i>Crystal Growth and Design</i> , 2021 , 21, 1946-1958	3.5	7
127	Aggregation Behavior of E-SARA Asphaltene Fractions Studied by Small-Angle Neutron Scattering. <i>Energy & Fuels</i> , 2020 , 34, 6894-6903	4.1	12
126	Measuring the Particle Packing of I-Glutamic Acid Crystals through X-ray Computed Tomography for Understanding Powder Flow and Consolidation Behavior. <i>Crystal Growth and Design</i> , 2020 , 20, 4252-4263	3.5	9
125	A Digital Workflow Supporting the Selection of Solvents for Optimizing the Crystallizability of p-Aminobenzoic Acid. <i>Organic Process Research and Development</i> , 2020 , 24, 500-507	3.9	7
124	A digital workflow from crystallographic structure to single crystal particle attributes for predicting the formulation properties of terbutaline sulfate. <i>CrystEngComm</i> , 2020 , 22, 3347-3360	3.3	2
123	Isothermal by Design: Comparison with an Established Isothermal Nucleation Kinetics Analysis Method. <i>Chemical Engineering and Technology</i> , 2020 , 43, 1971-1980	2	1
122	Molecular Characterization of Strongly and Weakly Interfacially Active Asphaltenes by High-Resolution Mass Spectrometry. <i>Energy & Fuels</i> , 2020 , 34, 13966-13976	4.1	13
121	Digital Design of Batch Cooling Crystallization Processes: Computational Fluid Dynamics Methodology for Modeling Free-Surface Hydrodynamics in Agitated Crystallizers. <i>Organic Process Research and Development</i> , 2020 , 24, 2565-2582	3.9	1
120	Evaluation of Force-Field Calculations of Lattice Energies on a Large Public Dataset, Assessment of Pharmaceutical Relevance, and Comparison to Density Functional Theory. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 4778-4792	6.1	11
119	Assessment of the Thermal Degradation of Sodium Lauroyl Isethionate Using Predictive Isoconversional Kinetics and a Temperature-Resolved Analysis of Evolved Gases. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 8112-8122	3.9	5

118	Molecular aggregation of L-isoleucine in aqueous solution and its impact on the determination of solubility and nucleation kinetics. <i>Journal of Crystal Growth</i> , 2019 , 519, 91-99	1.6	4
117	Habit Modification of the Active Pharmaceutical Ingredient Lovastatin Through a Predictive Solvent Selection Approach. <i>Journal of Pharmaceutical Sciences</i> , 2019 , 108, 1779-1787	3.9	22
116	Particle Informatics—Advancing Our Understanding of Particle Properties through Digital Design. <i>Crystal Growth and Design</i> , 2019 , 19, 5258-5266	3.5	8
115	Isothermal by Design: An Accelerated Approach to the Prediction of the Crystallizability of Slowly Nucleating Systems. <i>Organic Process Research and Development</i> , 2019 , 23, 1948-1959	3.9	8
114	Off-the-shelf DFT-DISPersion methods: Are they now "on-trend" for organic molecular crystals?. <i>Journal of Chemical Physics</i> , 2019 , 151, 044106	3.9	5
113	Solubility and Nucleation of Methyl Stearate as a Function of Crystallization Environment. <i>Energy & Fuels</i> , 2018 , 32, 3447-3459	4.1	5
112	Examination of inequivalent wetting on the crystal habit surfaces of RS-ibuprofen using grid-based molecular modelling. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 11622-11633	3.6	14
111	Kinetics of the Aqueous-Ethanol Solution Mediated Transformation between the Beta and Alpha Polymorphs of p-Aminobenzoic Acid. <i>Crystal Growth and Design</i> , 2018 , 18, 1117-1125	3.5	10
110	Process-Focused Synthesis, Crystallization, and Physicochemical Characterization of Sodium Lauroyl Isethionate. <i>ACS Sustainable Chemistry and Engineering</i> , 2018 , 6, 2667-2675	8.3	5
109	The thermal expansion coefficients of the alpha and beta polymorphic forms of p-aminobenzoic acid in relation to their bulk crystal chemistry. <i>CrystEngComm</i> , 2018 , 20, 4099-4102	3.3	1
108	Conformational and structural stability of the single molecule and hydrogen bonded clusters of para aminobenzoic acid in the gas and solution phases. <i>CrystEngComm</i> , 2018 , 20, 7543-7555	3.3	12
107	Combining Morphological Population Balances with Face-Specific Growth Kinetics Data to Model and Predict the Crystallization Processes for Ibuprofen. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 16379-16394	3.9	9
106	The Role of Solvent Composition and Polymorph Surface Chemistry in the Solution-Mediated Phase Transformation Process of Cefaclor. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 16925-16933	3.9	7
105	The influence of solid state information and descriptor selection on statistical models of temperature dependent aqueous solubility. <i>Journal of Cheminformatics</i> , 2018 , 10, 44	8.6	8
104	Characterization of the Structural Environment of Dithionate Ions Associated with Their Role in the Crystal Habit Modification of Sodium Chlorate. <i>Crystal Growth and Design</i> , 2018 , 18, 3328-3338	3.5	4
103	Data for crystallisation, dissolution and saturation temperatures of the ternary system: Hexadecane and octadecane representative in fuel solvents. <i>Data in Brief</i> , 2018 , 19, 1382-1392	1.2	
102	Solubility and crystallisability of the ternary system: Hexadecane and octadecane representative in fuel solvents. <i>Fuel</i> , 2018 , 226, 665-674	7.1	5
101	Crystal Morphology and Interfacial Stability of RS-Ibuprofen in Relation to Its Molecular and Synthonic Structure. <i>Crystal Growth and Design</i> , 2017 , 17, 3088-3099	3.5	31

100	Morphology and Growth of Methyl Stearate as a Function of Crystallization Environment. <i>Crystal Growth and Design</i> , 2017 , 17, 563-575	3.5	12
99	Influence of Solvent Composition on the Crystal Morphology and Structure of p-Aminobenzoic Acid Crystallized from Mixed Ethanol and Nitromethane Solutions. <i>Crystal Growth and Design</i> , 2017 , 17, 4151-4161	3.5	48
98	Crystallographic Structure, Intermolecular Packing Energetics, Crystal Morphology and Surface Chemistry of Salmeterol Xinafoate (Form I). <i>Journal of Pharmaceutical Sciences</i> , 2017 , 106, 882-891	3.9	8
97	Synthonic Engineering Modelling Tools for Product and Process Design. <i>NATO Science for Peace and Security Series A: Chemistry and Biology</i> , 2017 , 155-176	0.1	11
96	Crystallisation Route Map. <i>NATO Science for Peace and Security Series A: Chemistry and Biology</i> , 2017 , 179-213	0.1	6
95	Pharmaceutical Solid-State Characterisation Techniques. <i>NATO Science for Peace and Security Series A: Chemistry and Biology</i> , 2017 , 367-393	0.1	3
94	Crystal Growth and Morphology of Molecular Crystals. <i>NATO Science for Peace and Security Series A: Chemistry and Biology</i> , 2017 , 109-131	0.1	8
93	Synthonic Engineering 2016 , 175-210		8
92	The influence of solution environment on the nucleation kinetics and crystallisability of para-aminobenzoic acid. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 27507-27520	3.6	23
91	Formulation pre-screening of inhalation powders using computational atom-atom systematic search method. <i>Molecular Pharmaceutics</i> , 2015 , 12, 18-33	5.6	31
90	Towards an understanding of the nucleation of alpha-para amino benzoic acid from ethanolic solutions: a multi-scale approach. <i>Faraday Discussions</i> , 2015 , 179, 79-114	3.6	34
89	The solid state, surface and morphological properties of p-aminobenzoic acid in terms of the strength and directionality of its intermolecular synthons. <i>CrystEngComm</i> , 2015 , 17, 5768-5788	3.3	37
88	The crystal morphology and growth rates of triclinic N-docosane crystallising from N-dodecane solutions. <i>Journal of Crystal Growth</i> , 2015 , 416, 47-56	1.6	13
87	Nucleation mechanism and kinetics from the analysis of polythermal crystallisation data: methyl stearate from kerosene solutions. <i>CrystEngComm</i> , 2014 , 16, 974-991	3.3	33
86	X-ray Topographic and Polarized Optical Microscopy Studies of Inversion Twinning in Sodium Chlorate Single Crystals Grown in the Presence of Sodium Dithionate Impurities. <i>Crystal Growth and Design</i> , 2014 , 14, 6084-6092	3.5	5
85	Precision measurement of the growth rate and mechanism of ibuprofen {001} and {011} as a function of crystallization environment. <i>CrystEngComm</i> , 2014 , 16, 4568-4586	3.3	49
84	Direction of the polymorphic form of entacapone using an electrochemical tuneable surface template. <i>CrystEngComm</i> , 2014 , 16, 3487-3493	3.3	9
83	A comparative assessment of the influence of different crystallization screening methodologies on the solid forms of carbamazepine co-crystals. <i>CrystEngComm</i> , 2013 , 15, 3862	3.3	21

82	Morphology and Associated Surface Chemistry of l-Isoleucine Crystals Modeled under the Influence of l-Leucine Additive Molecules. <i>Crystal Growth and Design</i> , 2012 , 12, 2195-2203	3.5	19
81	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. <i>CrystEngComm</i> , 2012 , 14, 1069-1082	3.3	17
80	Free-surface turbulent flow induced by a Rushton turbine in an unbaffled dish-bottom stirred tank reactor: LDV measurements and CFD simulations. <i>Canadian Journal of Chemical Engineering</i> , 2011 , 89, 745-753	2.3	16
79	Molecular modelling of the incorporation of habit modifying additives: glycine in the presence of L-alanine. <i>CrystEngComm</i> , 2011 , 13, 4935	3.3	11
78	In-Process Monitoring and Control of Supersaturation in Seeded Batch Cooling Crystallisation of l-Glutamic Acid: From Laboratory to Industrial Pilot Plant. <i>Organic Process Research and Development</i> , 2011 , 15, 540-555	3.9	20
77	The breakage behaviour of Aspirin under quasi-static indentation and single particle impact loading: effect of crystallographic anisotropy. <i>International Journal of Pharmaceutics</i> , 2011 , 411, 49-63	6.5	46
76	A novel technique combining high-resolution synchrotron x-ray microtomography and x-ray diffraction for characterization of micro particulates. <i>Measurement Science and Technology</i> , 2011 , 22, 115703	2	5
75	Dependence of the critical undercooling for crystallization on the cooling rate. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 5441-6	3.4	35
74	Effect of cooling rate on the critical undercooling for crystallization. <i>Journal of Crystal Growth</i> , 2010 , 312, 698-704	1.6	83
73	An examination of binding motifs associated with inter-particle interactions between faceted nano-crystals of acetylsalicylic acid and ascorbic acid through the application of molecular grid-based search methods. <i>Journal of Pharmaceutical Sciences</i> , 2009 , 98, 4589-602	3.9	18
72	Measurements and modelling of free-surface turbulent flows induced by a magnetic stirrer in an unbaffled stirred tank reactor. <i>Chemical Engineering Science</i> , 2009 , 64, 4197-4209	4.4	49
71	Scalable solution cocrystallization: case of carbamazepine-nicotinamide I. <i>CrystEngComm</i> , 2009 , 11, 501-509	3.9	84
70	In Situ Measurement of Solution Concentration during the Batch Cooling Crystallization of l-Glutamic Acid using ATR-FTIR Spectroscopy Coupled with Chemometrics. <i>Crystal Growth and Design</i> , 2009 , 9, 692-706	3.5	62
69	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. <i>Organic Process Research and Development</i> , 2008 , 12, 860-868	3.9	1
68	Particle Shape Characterisation via Image Analysis: from Laboratory Studies to In-process Measurements Using an in Situ Particle Viewer System. <i>Organic Process Research and Development</i> , 2008 , 12, 837-849	3.9	24
67	An Examination of the Kinetics of the Solution-Mediated Polymorphic Phase Transformation between β and β' Forms of l-Glutamic Acid as Determined Using Online Powder X-ray Diffraction. <i>Crystal Growth and Design</i> , 2008 , 8, 2205-2216	3.5	32
66	Morphological population balance for modeling crystal growth in face directions. <i>AIChE Journal</i> , 2008 , 54, 209-222	3.6	63
65	Molecular Modeling of Crystal-Crystal Interactions between the β and β' Polymorphic Forms of l-Glutamic Acid Using Grid-Based Methods. <i>Crystal Growth and Design</i> , 2007 , 7, 875-884	3.5	25

64	Application of Grid-Based Molecular Methods for Modeling Solvent-Dependent Crystal Growth Morphology: Aspirin Crystallized from Aqueous Ethanolic Solution. <i>Crystal Growth and Design</i> , 2007 , 7, 1571-1574	3.5	54
63	Solid-state NMR and computational studies of 4-methyl-2-nitroacetanilide. <i>Magnetic Resonance in Chemistry</i> , 2006 , 44, 325-33	2.1	38
62	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. <i>Journal of Pharmaceutical Sciences</i> , 2006 , 95, 2361-72	3.9	22
61	Integration of crystal morphology modeling and on-line shape measurement. <i>AICHE Journal</i> , 2006 , 52, 2297-2305	3.6	43
60	Modeling Turbulent Flows with Free-Surface in Unbaffled Agitated Vessels. <i>Industrial & Engineering Chemistry Research</i> , 2006 , 45, 2881-2891	3.9	45
59	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. <i>Crystal Growth and Design</i> , 2006 , 6, 1324-1334	3.5	51
58	Polymorphic transformation of l-glutamic acid monitored using combined on-line video microscopy and X-ray diffraction. <i>Journal of Crystal Growth</i> , 2006 , 294, 35-40	1.6	41
57	Simulation of energetic stability of faceted l-glutamic acid nanocrystalline clusters in relation to their polymorphic phase stability as a function of crystal size. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 19550-2	3.4	39
56	An In-Situ Synchrotron X-ray Diffraction Tomography Study of Crystallization and Preferred Crystal Orientation in a Stirred Reactor. <i>Crystal Growth and Design</i> , 2005 , 5, 395-397	3.5	21
55	Scale up study of retreat curve impeller stirred tanks using LDA measurements and CFD simulation. <i>Chemical Engineering Journal</i> , 2005 , 108, 81-90	14.7	41
54	Real-time product morphology monitoring in crystallization using imaging technique. <i>AICHE Journal</i> , 2005 , 51, 1406-1414	3.6	80
53	Molecular Modelling of the Morphology of Organic Crystals in the Presence of Impurity Species: Recent Applications to Naphthalene, Phenanthrene, and Caprolactam Crystals. <i>Molecular Crystals and Liquid Crystals</i> , 2005 , 440, 235-257	0.5	8
52	Examination of the Process Scale Dependence of l-Glutamic Acid Batch Crystallized from Supersaturated Aqueous Solutions in Relation to Reactor Hydrodynamics. <i>Industrial & Engineering Chemistry Research</i> , 2004 , 43, 1227-1234	3.9	43
51	LDA Measurements and CFD Modeling of a Stirred Vessel with a Retreat Curve Impeller. <i>Industrial & Engineering Chemistry Research</i> , 2004 , 43, 6534-6547	3.9	28
50	An Examination into the Effect of Stirrer Material and Agitation Rate on the Nucleation of l-Glutamic Acid Batch Crystallized from Supersaturated Aqueous Solutions. <i>Crystal Growth and Design</i> , 2004 , 4, 1039-1044	3.5	44
49	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. <i>Crystal Growth and Design</i> , 2004 , 4, 1053-1060	3.5	40
48	On the Crystal Polymorphic Forms of l-Glutamic Acid Following Temperature Programmed Crystallization in a Batch Oscillatory Baffled Crystallizer. <i>Crystal Growth and Design</i> , 2004 , 4, 1129-1135	3.5	26
47	On-line monitoring of a crystallization process. <i>AICHE Journal</i> , 2003 , 49, 373-378	3.6	39

46	Molecular and Solid-State Modeling of the Crystal Purity and Morphology of ϵ -Caprolactam in the Presence of Synthesis Impurities and the Imino-Tautomeric Species Caprolactim. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 13262-13272	3-4	14
45	In Situ Ultrasonic Attenuation Spectroscopic Study of the Dynamic Evolution of Particle Size during Solution-Phase Crystallization of Urea. <i>Crystal Growth and Design</i> , 2003 , 3, 67-72	3-5	17
44	Molecular Modeling of Bulk Impurity Segregation and Impurity-Mediated Crystal Habit Modification of Naphthalene and Phenanthrene in the Presence of Heteroimpurity Species. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 4826-4833	3-4	21
43	In-Process ATR-FTIR Spectroscopy for Closed-Loop Supersaturation Control of a Batch Crystallizer Producing Monosodium Glutamate Crystals of Defined Size. <i>Industrial & Engineering Chemistry Research</i> , 2003 , 42, 198-206	3-9	119
42	Application of Systematic Search Methods to Studies of the Structures of UreaDihydroxy Benzene Cocrystals. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 11820-11826	3-4	30
41	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. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2002 , 217,	1	11
40	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. <i>Crystal Growth and Design</i> , 2002 , 2, 227-234	3-5	38
39	In Situ Small Angle X-ray Scattering (SAXS) Studies of Polymorphism with the Associated Crystallization of Cocoa Butter Fat Using Shearing Conditions. <i>Crystal Growth and Design</i> , 2002 , 2, 221-226	3-5	88
38	Determining the Crystal Structures of Organic Solids using X-Ray Powder Diffraction Together with Molecular and Solid State Modeling Techniques. <i>Molecular Crystals and Liquid Crystals</i> , 2001 , 356, 389-405		3
37	Nucleation, Growth, and Pseudo-Polymorphic Behavior of Citric Acid As Monitored in Situ by Attenuated Total Reflection Fourier Transform Infrared Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2001 , 105, 10723-10730	3-4	103
36	On-Line Analytical Techniques for Monitoring Crystallisation Processes of Organic Speciality Chemicals. <i>Molecular Crystals and Liquid Crystals</i> , 2001 , 356, 273-287		7
35	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. <i>Journal of Materials Chemistry</i> , 1999 , 9, 2385-2392		12
34	Application of a Computational Systematic Search Strategy to Study Polymorphism in Phenazine and Perylene. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 7762-7770	3-4	18
33	A NEXAFS Spectroscopic Examination of the Supramolecular Organization of a Red Reactive Azo Dye Adsorbed onto Cellulose Substrates. <i>Journal of Materials Science Letters</i> , 1998 , 17, 1223-1225		1
32	A NEXAFS Spectroscopic Examination of the Supramolecular Organization of a Red Reactive Azo Dye Adsorbed onto Cellulose Substrates. <i>Journal of Materials Science Letters</i> , 1998 , 17, 1871-1874		
31	Investigation into the structures of binary-, tertiary- and quaternary-mixtures of n-alkanes and real diesel waxes using high-resolution synchrotron X-ray powder diffraction. <i>Journal of Materials Chemistry</i> , 1998 , 8, 859-869		46
30	Prediction of the Polar Morphology of Sodium Chlorate Using a Surface-Specific Attachment Energy Model. <i>Journal of Physical Chemistry B</i> , 1998 , 102, 7044-7049	3-4	19
29	Structural Characterisation of Condensed Molecular Materials using Polarised NEXAFS Spectroscopy. <i>Molecular Crystals and Liquid Crystals</i> , 1998 , 313, 39-53		1

28	Modeling the crystal morphology of alpha-lactose monohydrate. <i>Journal of Pharmaceutical Sciences</i> , 1997 , 86, 135-41	3.9	41
27	An Examination of the Nucleation Kinetics of n-Alkanes in the Homologous Series C ₁₃ H ₂₈ to C ₃₂ H ₆₆ , and Their Relationship to Structural Type, Associated with Crystallization from Stagnant Melts. <i>Langmuir</i> , 1996 , 12, 5722-5728	4	52
26	Potential fitting to molecular ionic materials. <i>The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties</i> , 1996 , 73, 147-152		5
25	Chain length dependent polymorphism in even number n-alkanes: line profile analysis of synchrotron powder X-ray diffraction data. <i>Journal of Materials Science Letters</i> , 1996 , 15, 1193-1196		8
24	The Effect of Surface Molecular Conformational Change on Morphology: A Study of Benzil (0001). <i>Molecular Crystals and Liquid Crystals</i> , 1996 , 277, 29-37		4
23	Using Polarised, Ultra-Soft X-Ray Absorption Spectroscopy to Probe Molecular Orientation in Benzotriazole Films Adsorbed on Partly Oxidised Copper. <i>Molecular Crystals and Liquid Crystals</i> , 1996 , 278, 27-36		3
22	Investigating the Orientations of Langmuir Blodgett Films of Copper Tetra-t-Butyl Phthalocyanine Using Polarised, Ultra-Soft Xanes Spectroscopy. <i>Molecular Crystals and Liquid Crystals</i> , 1996 , 278, 157-164		4
21	Deriving empirical potentials for molecular ionic materials. <i>Mineralogical Magazine</i> , 1995 , 59, 617-622	1.7	31
20	Using X-ray Absorption Spectroscopy to Probe Structural Change in the Chemical Solid-State. <i>Molecular Crystals and Liquid Crystals</i> , 1994 , 248, 207-242		4
19	The Crystal Structure of Triphenioxazine as Solved by a New Ab Initio Method Utilising High Resolution Powder Diffraction and Computational Chemistry Techniques. <i>Molecular Crystals and Liquid Crystals</i> , 1994 , 248, 277-289		3
18	Computational Modelling Study of the Growth Morphology of the Normal Alkane Docosane and Its Mediation by Tailor-Made Additives. <i>Molecular Crystals and Liquid Crystals</i> , 1994 , 248, 243-276		9
17	Investigation of inter- and intra-molecular packing in the solid state for crystals of normal alkanes and homologous mixtures using FT-IR spectroscopy. <i>Journal of Materials Science</i> , 1994 , 29, 1915-1919	4.3	16
16	Investigation into the structures of some normal alkanes within the homologous series C ₁₃ H ₂₈ to C ₆₀ H ₁₂₂ using high-resolution synchrotron X-ray powder diffraction. <i>Journal of Materials Chemistry</i> , 1994 , 4, 977		102
15	Understanding the Solvent-Induced Habit Modification of Benzophenone in Terms of Molecular Recognition at the Crystal/Solution Interface.. <i>Chemistry of Materials</i> , 1994 , 6, 1099-1102	9.6	18
14	The importance of considering growth-induced conformational change in predicting the morphology of benzophenone. <i>Journal Physics D: Applied Physics</i> , 1993 , 26, B7-B21	3	41
13	Using Soft X-ray Absorption Spectroscopy to Examine the Structural Changes Taking Place around Si and Al Atoms in Kaolinite Following Flash Calcination. <i>Japanese Journal of Applied Physics</i> , 1993 , 32, 652	1.4	6
12	The application of an automated crystallization cell used to study the nucleation kinetics of potash alum. <i>Journal of Materials Science Letters</i> , 1993 , 12, 1741-1744		4
11	An examination of the 140°C phase transition in triammonium hydrogen sulphate (NH ₄) ₃ H(SO ₄) ₂ using synchrotron radiation white-beam topography. <i>Phase Transitions</i> , 1992 , 39, 171-185	1.3	7

10	In-situ X-ray diffraction studies of lead dioxide in sulphuric acid during potential cycling. <i>Phase Transitions</i> , 1992 , 39, 135-144	1.3	11
9	X-ray powder diffraction studies of n-alkanes: a re-examination of the unit-cell parameters of C ₂₄ H ₅₀ and C ₂₆ H ₅₄ . <i>Acta Crystallographica Section B: Structural Science</i> , 1992 , 48, 746-746		4
8	X-ray powder diffraction studies of alkanes: unit-cell parameters of the homologous series C ₁₈ H ₃₈ to C ₂₈ H ₅₈ . <i>Acta Crystallographica Section B: Structural Science</i> , 1991 , 47, 280-284		39
7	Application of Bravais-Friedel-Donnay-Harker, attachment energy and Ising models to predicting and understanding the morphology of molecular crystals. <i>Journal Physics D: Applied Physics</i> , 1991 , 24, 89-99	3	303
6	A fluorescence EXAFS study of the structure of copper-rich precipitates in FeCu and FeCuNi alloys. <i>Philosophical Magazine Letters</i> , 1990 , 61, 223-229	1	115
5	Environmental facility for synchrotron radiation topography. <i>Review of Scientific Instruments</i> , 1989 , 60, 2498-2501	1.7	5
4	Dislocations in energetic materials Dislocation characterization and post-growth motion in single crystals of cyclotrimethylene trinitramine. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , 1986 , 53, 531-542		25
3	Surface and bulk growth-induced strains in flux grown yttrium aluminium garnet. <i>Journal of Materials Science Letters</i> , 1982 , 1, 1-3		5
2	Synchrotron radiation damage in sodium bromate. <i>Journal of Materials Science Letters</i> , 1982 , 1, 300-302		8
1	The perfection of polybis (p-toluene sulphonate) diacetylene crystals. <i>Journal of Materials Science Letters</i> , 1982 , 1, 150-152		8