Robert B Hammond

List of Publications by Year
in descending order

72	1,810	293460	340414
papers	citations	24 h-index	39 g-index

76	76	76	1940
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The Structural Pathway from its Solvated Molecular State to the Solution Crystallisation of the Î±- and Î²-Polymorphic Forms of Para Amino Benzoic Acid. Faraday Discussions, 2022, , .	1.6	3
2	A Digital Mechanistic Workflow for Predicting Solvent-Mediated Crystal Morphology: The Î± and Î² Forms of <scp>l</scp>-Glutamic Acid. Crystal Growth and Design, 2022, 22, 3042-3059.	1.4	7
3	Influence of solution chemistry on the solubility, crystallisability and nucleation behaviour of eicosane in tolueneâ€‰:â€‰acetone mixed-solvents. CrystEngComm, 2021, 23, 3109-3125.	1.3	7
4	Crystallographic tomography and molecular modelling of structured organic polycrystalline powders. CrystEngComm, 2021, 23, 2520-2531.	1.3	8
5	Impact of Structural Binding Energies on Dissolution Rates for Single Faceted-Crystals. Crystal Growth and Design, 2021, 21, 1482-1495.	1.4	6
6	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.	1.4	22
7	Measured Growth Rates of Ibuprofen: Comparing Single Crystal and Bulk Suspensions Data. Chemical Engineering and Technology, 2021, 44, 1287-1293.	0.9	2
8	Automated In Silico Energy Mapping of Facet-Specific Interparticle Interactions. Crystal Growth and Design, 2021, 21, 5780-5791.	1.4	2
9	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.	1.3	18
10	A digital workflow from crystallographic structure to single crystal particle attributes for predicting the formulation properties of terbutaline sulfate. CrystEngComm, 2020, 22, 3347-3360.	1.3	6
11	Analysis of screw feeding of faceted particles by discrete element method. Powder Technology, 2020, 367, 474-486.	2.1	14
12	â€œParticle Informaticsâ€• Advancing Our Understanding of Particle Properties through Digital Design. Crystal Growth and Design, 2019, 19, 5258-5266.	1.4	14
13	DEM analysis of the effect of particle shape, cohesion and strain rate on powder rheometry. Powder Technology, 2019, 342, 653-663.	2.1	39
14	Molecular dynamics investigation of substrate wettability alteration and oil transport in a calcite nanopore. Fuel, 2019, 239, 1149-1161.	3.4	35
15	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.	1.4	12
16	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.	1.3	15
17	Molecular Dynamics Simulation of the Salinity Effect on the n-Decane/Water/Vapor Interfacial Equilibrium. Energy & Fuels, 2018, 32, 11080-11092.	2.5	33
18	Crystal Morphology and Interfacial Stability of RS-Ibuprofen in Relation to Its Molecular and Synthonic Structure. Crystal Growth and Design, 2017, 17, 3088-3099.	1.4	47

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19	Influence of shape and surface charge on the sedimentation of spheroidal, cubic and rectangular cuboid particles. Powder Technology, 2017, 322, 75-83.	2.1	20
20	Structures and orientation-dependent interaction forces of titania nanowires using molecular dynamics simulations. Journal of Nanoparticle Research, 2017, 19, 1.	0.8	3
21	Synthonic Engineering Modelling Tools for Product and Process Design. NATO Science for Peace and Security Series A: Chemistry and Biology, 2017, , 155-176.	0.5	13
22	Synthesis of nuclear waste simulants by reaction precipitation: Formation of caesium phosphomolybdate, zirconium molybdate and morphology modification with citratomolybdate complex. Polyhedron, 2015, 89, 129-141.	1.0	25
23	Molecular self-assembly and clustering in nucleation processes: general discussion. Faraday Discussions, 2015, 179, 155-197.	1.6	10
24	Nucleation in complex multi-component and multi-phase systems: general discussion. Faraday Discussions, 2015, 179, 503-542.	1.6	6
25	Probing Composition and Molecular Mobility in Thin Spherical Films Using Nuclear Magnetic Resonance Measurements of Diffusion. Industrial & Engineering Chemistry Research, 2015, 54, 6825-6830.	1.8	3
26	Formulation Pre-screening of Inhalation Powders Using Computational Atomâ€“Atom Systematic Search Method. Molecular Pharmaceutics, 2015, 12, 18-33.	2.3	43
27	Moving boundary models for the growth of crystalline deposits from undetected leakages of industrial process liquors. Computers and Chemical Engineering, 2014, 71, 331-346.	2.0	8
28	Nucleation mechanism and kinetics from the analysis of polythermal crystallisation data: methyl stearate from kerosene solutions. CrystEngComm, 2014, 16, 974-991.	1.3	43
29	Characterising highly active nuclear waste simulants. Chemical Engineering Research and Design, 2013, 91, 742-751.	2.7	14
30	A comparative assessment of the influence of different crystallization screening methodologies on the solid forms of carbamazepine co-crystals. CrystEngComm, 2013, 15, 3862.	1.3	26
31	Influence of size and temperature on the phase stability and thermophysical properties of anatase TiO2 nanoparticles: molecular dynamics simulation. Journal of Nanoparticle Research, 2013, 15, 1.	0.8	7
32	Molecular Dynamics Simulation of Anatase TiO₂ Nanoparticles. Journal of Nanoscience and Nanotechnology, 2013, 13, 1047-1052.	0.9	11
33	Characterisation of Nano-Particles in Colloids: Relationship Between Particle Size and Electrical Impedance Spectra. Journal of Nanoscience and Nanotechnology, 2013, 13, 808-812.	0.9	13
34	A meshless method for solving a twoâ€dimensional transient inverse geometric problem. International Journal of Numerical Methods for Heat and Fluid Flow, 2013, 23, 790-817.	1.6	8
35	Detection of a two-dimensional moving cavity. International Journal of Computer Mathematics, 2012, 89, 1569-1582.	1.0	2
36	Molecular Dynamics Study of Anatase TiO2 Nanoparticles in Water and Vacuum Environments. , 2012, , .		0

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37	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 â€˜crystallisabilityâ€™. CrystEngComm, 2012, 14, 1069-1082.	1.3	20
38	Molecular modelling of the incorporation of habit modifying additives: Î±-glycine in the presence of l-alanine. CrystEngComm, 2011, 13, 4935.	1.3	13
39	Direct Observation of the Dynamics of Bridge Formation between Urea Prills. Industrial & Engineering Chemistry Research, 2011, 50, 11728-11733.	1.8	10
40	Multi-dimensional advances for industrial process monitoring. Nuclear Engineering and Design, 2011, 241, 1937.	0.8	0
41	Characterization of crystallisation processes with electrical impedance spectroscopy. Nuclear Engineering and Design, 2011, 241, 1938-1944.	0.8	13
42	Effect of cooling rate on the critical undercooling for crystallization. Journal of Crystal Growth, 2010, 312, 698-704.	0.7	112
43	Dependence of the Critical Undercooling for Crystallization on the Cooling Rate. Journal of Physical Chemistry B, 2010, 114, 5441-5446.	1.2	45
44	Scalable solution cocrystallization: case of carbamazepine-nicotinamide I. CrystEngComm, 2009, 11, 501-509.	1.3	91
45	An Examination of the Influence of Divalent Cationic Dopants on the Bulk and Surface Properties of Ba(NO3)2 Associated with Crystallization. Crystal Growth and Design, 2009, 9, 2588-2594.	1.4	11
46	Comparison of the Crystal Chemistry, the Process Conditions for Crystallization and the Relative Structural Stability of Two Polymorphic Forms of N^G-monomethyl-<scp>l</scp>-arginine Hydrochloride. Organic Process Research and Development, 2008, 12, 860-868.	1.3	1
47	Behavior of Thin Films of Poly(oxyethylene)â^'Poly(oxybutylene) Copolymers Studied by Brewster Angle Microscopy and Atomic Force Microscopy. Langmuir, 2008, 24, 13470-13476.	1.6	1
48	An Examination of the Kinetics of the Solution-Mediated Polymorphic Phase Transformation between Î±- and Î²-Forms of <scp>l</scp>-Glutamic Acid as Determined Using Online Powder X-ray Diffraction. Crystal Growth and Design, 2008, 8, 2205-2216.	1.4	37
49	An examination of polymorphic stability and molecular conformational flexibility as a function of crystal size associated with the nucleation and growth of benzophenone. Faraday Discussions, 2007, 136, 91.	1.6	22
50	Quantifying solubility enhancement due to particle size reduction and crystal habit modification: Case study of acetyl salicylic acid. Journal of Pharmaceutical Sciences, 2007, 96, 1967-1973.	1.6	60
51	Structural Analysis of PEOâ^'PBO Copolymer Monolayers at the Airâ^'Water Interface. Langmuir, 2006, 22, 8821-8825.	1.6	7
52	A Structuralâ^'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.	1.4	57
53	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.	0.7	41
54	Solid-state NMR and computational studies of 4-methyl-2-nitroacetanilide. Magnetic Resonance in Chemistry, 2006, 44, 325-333.	1.1	43

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55	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, 2361-2372.	1.6	28
56	An examination of the thermal expansion of urea using high-resolution variable-temperature X-ray powder diffraction. Journal of Applied Crystallography, 2005, 38, 1038-1039.	1.9	12
57	Enhancing the Signal-to-Noise Ratio of X-ray Diffraction Profiles by Smoothed Principal Component Analysis. Analytical Chemistry, 2005, 77, 6563-6570.	3.2	23
58	Structural Studies of the Polymorphs of Carbamazepine, Its Dihydrate, and Two Solvates. Organic Process Research and Development, 2005, 9, 902-910.	1.3	117
59	Molecular Packing, Morphological Modeling, and Image Analysis of Cyanazine Crystals Precipitated from Aqueous Ethanol Solutions. Crystal Growth and Design, 2004, 4, 711-715.	1.4	8
60	Application of In-Process X-ray Powder Diffraction for the Identification of Polymorphic Forms during Batch Crystallization Reactions. Crystal Growth and Design, 2004, 4, 943-948.	1.4	18
61	Molecular and Solid-State Modeling of the Crystal Purity and Morphology of Îµ-Caprolactam in the Presence of Synthesis Impurities and the Imino-Tautomeric Species Caprolactim. Journal of Physical Chemistry B, 2003, 107, 13262-13272.	1.2	14
62	Dynamic In-Process Examination of Particle Size and Crystallographic Form under Defined Conditions of Reactant Supersaturation as Associated with the Batch Crystallization of Monosodium Glutamate from Aqueous Solution. Industrial & Engineering Chemistry Research, 2003, 42, 4888-4898.	1.8	37
63	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.	1.2	24
64	Application of Systematic Search Methods to Studies of the Structures of Ureaâ^'Dihydroxy Benzene Cocrystals. Journal of Physical Chemistry B, 2003, 107, 11820-11826.	1.2	38
65	Refinement of hydrogen atomic position in a hydrogen bond using a combination of solid-state NMR and computation. Chemical Communications, 2003, , 2834.	2.2	56
66	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.	1.2	92
67	On-Line Analytical Techniques for Monitoring Crystallisation Processes of Organic Speciality Chemicals. Molecular Crystals and Liquid Crystals, 2001, 356, 273-287.	0.3	9
68	Metastable Î²-phase of benzophenone: independent structure determinations via X-ray powder diffraction and single crystal studies. Acta Crystallographica Section B: Structural Science, 2000, 56, 486-496.	1.8	58
69	Application of a Computational Systematic Search Strategy to Study Polymorphism in Phenazine and Perylene. Journal of Physical Chemistry B, 1999, 103, 7762-7770.	1.2	22
70	Computationally Assisted Structure Determination for Molecular Materials from X-ray Powder Diffraction Data. Journal of Physical Chemistry B, 1997, 101, 6532-6536.	1.2	43
71	X-Form metal-free phthalocyanine: crystal structure determination using a combination of high-resolution X-ray powder diffraction and molecular modelling techniques. Journal of the Chemical Society Perkin Transactions II, 1996, , 1527.	0.9	44
72	An Ab Initio Approach to Crystal Structure Determination Using High-Resolution Powder Diffraction and Computational Chemistry Techniques: Application to 6,13-Dichlorotriphendioxazine. Chemistry of Materials, 1995, 7, 2322-2326.	3.2	21