Dirk Zahn

List of Publications by Year
in descending order

182	4,071	109321	155660
papers	citations	35 h-index	55 g-index

201	201	201	4842
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Uncovering Molecular Processes in Crystal Nucleation and Growth by Using Molecular Simulation. Angewandte Chemie - International Edition, 2011, 50, 1996-2013.	13.8	220
2	Enhancement of the Wolf Damped Coulomb Potential:Â Static, Dynamic, and Dielectric Properties of Liquid Water from Molecular Simulation. Journal of Physical Chemistry B, 2002, 106, 10725-10732.	2.6	131
3	Atomistic Mechanism of NaCl Nucleation from an Aqueous Solution. Physical Review Letters, 2004, 92, 040801.	7.8	127
4	Biomimetic Fluorapatiteâ€“Gelatine Nanocomposites: Pre-Structuring of Gelatine Matrices by Ion Impregnation and Its Effect on Form Development. Angewandte Chemie - International Edition, 2006, 45, 1905-1910.	13.8	125
5	Synthesis and Characterization of Gelatinâ€Based Magnetic Hydrogels. Advanced Functional Materials, 2014, 24, 3187-3196.	14.9	114
6	Intrinsic Electric Dipole Fields and the Induction of Hierarchical Form Developments in Fluorapatiteâ€“Gelatine Nanocomposites: A General Principle for Morphogenesis of Biominerals?. Angewandte Chemie - International Edition, 2006, 45, 1911-1915.	13.8	102
7	Computational study of interfaces between hydroxyapatite and water. Physical Chemistry Chemical Physics, 2003, 5, 4004.	2.8	99
8	Lithium Argyrodites with Phosphorus and Arsenic: Order and Disorder of Lithium Atoms, Crystal Chemistry, and Phase Transitions. Chemistry - A European Journal, 2010, 16, 2198-2206.	3.3	81
9	Thermodynamics and Kinetics of Prenucleation Clusters, Classical and Nonâ€Classical Nucleation. ChemPhysChem, 2015, 16, 2069-2075.	2.1	80
10	Nucleation and Growth in Pressure-Induced Phase Transitions from Molecular Dynamics Simulations: Mechanism of the Reconstructive Transformation of NaCl to the CsCl-Type Structure. Physical Review Letters, 2004, 92, 250201.	7.8	79
11	The Nucleation Mechanism of Fluorapatiteâ€“Collagen Composites: Ion Association and Motif Control by Collagen Proteins. Angewandte Chemie - International Edition, 2008, 47, 4982-4985.	13.8	73
12	Improving the Charge Transport in Self-Assembled Monolayer Field-Effect Transistors: From Theory to Devices. Journal of the American Chemical Society, 2013, 135, 4893-4900.	13.7	72
13	Magnetite nanoparticles as efficient materials for removal of glyphosate from water. Nature Sustainability, 2020, 3, 129-135.	23.7	72
14	Atomistic Mechanisms of ZnO Aggregation from Ethanolic Solution: Ion Association, Proton Transfer, and Self-Organization. Nano Letters, 2008, 8, 2336-2340.	9.1	68
15	Atomistic Characterisation of Li⁺ Mobility and Conductivity in Li_{7â”x}PS_{6â”x}I_x Argyrodites from Molecular Dynamics Simulations, Solidâ€State NMR, and Impedance Spectroscopy. Chemistry - A European Journal, 2010, 16, 8347-8354.	3.3	67
16	Robot-Based High-Throughput Screening of Antisolvents for Lead Halide Perovskites. Joule, 2020, 4, 1806-1822.	24.0	65
17	Theoretical Study of the Mechanisms of Acid-Catalyzed Amide Hydrolysis in Aqueous Solution. Journal of Physical Chemistry B, 2003, 107, 12303-12306.	2.6	63
18	An atomistic simulation scheme for modeling crystal formation from solution. Journal of Chemical Physics, 2006, 124, 024513.	3.0	63

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19	On the Role of Water in Amide Hydrolysis. European Journal of Organic Chemistry, 2004, 2004, 4020-4023.	2.4	62
20	The remediation of nano-/microplastics from water. Materials Today, 2021, 48, 38-46.	14.2	56
21	Atomistic Simulation Study of the Order/Disorder (Monoclinic to Hexagonal) Phase Transition of Hydroxyapatite. Chemistry of Materials, 2005, 17, 1978-1981.	6.7	53
22	Mechanism of the pressure-induced wurtzite to rocksalt transition of CdSe. Physical Review B, 2005, 72, .	3.2	52
23	Hydrolysis of a Basic Bismuth Nitrateâ€"Formation and Stability of Novel Bismuth Oxido Clusters. Chemistry - A European Journal, 2011, 17, 6985-6990.	3.3	52
24	How Does Water Boil?. Physical Review Letters, 2004, 93, 227801.	7.8	51
25	Polymorphic phase transitions: Macroscopic theory and molecular simulation. Advanced Drug Delivery Reviews, 2017, 117, 47-70.	13.7	49
26	Walking the Path fromB4- toB1-Type Structures in GaN. Physical Review Letters, 2007, 99, 125505.	7.8	46
27	Fullerene Van der Waals Oligomers as Electron Traps. Journal of the American Chemical Society, 2014, 136, 10890-10893.	13.7	46
28	Towards an atomistic understanding of apatiteâ€"collagen biomaterials: linking molecular simulation studies of complex-, crystal- and composite-formation to experimental findings. Journal of Materials Science, 2007, 42, 8966-8973.	3.7	41
29	On the composition and atomic arrangement of calcium-deficient hydroxyapatite: An ab-initio analysis. Journal of Solid State Chemistry, 2008, 181, 1712-1716.	2.9	41
30	Mimicking the Growth of a Pathologic Biomineral: Shape Development and Structures of Calcium Oxalate Dihydrate in the Presence of Polyacrylic Acid. Chemistry - A European Journal, 2012, 18, 4000-4009.	3.3	40
31	Carâ€"Parrinello molecular dynamics simulation of base-catalyzed amide hydrolysis in aqueous solution. Chemical Physics Letters, 2004, 383, 134-137.	2.6	39
32	A Novel Water-Soluble Hexanuclear Bismuth Oxido Cluster - Synthesis, Structure and Complexation with Polyacrylate. European Journal of Inorganic Chemistry, 2010, 2010, 4763-4769.	2.0	39
33	Indentation and Self-Healing Mechanisms of a Self-Assembled Monolayerâ€"A Combined Experimental and Modeling Study. Journal of the American Chemical Society, 2014, 136, 10718-10727.	13.7	37
34	Elucidation of the Conversion Reaction of CoMnFeO₄ Nanoparticles in Lithium Ion Battery Anode via Operando Studies. ACS Applied Materials & Interfaces, 2016, 8, 15320-15332.	8.0	35
35	Improved GAFF2 parameters for fluorinated alkanes and mixed hydro- and fluorocarbons. Journal of Molecular Modeling, 2019, 25, 39.	1.8	35
36	Superoleophilic Magnetic Iron Oxide Nanoparticles for Effective Hydrocarbon Removal from Water. Advanced Functional Materials, 2019, 29, 1805742.	14.9	32

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37	Quantumâ€“Classical Simulation of Proton Migration in Water. Israel Journal of Chemistry, 1999, 39, 469-482.	2.3	31
38	Molecular Simulation of Ag Nanoparticle Nucleation from Solution: Redox-Reactions Direct the Evolution of Shape and Structure. Nano Letters, 2014, 14, 4913-4917.	9.1	31
39	Low-dimensional sublattice melting by pressure: Superionic conduction in the phase interfaces of the fluorite-to-cotunnite transition ofCaF2. Physical Review B, 2006, 74, .	3.2	30
40	In situ investigation of two-step nucleation and growth of CdS nanoparticles from solution. Nanoscale, 2015, 7, 11328-11333.	5.6	30
41	Atomistic Mechanisms of Phase Separation and Formation of Solid Solutions:Â Model Studies of NaCl, NaClâ^'NaF, and Na(Cl1-xBrx) Crystallization from the Melt. Journal of Physical Chemistry B, 2007, 111, 5249-5253.	2.6	29
42	A group of cationic amphiphilic drugs activates MRGPRX2 and induces scratching behavior in mice. Journal of Allergy and Clinical Immunology, 2021, 148, 506-522.e8.	2.9	29
43	Putting the squeeze on NaCl: modelling and simulation of the pressure driven B1-B2 phase transition. Zeitschrift Fur Kristallographie - Crystalline Materials, 2004, 219, 339-344.	0.8	28
44	Mechanisms of Calcium and Phosphate Ion Association in Aqueous Solution. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2004, 630, 1507-1511.	1.2	28
45	Molecular mechanics modeling of azobenzene-based photoswitches. Journal of Molecular Modeling, 2012, 18, 2479-2482.	1.8	25
46	Fluctuations in surface pH of maturing rat incisor enamel are a result of cycles of H+-secretion by ameloblasts and variations in enamel buffer characteristics. Bone, 2014, 60, 227-234.	2.9	25
47	Chemical-recognition-driven selectivity of SnO2-nanowire-based gas sensors. Nano Today, 2021, 40, 101265.	11.9	25
48	Control of Channel Shapes in a Microporous Manganese(II)â€“Borophosphate Framework by Variation of Size and Shape of Organic Template Cations. Chemistry - A European Journal, 2007, 13, 1737-1745.	3.3	24
49	Quantumâ€“classical simulation of proton transport via a phospholipid bilayer. Physical Chemistry Chemical Physics, 2001, 3, 848-852.	2.8	23
50	Molecular dynamics investigation of the pressure induced B1 to B2 phase transitions of RbBr. Journal of Solid State Chemistry, 2004, 177, 3590-3594.	2.9	23
51	Multicenter multidomainB1â^'B2pressure-induced reconstructive phase transition in potassium fluoride. Physical Review B, 2005, 72, .	3.2	23
52	Multifunctional layered magnetic composites. Beilstein Journal of Nanotechnology, 2015, 6, 134-148.	2.8	22
53	Molecular dynamics simulations of phosphonic acidâ€“aluminum oxide self-organization and their evolution into ordered monolayers. Physical Chemistry Chemical Physics, 2017, 19, 5137-5144.	2.8	22
54	Investigation of the complex reaction coordinate of acid catalyzed amide hydrolysis from molecular dynamics simulations. Chemical Physics, 2004, 300, 79-83.	1.9	21

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55	From Composites to Solid Solutions: Modeling of Ionic Conductivity in the CaF₂â€“BaF₂ System. Chemistry - A European Journal, 2012, 18, 6225-6229.	3.3	20
56	Molecular dynamics study of water pores in a phospholipid bilayer. Chemical Physics Letters, 2002, 352, 441-446.	2.6	19
57	Motif Reconstruction in Clusters and Layers: Benchmarks for the Kawskaâ€“Zahn Approach to Model Crystal Formation. ChemPhysChem, 2010, 11, 847-852.	2.1	19
58	Thermoanalytical Evidence of Metastable Molecular Defects in Form I of Benzamide. Crystal Growth and Design, 2012, 12, 5365-5372.	3.0	19
59	On the Function of Saccharides during the Nucleation of Calcium Carbonateâ€“Protein Biocomposites. Crystal Growth and Design, 2013, 13, 4885-4889.	3.0	19
60	Collective displacements in a molecular crystal polymorphic transformation. RSC Advances, 2013, 3, 12810.	3.6	19
61	Improving the Performance of Organic Thinâ€Film Transistors by Ion Doping of Ethyleneâ€Glycolâ€Based Selfâ€Assembled Monolayer Hybrid Dielectrics. Advanced Materials, 2015, 27, 8023-8027.	21.0	19
62	The nano- and meso-scale structure of amorphous calcium carbonate. Scientific Reports, 2022, 12, 6870.	3.3	19
63	The Molecular Mechanism of Î±-Resorcinolâ€™s Asymmetric Crystal Growth from the Melt. Crystal Growth and Design, 2015, 15, 4026-4031.	3.0	18
64	Hydration breaking and chemical ordering in a levitated NaCl solution droplet beyond the metastable zone width limit: evidence for the early stage of two-step nucleation. Chemical Science, 2021, 12, 179-187.	7.4	18
65	The sense of balance in humans: Structural features of otoconia and their response to linear acceleration. PLoS ONE, 2017, 12, e0175769.	2.5	18
66	Exploring the Mechanisms of Reactions in Solution from Transition Path Sampling Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2006, 2, 107-114.	5.3	17
67	In situ X-ray monitoring of transport and chemistry of Ga-containing intermediates under ammonothermal growth conditions of GaN. Journal of Crystal Growth, 2018, 498, 214-223.	1.5	17
68	A Molecular Dynamics Simulation Study of (OH?) Schottky Defects in Hydroxyapatite. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2005, 631, 1134-1138.	1.2	16
69	Self-Assembled Monolayers Get Their Final Finish via a Quasi-Langmuirâ€“Blodgett Transfer. Langmuir, 2015, 31, 4678-4685.	3.5	16
70	Quantum/Classical Investigation of Amide Protonation in Aqueous Solution. Journal of Physical Chemistry A, 2002, 106, 7807-7812.	2.5	15
71	Unprejudiced identification of reaction mechanisms from biased transition path sampling. Journal of Chemical Physics, 2005, 123, 044104.	3.0	15
72	Mechanisms and Nucleation Characteristics of the Pressure-Induced B1â†’B2 Transition in Potassium Halides:Â A Question of Ion Hardness and Softness. Journal of Physical Chemistry B, 2006, 110, 10873-10877.	2.6	15

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73	A Molecular Simulation Approach to Bond Reorganization in Epoxy Resins: From Curing to Deformation and Fracture. ACS Polymers Au, 2021, 1, 165-174.	4.1	15
74	The Influence of Heteroatoms on the Extent of Double Bond Pyramidalization. European Journal of Organic Chemistry, 2003, 2003, 1111-1117.	2.4	14
75	Sizeâ€Ðependent Phase Stability of a Molecular Nanocrystal: a Proxy for Investigating the Early Stages of Crystallization. Chemistry - A European Journal, 2011, 17, 11186-11192.	3.3	14
76	Molecular Dynamics Modeling of Nanoscale CaF2/BaF2 Heterolayer Structures. Journal of Physical Chemistry C, 2009, 113, 1315-1319.	3.1	13
77	On the molecular mechanisms of the acid-induced dissociation of hydroxy-apatite in water. Journal of Molecular Modeling, 2011, 17, 1525-1528.	1.8	13
78	Nucleation Mechanisms of a Polymorphic Molecular Crystal: Solvent-Dependent Structural Evolution of Benzamide Aggregates. Crystal Growth and Design, 2014, 14, 2972-2976.	3.0	13
79	Investigations on the growth of bismuth oxido clusters and the nucleation to give metastable bismuth oxide modifications. Zeitschrift Fur Kristallographie - Crystalline Materials, 2017, 232, 185-207.	0.8	13
80	Mechanism of the pressure induced reconstructive transformation of KCl from the NaCl type to the CsCl type structure. Zeitschrift Fur Kristallographie - Crystalline Materials, 2004, 219, .	0.8	12
81	Competing Evaporation and Condensation Processes during the Boiling of Methane. Journal of Physical Chemistry B, 2006, 110, 19601-19604.	2.6	12
82	Molecular modeling of (101Ì„0) and (0001Ì„) zinc oxide surface growth from solution: islands, ridges and growth-controlling additives. CrystEngComm, 2015, 17, 6890-6894.	2.6	12
83	Two-Step Nucleation Rather than Self-Poisoning: An Unexpected Mechanism of Asymmetrical Molecular Crystal Growth. Crystal Growth and Design, 2015, 15, 5118-5123.	3.0	12
84	On the solvation of metal ions in liquid ammonia: a molecular simulation study of M(NH₂)_x(NH₃)_ycomplexes as a function of pH. RSC Advances, 2017, 7, 54063-54067.	3.6	12
85	Multifunctional and Tunable Surfaces Based on Pyrene Functionalized Nanoparticles. Advanced Materials Interfaces, 2019, 6, 1801930.	3.7	12
86	Supraparticles for Bareâ€Eye H₂ Indication and Monitoring: Design, Working Principle, and Molecular Mobility. Advanced Functional Materials, 2022, 32, .	14.9	12
87	From Amorphous Aggregates to Crystallites: Modelling Studies of Crystal Growth in Vacuum. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2005, 631, 1172-1176.	1.2	11
88	The Role of Substitutional Defects in Order/Disorder Phenomena of OHâ^' Ions in Hydroxyapatite. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2006, 632, 79-83.	1.2	11
89	The evolution of crystalline ordering for ligand-ornamented zinc oxide nanoparticles. CrystEngComm, 2016, 18, 2163-2172.	2.6	11
90	Elucidating water dynamics in MgCl 2 hydrates from molecular dynamics simulation. Solid State Sciences, 2017, 69, 64-70.	3.2	11

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91	Polarization Effects in Dynamic Interfaces of Platinum Electrodes and Ionic Liquid Phases: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2020, 124, 2002-2007.	3.1	11
92	Molecular Simulation of Thermosetting Polymer Hardening: Reactive Events Enabled by Controlled Topology Transfer. Macromolecules, 2020, 53, 9698-9705.	4.8	11
93	On the photophysics of nanographenes â€“ investigation of functionalized hexa-peri-hexabenzocoronenes as model systems. Nanoscale, 2021, 13, 801-809.	5.6	11
94	Atomistic Simulation Study of the Pressure Induced Incorporation of Helium into C60. Journal of Physical Chemistry B, 2004, 108, 16495-16498.	2.6	10
95	Atomistic Simulation Study of Calcium, Phosphate and Fluoride Ion Association to the Teleopeptide-Tails of Collagen â€“ Initial Steps to Biomineral Formation. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2007, 633, 411-414.	1.2	10
96	Extending the scope of â€˜in silico experimentsâ€™: Theoretical approaches for the investigation of reaction mechanisms, nucleation events and phase transitions. Science and Technology of Advanced Materials, 2007, 8, 434-441.	6.1	10
97	Barium titanate nanoparticle self-organization in an external electric field. Journal of Materials Chemistry, 2011, 21, 16978.	6.7	10
98	A new polymorph (IV) of benzamide: Structural characterization and mechanism of the Iâ†”IV phase transition. Chemical Physics Letters, 2011, 514, 274-277.	2.6	10
99	Molecular dynamics simulation of ionic conductors: perspectives and limitations. Journal of Molecular Modeling, 2011, 17, 1531-1535.	1.8	10
100	Solvation structure and dynamics of Ag+ in aqueous ammonia solutions: A molecular simulation study. Journal of Chemical Physics, 2017, 147, 114506.	3.0	10
101	Mixed Organic Ligand Shells: Controlling the Nanoparticle Surface Morphology toward Tuning the Optoelectronic Properties. Small, 2020, 16, e1903729.	10.0	10
102	Atomic mechanisms of superionic conductivity in fluorite. Solid State Ionics, 2009, 180, 116-119.	2.7	9
103	Surface Effects in the Pressureâ€Induced Structural Transformation of a ZnO NanorodÂ. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2009, 635, 1773-1776.	1.2	9
104	Atomistic modeling of apatite-collagen composites from molecular dynamics simulations extended to hyperspace. Journal of Molecular Modeling, 2011, 17, 73-79.	1.8	9
105	From oligomers towards a racemic crystal: molecular simulation of<scp>dl</scp>-norleucine crystal nucleation from solution. CrystEngComm, 2015, 17, 6884-6889.	2.6	9
106	On the Role of Silica Carrier Curvature for the Unloading of Small Drug Molecules: A Molecular Dynamics Simulation Study. Journal of Pharmaceutical Sciences, 2020, 109, 2018-2023.	3.3	9
107	A Molecular View of the Ionic Liquid Catalyst Interface of SCILLs: Coverage-Dependent Adsorption Motifs of [C₄C₁Pyr][NTf₂] on Pd Single Crystals and Nanoparticles. Journal of Physical Chemistry C, 2021, 125, 13264-13272.	3.1	9
108	A Molecular Rationale of Shock Absorption and Selfâ€Healing in a Biomimetic Apatiteâ€“Collagen Composite under Mechanical Load. Angewandte Chemie - International Edition, 2010, 49, 9405-9407.	13.8	8

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109	A test of improved force field parameters for urea: molecular-dynamics simulations of urea crystals. Journal of Molecular Modeling, 2012, 18, 3455-3466.	1.8	8
110	Analysis of the molecular interactions governing the polymorphism of benzamide â€“ a guide to syntheses?. Physical Chemistry Chemical Physics, 2013, 15, 9219.	2.8	8
111	A molecular simulation study of the auto-protolysis of ammonia as a function of temperature. Chemical Physics Letters, 2017, 682, 55-59.	2.6	8
112	Molecular Mechanisms of Solvent-Controlled Assembly of Phosphonate Monolayers on Oxide Surfaces. Journal of Physical Chemistry C, 2017, 121, 18012-18020.	3.1	8
113	Molecular mechanisms of mesoporous silica formation from colloid solution: Ripening-reactions arrest hollow network structures. PLoS ONE, 2019, 14, e0212731.	2.5	8
114	Red light-triggered photoreduction on a nucleic acid template. Chemical Communications, 2020, 56, 10026-10029.	4.1	8
115	Interaction Models and Molecular Simulation Systems of Steelâ€“Organic Friction Modifier Interfaces. Tribology Letters, 2021, 69, 1.	2.6	8
116	Length-dependent nucleation mechanisms rule the vaporization of n-alkanes. Chemical Physics Letters, 2008, 467, 80-83.	2.6	7
117	On the mechanisms of ionic conductivity in BaLiF3: a molecular dynamics study. Physical Chemistry Chemical Physics, 2011, 13, 21492.	2.8	7
118	Nucleation mechanism and kinetics of the perovskite to post-perovskite transition of MgSiO3 under extreme conditions. Chemical Physics Letters, 2013, 573, 5-7.	2.6	7
119	Molecular Mechanisms of [Bi6O4(OH)4](NO3)6Precursor Activation, Agglomeration, and Ripening towards Bismuth Oxide Nuclei. European Journal of Inorganic Chemistry, 2015, 2015, 1178-1181.	2.0	7
120	Multi-scale simulations of apatiteâ€“collagen composites: from molecules to materials. Frontiers of Materials Science, 2017, 11, 1-12.	2.2	7
121	Directed Dehydration as Synthetic Tool for Generation of a New Na₄SnS₄ Polymorph: Crystal Structure, Na⁺ Conductivity, and Influence of Sbâ€Substitution. Angewandte Chemie - International Edition, 2022, 61, .	13.8	7
122	A comparative study of proton migration in water and deuteron transport in heavy water by means of mixed quantum/classical molecular dynamics simulation. Chemical Physics Letters, 2000, 331, 224-228.	2.6	6
123	Minimum energy pathways of brittle and ductile deformation/fracture processes. Journal of Chemical Physics, 2008, 128, 184707.	3.0	6
124	Structure and interactions in benzamide molecular crystals. Molecular Simulation, 2013, 39, 1079-1083.	2.0	6
125	Approaching Dissolved Species in Ammonoacidic GaN Crystal Growth: A Combined Solution NMR and Computational Study. Chemistry - A European Journal, 2020, 26, 7008-7017.	3.3	6
126	Nonclassical Nucleationâ€”Role of Metastable Intermediate Phase in Crystal Nucleation: An Editorial Prefix. Crystals, 2021, 11, 174.	2.2	6

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127	Modeling of dislocation patterns of small- and high-angle grain boundaries in aluminum. Computational Materials Science, 2009, 46, 293-296.	3.0	5
128	Fluorapatiteâ€“Gelatine Nanocomposite Superstructures: New Insights into a Biomimetic System of High Complexity. ChemPhysChem, 2010, 11, 1851-1853.	2.1	5
129	Atomistic In Situ Investigation of the Morphogenesis of Grains during Pressure-Induced Phase Transitions: Molecular Dynamics Simulations of the B1-B2 Transformation of RbCl. Chemistry - A European Journal, 2010, 16, 13385-13389.	3.3	5
130	High-pressure high-temperature synthesis and crystal structure of the isotypic rare earth (RE)â€“thioborateâ€“sulfides RE9[BS3]2[BS4]3S3, (RE=Dyâ€“Lu). Journal of Solid State Chemistry, 2011, 184, 296-303.	2.9	5
131	Charge distribution analysis in Ag n m + $$ {mathbf{Ag}}_{mathbf{n}}^{mathbf{m}+} $$ clusters: molecular modeling and DFT calculations. Journal of Molecular Modeling, 2014, 20, 2111.	1.8	5
132	Molecular Mechanisms of ZnO Nanoparticle Dispersion in Solution: Modeling of Surfactant Association, Electrostatic Shielding and Counter Ion Dynamics. PLoS ONE, 2015, 10, e0125872.	2.5	5
133	Defect-driven water migration in MgCl2 tetra- and hexahydrates. Journal of Solid State Chemistry, 2019, 277, 221-228.	2.9	5
134	Bioinspired multifunctional layered magnetic hybrid materials. Bioinspired, Biomimetic and Nanobiomaterials, 2019, 8, 28-46.	0.9	5
135	Assessing the mechanical properties of molecular materials from atomic simulation. AIMS Materials Science, 2021, 8, 867-880.	1.4	5
136	On the mechanism of Zn4O-acetate precursors ripening to ZnO: How dimerization is promoted by hydroxide incorporation. Journal of Chemical Physics, 2015, 143, 064501.	3.0	4
137	Atomistic modeling of a KRT35/KRT85 keratin dimer: folding in aqueous solution and unfolding under tensile load. Physical Chemistry Chemical Physics, 2015, 17, 21880-21884.	2.8	4
138	A Surfactants Walk to Work: Modes of Action of Citrate Controlling (10-10) and (000-1) Zinc Oxide Surface Growth from Solution. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2016, 642, 902-905.	1.2	4
139	Fundamental theoretical and practical investigations of the polymorph formation of small amphiphilic molecules, their co-crystals and salts. Zeitschrift Fur Kristallographie - Crystalline Materials, 2017, 232, 55-67.	0.8	4
140	Size-Dependent Local Ordering in Melanin Aggregates and Its Implication on Optical Properties. Journal of Physical Chemistry A, 2019, 123, 9403-9412.	2.5	4
141	Interface between Waterâ€“Solvent Mixtures and a Hydrophobic Surface. Langmuir, 2020, 36, 12077-12086.	3.5	4
142	Interaction potentials for modelling GaN precipitation and solid state polymorphism. Journal of Physics Condensed Matter, 2020, 32, 205401.	1.8	4
143	Tailoring mesoporous silica nanomaterials from molecular simulation: Modelling the interplay of condensation reactions, surfactants and space-fillers during self assembly. Microporous and Mesoporous Materials, 2021, 320, 111114.	4.4	4
144	Multi-Scale Modelling of Deformation and Fracture in a Biomimetic Apatite-Protein Composite: Molecular-Scale Processes Lead to Resilience at the Î¼m-Scale. PLoS ONE, 2016, 11, e0157241.	2.5	4

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145	Deciphering the molecular mechanism of water boiling at heterogeneous interfaces. Scientific Reports, 2021, 11, 19858.	3.3	4
146	On the Atomistic Mechanisms of Alkane (Methaneâ^'Pentane) Separation by Distillation:â€‰ A Molecular Dynamics Study. Journal of Physical Chemistry B, 2007, 111, 12518-12523.	2.6	3
147	Molecular dynamics simulation of optimized shearing routes in single- and polycrystalline aluminum. Computational Materials Science, 2009, 45, 845-848.	3.0	3
148	Shearing mechanisms of MgSiO3at conditions of the Earth's Dâ€³ layer. Geophysical Research Letters, 2011, 38, n/a-n/a.	4.0	3
149	A first-principles based force-field for Li+ and OHâ^' in ethanolic solution. Journal of Chemical Physics, 2013, 139, 144506.	3.0	3
150	Molecular modeling of amorphous, non-woven polymer networks. Journal of Molecular Modeling, 2015, 21, 263.	1.8	3
151	From bismuth oxide/hydroxide precursor clusters towards stable oxides: Proton transfer reactions and structural reorganization govern the stability of [Bi18O13(OH)10]-nitrate clusters. Chemical Physics Letters, 2018, 691, 87-90.	2.6	3
152	Shearing in a Biomimetic Apatite-Protein Composite: Molecular Dynamics of Slip Zone Formation, Plastic Flow and Backcreep Mechanisms. PLoS ONE, 2014, 9, e93309.	2.5	3
153	Atomistic Simulation Study of Cu0.327Ni0.673Alloys: from Solid Solution to Phase Segregation. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2008, 634, 2562-2566.	1.2	2
154	Motif Identification in Materials Simulations. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2009, 635, 649-652.	1.2	2
155	Tackling time-reversibility in transition path sampling molecular dynamics simulations. Molecular Simulation, 2012, 38, 211-217.	2.0	2
156	Molecular simulations of crystal growth: From understanding to tailoring. Advances in Inorganic Chemistry, 2019, , 507-529.	1.0	2
157	Polar Structure Formation in Solid Solution of Strontium-Substituted Fluorapatiteâ€“Gelatin Composites: From Structural and Morphogenetic Aspects to Pyroelectric Properties. Chemistry of Materials, 2020, 32, 8619-8632.	6.7	2
158	Molecular dynamics simulation study of NH4+ and NH2â^' in liquid ammonia: interaction potentials, structural and dynamical properties. Journal of Molecular Modeling, 2022, 28, 127.	1.8	2
159	Molecular Dynamics Simulations of Nitrate/MgO Interfaces and Understanding Metastability of Thermochemical Materials. ACS Omega, 2022, 7, 16371-16379.	3.5	2
160	On the Role of Amides and Imides for Understanding GaN Syntheses from Ammonia Solution: Molecular Mechanics Models of Ammonia, Amide and Imide Interactions with Gallium Nitride. ChemPhysChem, 2022, 23, e202200117.	2.1	2
161	Atomistic Simulation Study of the Order/Disorder (Monoclinic to Hexagonal) Phase Transition of Hydroxyapatite.. ChemInform, 2005, 36, no.	0.0	1
162	Modeling martensic transformations in crystalline solids: validity and redesign of geometric approaches. Zeitschrift FÃ¼r Kristallographie, 2011, 226, 568-575.	1.1	1

#	Article	IF	Citations
163	The formation of CdS quantum dots and Au nanoparticles. Zeitschrift Fur Kristallographie - Crystalline Materials, 2017, 232, 39-46.	0.8	1
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181	An embedded atom model for Gaâ€“Pd systems: From intermetallic crystals to liquid alloys. Journal of Chemical Physics, 2021, 154, 014109.	3.0	0
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