

Andrew L Rohl

List of Publications by Year in descending order

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126
papers

6,900
citations

81900

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62596

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129
all docs

129
docs citations

129
times ranked

7102
citing authors

#	ARTICLE	IF	CITATIONS
1	A self-supervised learning based approach to analyze Martian water-ice cloud properties for planetary atmospheric applications. <i>Acta Astronautica</i> , 2021, 181, 1-13.	3.2	3
2	Stabilization of Aragonite: Role of Mg ²⁺ and Other Impurity Ions. <i>Crystal Growth and Design</i> , 2020, 20, 5006-5017.	3.0	24
3	Tip dependence of three-dimensional scanning force microscopy images of calcite-water interfaces investigated by simulation and experiments. <i>Nanoscale</i> , 2020, 12, 12856-12868.	5.6	15
4	Why Are Some Crystals Straight?. <i>Journal of Physical Chemistry C</i> , 2020, 124, 15616-15624.	3.1	26
5	Using Molecular Modelling to Understand and Predict the Impact of Organic Additives as Crystal Growth Modifiers. <i>Australian Journal of Chemistry</i> , 2020, 73, 724.	0.9	3
6	Can macrocyclic phosphonate molecules inhibit barium sulfate crystallization?. <i>CrystEngComm</i> , 2019, 21, 807-815.	2.6	4
7	Atomistic Simulation of Atomic Force Microscopy Imaging of Hydration Layers on Calcite, Dolomite, and Magnesite Surfaces. <i>Journal of Physical Chemistry C</i> , 2019, 123, 14985-14992.	3.1	30
8	Resolving Point Defects in the Hydration Structure of Calcite (10.4) with Three-Dimensional Atomic Force Microscopy. <i>Physical Review Letters</i> , 2018, 120, 116101.	7.8	58
9	Timoshenko Bending and Eshelby Twisting Predicted in Molecular Nanocrystals. <i>Journal of Physical Chemistry C</i> , 2018, 122, 25085-25091.	3.1	9
10	Molecular Dynamics Visualization (MDV): Stereoscopic 3D Display of Biomolecular Structure and Interactions Using the Unity Game Engine. <i>Journal of Integrative Bioinformatics</i> , 2018, 15, .	1.5	22
11	Atomic force microscope adhesion measurements and atomistic molecular dynamics simulations at different humidities. <i>Measurement Science and Technology</i> , 2017, 28, 034004.	2.6	6
12	Synthesis, Stereochemistry and Antiparasitic Activity of Derivatives of (4 <i>R</i>)-4,6-Dihydroxy- <i>N</i> -methyl-1,2,3,4-tetrahydroisoquinoline. <i>ChemistrySelect</i> , 2017, 2, 2006-2013.	1.5	4
13	Powder diffraction and crystal structure prediction identify four new coumarin polymorphs. <i>Chemical Science</i> , 2017, 8, 4926-4940.	7.4	97
14	The controlled disassembly of mesostructured perovskites as an avenue to fabricating high performance nanohybrid catalysts. <i>Nature Communications</i> , 2017, 8, 15553.	12.8	65
15	Difference Hirshfeld fingerprint plots: a tool for studying polymorphs. <i>CrystEngComm</i> , 2017, 19, 2207-2215.	2.6	20
16	Atomistic simulation of the measurement of mechanical properties of gold nanorods by AFM. <i>Scientific Reports</i> , 2017, 7, 16257.	3.3	6
17	A Supramolecular Ice Growth Inhibitor. <i>Journal of the American Chemical Society</i> , 2016, 138, 13396-13401.	13.7	83
18	Structure, Energetics, and Dynamics of Screw Dislocations in Even <i>n</i> -Alkane Crystals. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3112-3117.	4.6	11

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19	Can Point Defects in Surfaces in Solution be Atomically Resolved by Atomic Force Microscopy?. <i>Physical Review Letters</i> , 2016, 117, 226101.	7.8	18
20	Understanding 2D atomic resolution imaging of the calcite surface in water by frequency modulation atomic force microscopy. <i>Nanotechnology</i> , 2016, 27, 415709.	2.6	20
21	Resorcinol Crystallization from the Melt: A New Ambient Phase and New "Riddles". <i>Journal of the American Chemical Society</i> , 2016, 138, 4881-4889.	13.7	74
22	Silver(i), gold(i) and palladium(ii) complexes of a NHC-pincer ligand with an aminotriazine core: a comparison with pyridyl analogues. <i>Dalton Transactions</i> , 2016, 45, 1484-1495.	3.3	15
23	Dislocation-Actuated Growth and Inhibition of Hexagonal α -Cystine Crystallization at the Molecular Level. <i>Crystal Growth and Design</i> , 2015, 15, 921-934.	3.0	28
24	Benchmarking Calculated Lattice Parameters and Energies of Molecular Crystals Using van der Waals Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3423-3437.	5.3	56
25	van der Waals corrected density functional calculations of the adsorption of benzene on the Cu (111) surface. <i>Journal of Computational Chemistry</i> , 2014, 35, 2263-2271.	3.3	11
26	Effect of Lanthanum on the Crystal Growth of Barium Sulfate. <i>Crystal Growth and Design</i> , 2014, 14, 1650-1658.	3.0	20
27	Structural Correspondence of Solution, Liquid Crystal, and Crystalline Phases of the Chromonic Mesogen Sunset Yellow. <i>Crystal Growth and Design</i> , 2014, 14, 4166-4176.	3.0	21
28	Twisted Aspirin Crystals. <i>Journal of the American Chemical Society</i> , 2013, 135, 3395-3398.	13.7	86
29	Chemical evolution via beta decay: a case study in strontium-90. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 065504.	1.8	17
30	Electronic structure of phosphorus and arsenic ³⁻ -doped germanium. <i>Physical Review B</i> , 2013, 88, .	3.2	4
31	Noncovalent Interactions in SIESTA Using the vdW-DF Functional: S22 Benchmark and Macrocyclic Structures. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 281-289.	5.3	26
32	Prediction of Soai Reaction Enantioselectivity Induced by Crystals of N -(2-Thienylcarbonyl)glycine. <i>Crystal Growth and Design</i> , 2012, 12, 2138-2145.	3.0	32
33	Computational methodology for chirality determination in the Soai reaction by crystals: $\hat{1}^3$ -glycine. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	3
34	<i>Ab Initio</i> Molecular Dynamics Simulations of (101) Surfaces of Potassium Dihydrogenphosphate. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1604-1609.	5.3	8
35	Investigation into the effects of phosphonic inhibitors on the formation of calcium sulfate scales. <i>Desalination and Water Treatment</i> , 2011, 29, 294-301.	1.0	10
36	Controlling Mesoscale Crystal Helicity with Additives, Again. <i>Crystal Growth and Design</i> , 2011, 11, 2070-2073.	3.0	31

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37	Effects of Process Parameters on Gypsum Scale Formation in Pipes. <i>Chemical Engineering and Technology</i> , 2011, 34, 1003-1009.	1.5	20
38	Implications of transmutation on the defect chemistry in crystalline waste forms. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2010, 268, 3261-3264.	1.4	14
39	A NOVEL SPINNING DISC CONTINUOUS STIR TANK AND SETTLER REACTOR (SDCSTR) MODEL FOR CONTINUOUS SYNTHESIS OF TITANIA: A PHENOMENOLOGICAL MODEL. <i>Chemical Engineering Communications</i> , 2010, 198, 73-84.	2.6	4
40	Effects of Organic Additives on Calcium Sulfate Scaling in Pipes. <i>Australian Journal of Chemistry</i> , 2009, 62, 927.	0.9	21
41	Understanding barium sulfate precipitation onto stainless steel. <i>Applied Surface Science</i> , 2008, 254, 3459-3468.	6.1	18
42	Growth modification of hematite by phosphonate additives. <i>Journal of Crystal Growth</i> , 2008, 310, 688-698.	1.5	11
43	Hirshfeld Surfaces Identify Inadequacies in Computations of Intermolecular Interactions in Crystals: Pentamorphic 1,8-Dihydroxyanthraquinone. <i>Crystal Growth and Design</i> , 2008, 8, 4517-4525.	3.0	482
44	A study of the high-pressure polymorphs of L-serine using ab initio structures and PIXEL calculations. <i>CrystEngComm</i> , 2008, 10, 1154.	2.6	48
45	An efficient technique for the prediction of solvent-dependent morphology: the COSMIC method. <i>Molecular Simulation</i> , 2007, 33, 1237-1246.	2.0	24
46	Mechanisms of Dye Incorporation into Potassium Sulfate: Computational and Experimental Studies. <i>Journal of Physical Chemistry C</i> , 2007, 111, 9283-9289.	3.1	8
47	Effects of temperature on the scaling of calcium sulphate in pipes. <i>Powder Technology</i> , 2007, 179, 31-37.	4.2	106
48	The interaction of EDTA with barium sulfate. <i>Journal of Colloid and Interface Science</i> , 2007, 316, 553-561.	9.4	60
49	Understanding the mechanism by which nitrilotriacetic acid interacts with precipitating barium sulfate. <i>CrystEngComm</i> , 2006, 8, 869.	2.6	18
50	Molecular Modeling of Phosphonate Molecules onto Barium Sulfate Terraced Surfaces. <i>Journal of Physical Chemistry B</i> , 2006, 110, 7414-7424.	2.6	55
51	Ab Initio Simulations of the (101) Surfaces of Potassium Dihydrogenphosphate (KDP). <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 797-800.	5.3	5
52	Comment on "Examination of Spinel and Nonspinel Structural Models for $\hat{\Gamma}^3$ -Al ₂ O ₃ by DFT and Rietveld Refinement Simulations". <i>Journal of Physical Chemistry B</i> , 2006, 110, 20721-20723.	2.6	33
53	What is Syncrystallization? States of the pH Indicator Methyl Red in Crystals of Phthalic Acid. <i>Journal of the American Chemical Society</i> , 2006, 128, 5548-5559.	13.7	28
54	The interstellar gas-phase formation of CO ₂ " Assisted or not by water molecules?. <i>Chemical Physics</i> , 2006, 320, 214-228.	1.9	28

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55	Robert Boyle's chiral crystal chemistry: Computational re-evaluation of enantioselective adsorption on quartz. <i>Chirality</i> , 2006, 18, 127-133.	2.6	15
56	Quantum mechanical vs. empirical potential modeling of uranium dioxide (UO ₂) surfaces: (111), (110), and (100). <i>American Mineralogist</i> , 2006, 91, 1761-1772.	1.9	47
57	Incorporation of impurity anions into DSP: insights into structure and stability from computer modelling. <i>Molecular Simulation</i> , 2006, 32, 35-44.	2.0	8
58	Calculation of Attachment Energies and Relative Volume Growth Rates As an Aid to Polymorph Prediction. <i>Crystal Growth and Design</i> , 2005, 5, 879-885.	3.0	52
59	Linking Additive Structures to Nanoparticle Properties. <i>Journal of Metastable and Nanocrystalline Materials</i> , 2005, 23, 51-54.	0.1	0
60	Empirical molecular modelling of crystal growth modifiers. <i>Molecular Simulation</i> , 2005, 31, 393-398.	2.0	10
61	Comparison of the effect growth inhibitors have on an isostructural pair of salts. <i>CrystEngComm</i> , 2005, 7, 320.	2.6	5
62	Interatomic Potentials for Simulating MnO ₂ Polymorphs. <i>Molecular Simulation</i> , 2005, 31, 25-32.	2.0	4
63	Determination of the structure of γ -alumina from interatomic potential and first-principles calculations: The requirement of significant numbers of nonspinel positions to achieve an accurate structural model. <i>Physical Review B</i> , 2005, 71, .	3.2	139
64	GDIS: a visualization program for molecular and periodic systems. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2005, 220, .	0.8	97
65	The Epitaxial Growth of Cholesterol Crystals from Bile Solutions on Calcite Substrates. <i>Journal of the American Chemical Society</i> , 2004, 126, 7915-7924.	13.7	38
66	Luminescent Probes of Crystal Growth: Surface Charge and Polar Axis Sense in Dye-Doped Potassium Hydrogen Phthalate. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 5328-5331.	13.8	34
67	Boehmite Derived γ -Alumina System. Part 1. Structural Evolution with Temperature, with the Identification and Structural Determination of a New Transition Phase, γ -Alumina.. <i>ChemInform</i> , 2004, 35, no.	0.0	0
68	The effect of calcium ions on the precipitation of barium sulphate 1: calcium ions in the absence of organic additives. <i>Journal of Crystal Growth</i> , 2004, 262, 572-580.	1.5	32
69	The effect of calcium cations on the precipitation of barium sulfate 2: calcium ions in the presence of organic additives. <i>Journal of Crystal Growth</i> , 2004, 270, 593-603.	1.5	18
70	Boehmite Derived γ -Alumina System. 1. Structural Evolution with Temperature, with the Identification and Structural Determination of a New Transition Phase, γ -Alumina. <i>Chemistry of Materials</i> , 2004, 16, 220-236.	6.7	176
71	Boehmite-Derived γ -Alumina System. 2. Consideration of Hydrogen and Surface Effects. <i>Chemistry of Materials</i> , 2004, 16, 1914-1923.	6.7	70
72	The role of phosphonate speciation on the inhibition of barium sulfate precipitation. <i>Journal of Crystal Growth</i> , 2003, 249, 584-593.	1.5	38

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73	Adsorption energetics of potassium sulfate dye inclusion crystals. <i>Journal of Molecular Structure</i> , 2003, 647, 65-73.	3.6	6
74	The General Utility Lattice Program (GULP). <i>Molecular Simulation</i> , 2003, 29, 291-341.	2.0	1,921
75	Computer prediction of crystal morphology. <i>Current Opinion in Solid State and Materials Science</i> , 2003, 7, 21-26.	11.5	57
76	Evidence from surface phonons for the (2 Å ⁻¹) reconstruction of the (101̄...4) surface of calcite from computer simulation. <i>American Mineralogist</i> , 2003, 88, 921-925.	1.9	100
77	Incorporation of Cyano Transition Metal Complexes in KCl Crystals—Experimental and Computational Studies. <i>Australian Journal of Chemistry</i> , 2003, 56, 675.	0.9	8
78	IN SITU CHARACTERISATION OF CALCITE GROWTH AND INHIBITION USING ATOMIC FORCE MICROSCOPY. <i>International Journal of Modern Physics B</i> , 2002, 16, 25-33.	2.0	20
79	Toward a Fundamental Understanding of Molecular Recognition: A Synthetic and Computational Study of Morphological Control of Ca ₃ Al ₂ (OH) ₁₂ . <i>Journal of Physical Chemistry B</i> , 2002, 106, 5820-5826.	2.6	9
80	Morphological control of Ca ₃ Al ₂ (OH) ₁₂ . <i>Journal of Crystal Growth</i> , 2002, 234, 255-262.	1.5	12
81	Investigation into the effect of phosphonate inhibitors on barium sulfate precipitation. <i>Journal of Crystal Growth</i> , 2002, 237-239, 424-429.	1.5	54
82	An ab initio study of the influence of crystal packing on the host-guest interactions of calix[4]arene crystal structures. <i>Chemical Communications</i> , 2001, , 1626-1627.	4.1	18
83	An ab Initio Study of the Structure and Properties of Aluminum Hydroxide: Gibbsite and Bayerite. <i>Journal of Physical Chemistry B</i> , 2001, 105, 10236-10242.	2.6	86
84	A computational investigation of the structure of γ -alumina using interatomic potentials. <i>Journal of Materials Chemistry</i> , 2001, 11, 3310-3316.	6.7	8
85	Anomalous behaviour within a systematic series of barium sulfate growth modifiers. <i>CrystEngComm</i> , 2001, 3, 165.	2.6	9
86	Atomistic Modeling of Gibbsite: Cation Incorporation. <i>Journal of Physical Chemistry B</i> , 2001, 105, 5099-5105.	2.6	19
87	Imaging problems on insulators: What can be learnt from NC-AFM modelling on CaF ₂ ?. <i>Applied Physics A: Materials Science and Processing</i> , 2001, 72, S31-S34.	2.3	13
88	Modelling non-stationary precipitation systems: sources of error and their propagation. <i>Chemical Engineering Science</i> , 2000, 55, 6037-6047.	3.8	8
89	Atomistic modelling of gibbsite: surface structure and morphology. <i>Journal of Crystal Growth</i> , 2000, 209, 159-166.	1.5	33
90	Molecular modeling of water adsorption on hematite. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 3209-3216.	2.8	74

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91	Model of noncontact scanning force microscopy on ionic surfaces. <i>Physical Review B</i> , 1999, 59, 2436-2448.	3.2	134
92	Contrast mechanism in non-contact SFM imaging of ionic surfaces. <i>Applied Surface Science</i> , 1999, 140, 327-332.	6.1	29
93	Crystallisation of β -lactose monohydrate from dimethyl sulfoxide (DMSO) solutions: influence of β -lactose. <i>Journal of Crystal Growth</i> , 1999, 205, 368-374.	1.5	60
94	Predicting Guest Orientations in Layered Double Hydroxide Intercalates. <i>Chemistry of Materials</i> , 1999, 11, 1194-1200.	6.7	63
95	Structure, stability and morphology of stoichiometric ceria crystallites. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1998, 94, 427-434.	1.7	109
96	Ionic structure in caustic aluminate solutions and the precipitation of gibbsite. <i>Journal of the Chemical Society Dalton Transactions</i> , 1998, , 3911-3918.	1.1	41
97	Incorporation of growth-inhibiting diphosphonates into steps on the calcite cleavage plane surface. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1998, 94, 3685-3693.	1.7	51
98	Theoretical Investigation of the Nature of Aluminum-Containing Species Present in Alkaline Solution. <i>Journal of Physical Chemistry B</i> , 1998, 102, 10372-10382.	2.6	41
99	Does AFM Really See Atoms at the Surface?. <i>Materials Science Forum</i> , 1997, 239-241, 651-656.	0.3	0
100	Predicting the occurrence of reflection twins. <i>Journal of Crystal Growth</i> , 1997, 178, 402-409.	1.5	18
101	Hydrogen Dissociation on Reconstructed ZnO Surfaces. <i>The Journal of Physical Chemistry</i> , 1996, 100, 9054-9063.	2.9	57
102	Interactions at the Organic/Inorganic Interface: A Molecular Modeling of the Interaction between Diphosphonates and the Surfaces of Barite Crystals. <i>Journal of the American Chemical Society</i> , 1996, 118, 642-648.	13.7	77
103	Computer modelling of V ₂ O ₅ : surface structures, crystal morphology and ethene sorption. <i>Journal of Materials Chemistry</i> , 1996, 6, 653.	6.7	26
104	Molecular Mechanics Study of Oligomeric Models for Poly(ferrocenylsilanes) Using the Extensible Systematic Forcefield (ESFF). <i>Journal of the American Chemical Society</i> , 1996, 118, 7578-7592.	13.7	132
105	Molecular-mechanics study of oligomeric models for poly(ferrocenylsilanes) using the ESFF forcefield. <i>Chemical Communications</i> , 1996, , 257.	4.1	17
106	Simulating the structures of crystals and their surfaces. <i>Topics in Catalysis</i> , 1996, 3, 135-167.	2.8	7
107	A model of the interaction of ionic tips with ionic surfaces for interpretation of scanning force microscope images. <i>Topics in Catalysis</i> , 1996, 3, 221-247.	2.8	14
108	Calculating the effects of surface relaxation on morphology. <i>Journal of Crystal Growth</i> , 1996, 166, 84-90.	1.5	32

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109	Theoretical Models of the Polar Cu ₂ O(100) Cu ⁺ -Terminated Surface. <i>The Journal of Physical Chemistry</i> , 1996, 100, 294-298.	2.9	30
110	Structure of small Ni clusters on SiO ₂ . <i>Catalysis Letters</i> , 1995, 30, 77-85.	2.6	12
111	Model of scanning force microscopy on ionic surfaces. <i>Physical Review B</i> , 1995, 52, 11398-11411.	3.2	19
112	Properties of small clusters at ionic surfaces: (NaCl) _n clusters (n=1-48) at the (100) MgO surface. <i>Physical Review B</i> , 1995, 51, 13631-13644.	3.2	22
113	Theoretical study of nanoclusters at ionic surfaces: Properties of (NaCl) _n clusters (n=1-48) at the (100) MgO surface. <i>Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena</i> , 1995, 13, 1190.	1.6	5
114	Atomistic modeling of imaging of ionic surfaces with a scanning force microscope. <i>Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena</i> , 1995, 13, 1155.	1.6	10
115	Lateral and friction forces originating during force microscope scanning of ionic surfaces. <i>Surface Science</i> , 1995, 343, 273-287.	1.9	32
116	Computational investigation of surface structural relaxation in crystalline urea. <i>Journal of Materials Chemistry</i> , 1995, 5, 133.	6.7	29
117	MARVIN: a new computer code for studying surfaces and interfaces and its application to calculating the crystal morphologies of corundum and zircon. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1995, 91, 925.	1.7	246
118	Modelling the morphology of minerals by computer. <i>Mineralogical Magazine</i> , 1995, 59, 607-615.	1.4	6
119	Atomistic theory of the interaction between AFM tips and ionic surfaces. <i>Journal of Physics Condensed Matter</i> , 1994, 6, 1825-1846.	1.8	66
120	Calculation of the morphology of silica sodalite. <i>Journal of the Chemical Society Chemical Communications</i> , 1994, , 1369.	2.0	25
121	Size and shape of molecular ions and their relevance to the packing of the "soft salts". <i>Inorganica Chimica Acta</i> , 1993, 212, 5-13.	2.4	12
122	Calculated bulk and surface properties of sulfates. <i>Faraday Discussions</i> , 1993, 95, 273.	3.2	108
123	Relationships between computed and experimentally determined molecular volumes and radii. <i>Journal of the Chemical Society Dalton Transactions</i> , 1993, , 423.	1.1	13
124	The size and shape of molecular ions and their relevance to the packing of the hexafluorophosphate salts. <i>Journal of the Chemical Society Dalton Transactions</i> , 1992, , 3541.	1.1	15
125	Size and shape characteristics of inorganic molecules and ions and their relevance to molecular packing problems. <i>Journal of the Chemical Society Dalton Transactions</i> , 1991, , 3419.	1.1	77
126	Size and shape characteristics of inorganic molecular ions and their relevance to crystallization problems. <i>Inorganic Chemistry</i> , 1991, 30, 3769-3771.	4.0	78