Andrew L Rohl

List of Publications by Year
in descending order

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126 papers	6,900 citations	81900 39 h-index	62596 80 g-index
129 all docs	129 docs citations	129 times ranked	7102 citing authors

#	Article	IF	Citations
1	The General Utility Lattice Program (GULP). Molecular Simulation, 2003, 29, 291-341.	2.0	1,921
2	Hirshfeld Surfaces Identify Inadequacies in Computations of Intermolecular Interactions in Crystals: Pentamorphic 1,8-Dihydroxyanthraquinone. Crystal Growth and Design, 2008, 8, 4517-4525.	3.0	482
3	MARVIN: a new computer code for studying surfaces and interfaces and its application to calculating the crystal morphologies of corundum and zircon. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 925.	1.7	246
4	Boehmite Derived Î³-Alumina System. 1. Structural Evolution with Temperature, with the Identification and Structural Determination of a New Transition Phase, Î³â€˜-Alumina. Chemistry of Materials, 2004, 16, 220-236.	6.7	176
5	Determination of the structure ofÎ³-alumina from interatomic potential and first-principles calculations: The requirement of significant numbers of nonspinel positions to achieve an accurate structural model. Physical Review B, 2005, 71, .	3.2	139
6	Model of noncontact scanning force microscopy on ionic surfaces. Physical Review B, 1999, 59, 2436-2448.	3.2	134
7	Molecular Mechanics Study of Oligomeric Models for Poly(ferrocenylsilanes) Using the Extensible Systematic Forcefield (ESFF). Journal of the American Chemical Society, 1996, 118, 7578-7592.	13.7	132
8	Structure, stability and morphology of stoichiometric ceria crystallites. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 427-434.	1.7	109
9	Calculated bulk and surface properties of sulfates. Faraday Discussions, 1993, 95, 273.	3.2	108
10	Effects of temperature on the scaling of calcium sulphate in pipes. Powder Technology, 2007, 179, 31-37.	4.2	106
11	Evidence from surface phonons for the (2 Ã— 1) reconstruction of the (101Ì…4) surface of calcite from computer simulation. American Mineralogist, 2003, 88, 921-925.	1.9	100
12	GDIS: a visualization program for molecular and periodic systems. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.8	97
13	Powder diffraction and crystal structure prediction identify four new coumarin polymorphs. Chemical Science, 2017, 8, 4926-4940.	7.4	97
14	An ab Initio Study of the Structure and Properties of Aluminum Hydroxide:Â Gibbsite and Bayerite. Journal of Physical Chemistry B, 2001, 105, 10236-10242.	2.6	86
15	Twisted Aspirin Crystals. Journal of the American Chemical Society, 2013, 135, 3395-3398.	13.7	86
16	A Supramolecular Ice Growth Inhibitor. Journal of the American Chemical Society, 2016, 138, 13396-13401.	13.7	83
17	Size and shape characteristics of inorganic molecular ions and their relevance to crystallization problems. Inorganic Chemistry, 1991, 30, 3769-3771.	4.0	78
18	Size and shape characteristics of inorganic molecules and ions and their relevance to molecular packing problems. Journal of the Chemical Society Dalton Transactions, 1991, , 3419.	1.1	77

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19	Interactions at the Organic/Inorganic Interface:Â Molecular Modeling of the Interaction between Diphosphonates and the Surfaces of Barite Crystals. Journal of the American Chemical Society, 1996, 118, 642-648.	13.7	77
20	Molecular modeling of water adsorption on hematite. Physical Chemistry Chemical Physics, 2000, 2, 3209-3216.	2.8	74
21	Resorcinol Crystallization from the Melt: A New Ambient Phase and New â€œRiddlesâ€• Journal of the American Chemical Society, 2016, 138, 4881-4889.	13.7	74
22	Boehmite-Derived Î³-Alumina System. 2. Consideration of Hydrogen and Surface Effects. Chemistry of Materials, 2004, 16, 1914-1923.	6.7	70
23	Atomistic theory of the interaction between AFM tips and ionic surfaces. Journal of Physics Condensed Matter, 1994, 6, 1825-1846.	1.8	66
24	The controlled disassembly of mesostructured perovskites as an avenue to fabricating high performance nanohybrid catalysts. Nature Communications, 2017, 8, 15553.	12.8	65
25	Predicting Guest Orientations in Layered Double Hydroxide Intercalates. Chemistry of Materials, 1999, 11, 1194-1200.	6.7	63
26	Crystallisation of Î±-lactose monohydrate from dimethyl sulfoxide (DMSO) solutions: influence of Î²-lactose. Journal of Crystal Growth, 1999, 205, 368-374.	1.5	60
27	The interaction of EDTA with barium sulfate. Journal of Colloid and Interface Science, 2007, 316, 553-561.	9.4	60
28	Resolving Point Defects in the Hydration Structure of Calcite (10.4) with Three-Dimensional Atomic Force Microscopy. Physical Review Letters, 2018, 120, 116101.	7.8	58
29	Hydrogen Dissociation on Reconstructed ZnO Surfaces. The Journal of Physical Chemistry, 1996, 100, 9054-9063.	2.9	57
30	Computer prediction of crystal morphology. Current Opinion in Solid State and Materials Science, 2003, 7, 21-26.	11.5	57
31	Benchmarking Calculated Lattice Parameters and Energies of Molecular Crystals Using van der Waals Density Functionals. Journal of Chemical Theory and Computation, 2014, 10, 3423-3437.	5.3	56
32	Molecular Modeling of Phosphonate Molecules onto Barium Sulfate Terraced Surfaces. Journal of Physical Chemistry B, 2006, 110, 7414-7424.	2.6	55
33	Investigation into the effect of phosphonate inhibitors on barium sulfate precipitation. Journal of Crystal Growth, 2002, 237-239, 424-429.	1.5	54
34	Calculation of Attachment Energies and Relative Volume Growth Rates As an Aid to Polymorph Prediction. Crystal Growth and Design, 2005, 5, 879-885.	3.0	52
35	Incorporation of growth-inhibiting diphosphonates into steps on the calcite cleavage plane surface. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 3685-3693.	1.7	51
36	A study of the high-pressure polymorphs of L-serine using ab initio structures and PIXEL calculations. CrystEngComm, 2008, 10, 1154.	2.6	48

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37	Quantum mechanical vs. empirical potential modeling of uranium dioxide (UO2) surfaces: (111), (110), and (100). American Mineralogist, 2006, 91, 1761-1772.	1.9	47
38	Ionic structure in caustic aluminate solutions and the precipitation of gibbsite. Journal of the Chemical Society Dalton Transactions, 1998, , 3911-3918.	1.1	41
39	Theoretical Investigation of the Nature of Aluminum-Containing Species Present in Alkaline Solution. Journal of Physical Chemistry B, 1998, 102, 10372-10382.	2.6	41
40	The role of phosphonate speciation on the inhibition of barium sulfate precipitation. Journal of Crystal Growth, 2003, 249, 584-593.	1.5	38
41	The Epitaxial Growth of Cholesterol Crystals from Bile Solutions on Calcite Substrates. Journal of the American Chemical Society, 2004, 126, 7915-7924.	13.7	38
42	Luminescent Probes of Crystal Growth: Surface Charge and Polar Axis Sense in Dye-Doped Potassium Hydrogen Phthalate. Angewandte Chemie - International Edition, 2004, 43, 5328-5331.	13.8	34
43	Atomistic modelling of gibbsite: surface structure and morphology. Journal of Crystal Growth, 2000, 209, 159-166.	1.5	33
44	Comment on â€œExamination of Spinel and Nonspinel Structural Models for Î³-Al2O3by DFT and Rietveld Refinement Simulationsâ€• Journal of Physical Chemistry B, 2006, 110, 20721-20723.	2.6	33
45	Lateral and friction forces originating during force microscope scanning of ionic surfaces. Surface Science, 1995, 343, 273-287.	1.9	32
46	Calculating the effects of surface relaxation on morphology. Journal of Crystal Growth, 1996, 166, 84-90.	1.5	32
47	The effect of calcium ions on the precipitation of barium sulphate 1: calcium ions in the absence of organic additives. Journal of Crystal Growth, 2004, 262, 572-580.	1.5	32
48	Prediction of Soai Reaction Enantioselectivity Induced by Crystals of N-(2-Thienylcarbonyl)glycine. Crystal Growth and Design, 2012, 12, 2138-2145.	3.0	32
49	Controlling Mesoscale Crystal Helicity with Additives, Again. Crystal Growth and Design, 2011, 11, 2070-2073.	3.0	31
50	Theoretical Models of the Polar Cu2O(100) Cu+-Terminated Surface. The Journal of Physical Chemistry, 1996, 100, 294-298.	2.9	30
51	Atomistic Simulation of Atomic Force Microscopy Imaging of Hydration Layers on Calcite, Dolomite, and Magnesite Surfaces. Journal of Physical Chemistry C, 2019, 123, 14985-14992.	3.1	30
52	Computational investigation of surface structural relaxation in crystalline urea. Journal of Materials Chemistry, 1995, 5, 133.	6.7	29
53	Contrast mechanism in non-contact SFM imaging of ionic surfaces. Applied Surface Science, 1999, 140, 327-332.	6.1	29
54	What is Syncrystallization? States of the pH Indicator Methyl Red in Crystals of Phthalic Acid. Journal of the American Chemical Society, 2006, 128, 5548-5559.	13.7	28

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55	The interstellar gas-phase formation of CO2 â€“ Assisted or not by water molecules?. Chemical Physics, 2006, 320, 214-228.	1.9	28
56	Dislocation-Actuated Growth and Inhibition of Hexagonal <scp>l</scp>-Cystine Crystallization at the Molecular Level. Crystal Growth and Design, 2015, 15, 921-934.	3.0	28
57	Computer modelling of V2O5: surface structures, crystal morphology and ethene sorption. Journal of Materials Chemistry, 1996, 6, 653.	6.7	26
58	Noncovalent Interactions in SIESTA Using the vdW-DF Functional: S22 Benchmark and Macrocyclic Structures. Journal of Chemical Theory and Computation, 2012, 8, 281-289.	5.3	26
59	Why Are Some Crystals Straight?. Journal of Physical Chemistry C, 2020, 124, 15616-15624.	3.1	26
60	Calculation of the morphology of silica sodalite. Journal of the Chemical Society Chemical Communications, 1994, , 1369.	2.0	25
61	An efficient technique for the prediction of solvent-dependent morphology: the COSMIC method. Molecular Simulation, 2007, 33, 1237-1246.	2.0	24
62	Stabilization of Aragonite: Role of Mg²⁺ and Other Impurity Ions. Crystal Growth and Design, 2020, 20, 5006-5017.	3.0	24
63	Properties of small clusters at ionic surfaces: (NaCl)nclusters (n=1â€“48) at the (100) MgO surface. Physical Review B, 1995, 51, 13631-13644.	3.2	22
64	Molecular Dynamics Visualization (MDV): Stereoscopic 3D Display of Biomolecular Structure and Interactions Using the Unity Game Engine. Journal of Integrative Bioinformatics, 2018, 15, .	1.5	22
65	Effects of Organic Additives on Calcium Sulfate Scaling in Pipes. Australian Journal of Chemistry, 2009, 62, 927.	0.9	21
66	Structural Correspondence of Solution, Liquid Crystal, and Crystalline Phases of the Chromonic Mesogen Sunset Yellow. Crystal Growth and Design, 2014, 14, 4166-4176.	3.0	21
67	IN SITU CHARACTERISATION OF CALCITE GROWTH AND INHIBITION USING ATOMIC FORCE MICROSCOPY. International Journal of Modern Physics B, 2002, 16, 25-33.	2.0	20
68	Effects of Process Parameters on Gypsum Scale Formation in Pipes. Chemical Engineering and Technology, 2011, 34, 1003-1009.	1.5	20
69	Effect of Lanthanum on the Crystal Growth of Barium Sulfate. Crystal Growth and Design, 2014, 14, 1650-1658.	3.0	20
70	Understanding 2D atomic resolution imaging of the calcite surface in water by frequency modulation atomic force microscopy. Nanotechnology, 2016, 27, 415709.	2.6	20
71	Difference Hirshfeld fingerprint plots: a tool for studying polymorphs. CrystEngComm, 2017, 19, 2207-2215.	2.6	20
72	Model of scanning force microscopy on ionic surfaces. Physical Review B, 1995, 52, 11398-11411.	3.2	19

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73	Atomistic Modeling of Gibbsite:Â Cation Incorporation. Journal of Physical Chemistry B, 2001, 105, 5099-5105.	2.6	19
74	Predicting the occurrence of reflection twins. Journal of Crystal Growth, 1997, 178, 402-409.	1.5	18
75	An ab initio study of the influence of crystal packing on the hostâ€“guest interactions of calix[4]arene crystal structures. Chemical Communications, 2001, , 1626-1627.	4.1	18
76	The effect of calcium cations on the precipitation of barium sulfate 2: calcium ions in the presence of organic additives. Journal of Crystal Growth, 2004, 270, 593-603.	1.5	18
77	Understanding the mechanism by which nitrilotriacetic acid interacts with precipitating barium sulfate. CrystEngComm, 2006, 8, 869.	2.6	18
78	Understanding barium sulfate precipitation onto stainless steel. Applied Surface Science, 2008, 254, 3459-3468.	6.1	18
79	Can Point Defects in Surfaces in Solution be Atomically Resolved by Atomic Force Microscopy?. Physical Review Letters, 2016, 117, 226101.	7.8	18
80	Molecular-mechanics study of oligomeric models for poly(ferrocenylsilanes) using the ESFF forcefield. Chemical Communications, 1996, , 257.	4.1	17
81	Chemical evolution via beta decay: a case study in strontium-90. Journal of Physics Condensed Matter, 2013, 25, 065504.	1.8	17
82	The size and shape of molecular ions and their relevance to the packing of the hexafluorophosphate salts. Journal of the Chemical Society Dalton Transactions, 1992, , 3541.	1.1	15
83	Robert Boyle's chiral crystal chemistry: Computational re-evaluation of enantioselective adsorption on quartz. Chirality, 2006, 18, 127-133.	2.6	15
84	Silver(i), gold(i) and palladium(ii) complexes of a NHC-pincer ligand with an aminotriazine core: a comparison with pyridyl analogues. Dalton Transactions, 2016, 45, 1484-1495.	3.3	15
85	Tip dependence of three-dimensional scanning force microscopy images of calciteâ€“water interfaces investigated by simulation and experiments. Nanoscale, 2020, 12, 12856-12868.	5.6	15
86	A model of the interaction of ionic tips with ionic surfaces for interpretation of scanning force microscope images. Topics in Catalysis, 1996, 3, 221-247.	2.8	14
87	Implications of transmutation on the defect chemistry in crystalline waste forms. Nuclear Instruments & Methods in Physics Research B, 2010, 268, 3261-3264.	1.4	14
88	Relationships between computed and experimentally determined molecular volumes and radii. Journal of the Chemical Society Dalton Transactions, 1993, , 423.	1.1	13
89	Imaging problems on insulators: What can be learnt from NC-AFM modelling on CaF2?. Applied Physics A: Materials Science and Processing, 2001, 72, S31-S34.	2.3	13
90	Size and shape of molecular ions and their relevance to the packing of the â€˜soft saltsâ€™. Inorganica Chimica Acta, 1993, 212, 5-13.	2.4	12

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91	Structure of small Ni clusters on SiO2. Catalysis Letters, 1995, 30, 77-85.	2.6	12
92	Morphological control of Ca3Al2(OH)12. Journal of Crystal Growth, 2002, 234, 255-262.	1.5	12
93	Growth modification of hematite by phosphonate additives. Journal of Crystal Growth, 2008, 310, 688-698.	1.5	11
94	van der <scp>W</scp>aals corrected density functional calculations of the adsorption of benzene on the Cu (111) surface. Journal of Computational Chemistry, 2014, 35, 2263-2271.	3.3	11
95	Structure, Energetics, and Dynamics of Screw Dislocations in Even n-Alkane Crystals. Journal of Physical Chemistry Letters, 2016, 7, 3112-3117.	4.6	11
96	Atomistic modeling of imaging of ionic surfaces with a scanning force microscope. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 1995, 13, 1155.	1.6	10
97	Empirical molecular modelling of crystal growth modifiers. Molecular Simulation, 2005, 31, 393-398.	2.0	10
98	Investigation into the effects of phosphonic inhibitors on the formation of calcium sulfate scales. Desalination and Water Treatment, 2011, 29, 294-301.	1.0	10
99	Anomalous behaviour within a systematic series of barium sulfate growth modifiers. CrystEngComm, 2001, 3, 165.	2.6	9
100	Toward a Fundamental Understanding of Molecular Recognition:Â A Synthetic and Computational Study of Morphological Control of Ca3Al2(OH)12. Journal of Physical Chemistry B, 2002, 106, 5820-5826.	2.6	9
101	Timoshenko Bending and Eshelby Twisting Predicted in Molecular Nanocrystals. Journal of Physical Chemistry C, 2018, 122, 25085-25091.	3.1	9
102	Modelling non-stationary precipitation systems: sources of error and their propagation. Chemical Engineering Science, 2000, 55, 6037-6047.	3.8	8
103	A computational investigation of the structure of Î²-alumina using interatomic potentials. Journal of Materials Chemistry, 2001, 11, 3310-3316.	6.7	8
104	Incorporation of Cyano Transition Metal Complexes in KCl Crystalsâ€"Experimental and Computational Studies. Australian Journal of Chemistry, 2003, 56, 675.	0.9	8
105	Incorporation of impurity anions into DSP: insights into structure and stability from computer modelling. Molecular Simulation, 2006, 32, 35-44.	2.0	8
106	Mechanisms of Dye Incorporation into Potassium Sulfate: Computational and Experimental Studies. Journal of Physical Chemistry C, 2007, 111, 9283-9289.	3.1	8
107	Ab Initio Molecular Dynamics Simulations of (101) Surfaces of Potassium Dihydrogenphosphate. Journal of Chemical Theory and Computation, 2011, 7, 1604-1609.	5.3	8
108	Simulating the structures of crystals and their surfaces. Topics in Catalysis, 1996, 3, 135-167.	2.8	7

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109	Adsorption energetics of potassium sulfate dye inclusion crystals. Journal of Molecular Structure, 2003, 647, 65-73.	3.6	6
110	Atomic force microscope adhesion measurements and atomistic molecular dynamics simulations at different humidities. Measurement Science and Technology, 2017, 28, 034004.	2.6	6
111	Atomistic simulation of the measurement of mechanical properties of gold nanorods by AFM. Scientific Reports, 2017, 7, 16257.	3.3	6
112	Modelling the morphology of minerals by computer. Mineralogical Magazine, 1995, 59, 607-615.	1.4	6
113	Theoretical study of nanoclusters at ionic surfaces: Properties of (NaCl)n clusters (n=1â€“48) at the (100) MgO surface. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 1995, 13, 1190.	1.6	5
114	Comparison of the effect growth inhibitors have on an isostructural pair of salts. CrystEngComm, 2005, 7, 320.	2.6	5
115	Ab Initio Simulations of the (101) Surfaces of Potassium Dihydrogenphosphate (KDP). Journal of Chemical Theory and Computation, 2006, 2, 797-800.	5.3	5
116	Interatomic Potentials for Simulating MnO2Polymorphs. Molecular Simulation, 2005, 31, 25-32.	2.0	4
117	A NOVEL SPINNING DISC CONTINUOUS STIR TANK AND SETTLER REACTOR (SDCSTR) MODEL FOR CONTINUOUS SYNTHESIS OF TITANIA: A PHENOMENOLOGICAL MODEL. Chemical Engineering Communications, 2010, 198, 73-84.	2.6	4
118	Electronic structure of phosphorus and arsenicÎ´-doped germanium. Physical Review B, 2013, 88, .	3.2	4
119	Synthesis, Stereochemistry and Antiparasitic Activity of Derivatives of (4R)-4,6-Dihydroxy-N-methyl-1,2,3,4-tetrahydroisoquinoline. ChemistrySelect, 2017, 2, 2006-2013.	1.5	4
120	Can macrocyclic phosphonate molecules inhibit barium sulfate crystallization?. CrystEngComm, 2019, 21, 807-815.	2.6	4
121	Computational methodology for chirality determination in the Soai reaction by crystals: Î³-glycine. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	3
122	A self-supervised learning based approach to analyze Martian waterâ€“ice cloud properties for planetary atmospheric applications. Acta Astronautica, 2021, 181, 1-13.	3.2	3
123	Using Molecular Modelling to Understand and Predict the Impact of Organic Additives as Crystal Growth Modifiers. Australian Journal of Chemistry, 2020, 73, 724.	0.9	3
124	Does AFM Really See Atoms at the Surface?. Materials Science Forum, 1997, 239-241, 651-656.	0.3	0
125	Boehmite Derived Î³-Alumina System. Part 1. Structural Evolution with Temperature, with the Identification and Structural Determination of a New Transition Phase, Î³â€²-Alumina.. ChemInform, 2004, 35, no.	0.0	0
126	Linking Additive Structures to Nanoparticle Properties. Journal of Metastable and Nanocrystalline Materials, 2005, 23, 51-54.	0.1	0