Andrey G Kalinichev

List of Publications by Year
in descending order

94 papers	7,825 citations	57631 44 h-index	51492 86 g-index
97 all docs	97 docs citations	97 times ranked	5124 citing authors

#	Article	IF	Citations
1	Molecular Models of Hydroxide, Oxyhydroxide, and Clay Phases and the Development of a General Force Field. Journal of Physical Chemistry B, 2004, 108, 1255-1266.	1.2	2,281
2	Effects of substrate structure and composition on the structure, dynamics, and energetics of water at mineral surfaces: A molecular dynamics modeling study. Geochimica Et Cosmochimica Acta, 2006, 70, 562-582.	1.6	250
3	Molecular Dynamics Modeling of Chloride Binding to the Surfaces of Calcium Hydroxide, Hydrated Calcium Aluminate, and Calcium Silicate Phases. Chemistry of Materials, 2002, 14, 3539-3549.	3.2	249
4	Molecular models and simulations of layered materials. Journal of Materials Chemistry, 2009, 19, 2470.	6.7	244
5	Molecular dynamics modeling of the structure, dynamics and energetics of mineralâ€“water interfaces: Application to cement materials. Cement and Concrete Research, 2007, 37, 337-347.	4.6	226
6	Structure, Energetics, and Dynamics of Water Adsorbed on the Muscovite (001) Surface:Â A Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2005, 109, 15893-15905.	1.2	202
7	Hydrogen Bonding in Supercritical Water. 1. Experimental Results. The Journal of Physical Chemistry, 1995, 99, 5336-5340.	2.9	189
8	Hydrogen Bonding in Supercritical Water. 2. Computer Simulations. Journal of Physical Chemistry A, 1997, 101, 9720-9727.	1.1	189
9	: A force field database for cementitious materials including validations, applications and opportunities. Cement and Concrete Research, 2017, 102, 68-89.	4.6	186
10	Effects of background cations on the fouling of polyethersulfone membranes by natural organic matter: Experimental and molecular modeling study. Journal of Membrane Science, 2008, 309, 128-140.	4.1	169
11	Metal Cation Complexation with Natural Organic Matter in Aqueous Solutions: Molecular Dynamics Simulations and Potentials of Mean Force. Langmuir, 2010, 26, 15909-15919.	1.6	155
12	Molecular dynamics simulation of cationic complexation with natural organic matter. European Journal of Soil Science, 2007, 58, 909-917.	1.8	151
13	Molecular modeling of water structure in nano-pores between brucite (001) surfaces. Geochimica Et Cosmochimica Acta, 2004, 68, 3351-3365.	1.6	148
14	Molecular Modeling of the Structure and Energetics of Hydrotalcite Hydration. Chemistry of Materials, 2001, 13, 145-150.	3.2	126
15	Structural Arrangements of Isomorphic Substitutions in Smectites: Molecular Simulation of the Swelling Properties, Interlayer Structure, and Dynamics of Hydrated Csâ€“Montmorillonite Revisited with New Clay Models. Journal of Physical Chemistry C, 2014, 118, 12758-12773.	1.5	118
16	Hydrogen bonding in supercritical water: a Monte Carlo simulation. Chemical Physics Letters, 1994, 231, 301-307.	1.2	112
17	Structure, Energetics, and Dynamics of Smectite Clay Interlayer Hydration: Molecular Dynamics and Metadynamics Investigation of Na-Hectorite. Journal of Physical Chemistry C, 2013, 117, 5172-5187.	1.5	102
18	Molecular modeling of the structure and dynamics of the interlayer and surface species of mixed-metal layered hydroxides: Chloride and water in hydrocalumite (Friedelâ€™s salt). American Mineralogist, 2000, 85, 1046-1052.	0.9	101

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19	Hydration, Swelling, Interlayer Structure, and Hydrogen Bonding in Organolayered Double Hydroxides:Â Insights from Molecular Dynamics Simulation of Citrate-Intercalated Hydrotalcite. Journal of Physical Chemistry B, 2006, 110, 3841-3844.	1.2	95
20	Advances in Clayff Molecular Simulation of Layered and Nanoporous Materials and Their Aqueous Interfaces. Journal of Physical Chemistry C, 2021, 125, 17573-17589.	1.5	95
21	Size and topology of molecular clusters in supercritical water: a molecular dynamics simulation. Chemical Physics Letters, 1999, 302, 411-417.	1.2	92
22	Molecular Simulations of Liquid and Supercritical Water: Thermodynamics, Structure, and Hydrogen Bonding. Reviews in Mineralogy and Geochemistry, 2001, 42, 83-129.	2.2	92
23	Structure of Hydrated Gibbsite and Brucite Edge Surfaces: DFT Results and Further Development of the ClayFF Classical Force Field with Metalâ€“Oâ€“H Angle Bending Terms. Journal of Physical Chemistry C, 2017, 121, 14757-14771.	1.5	91
24	Asymmetric Hydrogen Bonding and Orientational Ordering of Water at Hydrophobic and Hydrophilic Surfaces: A Comparison of Water/Vapor, Water/Talc, and Water/Mica Interfaces. Journal of Physical Chemistry C, 2009, 113, 11077-11085.	1.5	90
25	Hydrogen-Bonding Structure and Dynamics of Aqueous Carbonate Species from Carâ€“Parrinello Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 794-802.	1.2	86
26	Molecular Dynamics Simulation of the Energetics and Structure of Layered Double Hydroxides Intercalated with Carboxylic Acids. Journal of Physical Chemistry C, 2007, 111, 13517-13523.	1.5	74
27	Effects of Ca2+ on supramolecular aggregation of natural organic matter in aqueous solutions: A comparison of molecular modeling approaches. Geoderma, 2011, 169, 27-32.	2.3	74
28	Interlayer structure and dynamics of Cl-bearing hydrotalcite: far infrared spectroscopy and molecular dynamics modeling. American Mineralogist, 2003, 88, 398-409.	0.9	73
29	Structure and Hydrogen Bonding in Liquid and Supercritical Aqueous NaCl Solutions at a Pressure of 1000 bar and Temperatures up to 500 Â°C:â€‰ A Comprehensive Experimental and Computational Study. Journal of Physical Chemistry A, 2006, 110, 4042-4052.	1.1	66
30	Molecular dynamics modelling of hydrated mineral interlayers and surfaces: structure and dynamics. Mineralogical Magazine, 2005, 69, 289-308.	0.6	63
31	Comparison of proton field-cycling relaxometry and molecular dynamics simulations for protonâ€“water surface dynamics in cement-based materials. Cement and Concrete Research, 2007, 37, 348-350.	4.6	63
32	Structure of Hydrated Kaolinite Edge Surfaces: DFT Results and Further Development of the ClayFF Classical Force Field with Metalâ€“Oâ€“H Angle Bending Terms. Journal of Physical Chemistry C, 2019, 123, 11628-11638.	1.5	61
33	Elastic properties of tetragonal PbTiO₃ single crystals by Brillouin scattering. Journal of Materials Research, 1997, 12, 2623-2627.	1.2	60
34	Structure, Energetics, and Dynamics of Cs⁺ and H₂O in Hectorite: Molecular Dynamics Simulations with an Unconstrained Substrate Surface. Journal of Physical Chemistry C, 2016, 120, 10298-10310.	1.5	60
35	Thermodynamics and structure of molecular clusters in supercritical water. Fluid Phase Equilibria, 2001, 183-184, 271-278.	1.4	59
36	Dissociation of carbonic acid: Gas phase energetics and mechanism from ab initio metadynamics simulations. Journal of Chemical Physics, 2007, 126, 204315.	1.2	58

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37	Interlayer Structure and Dynamics of Cl-â˜LiAl2-Layered Double Hydroxide:Â35Cl NMR Observations and Molecular Dynamics Modeling. Chemistry of Materials, 2002, 14, 2078-2085.	3.2	54
38	Molecular dynamics of supercritical water: A computer simulation of vibrational spectra with the flexible BJH potential. Geochimica Et Cosmochimica Acta, 1995, 59, 641-650.	1.6	53
39	Molecular dynamics computer simulations of the effects of hydrogen bonding on the properties of layered double hydroxides intercalated with organic acids. Philosophical Magazine, 2010, 90, 2475-2488.	0.7	52
40	133Cs and 35Cl NMR spectroscopy and molecular dynamics modeling of Cs+ and Clâ˜ complexation with natural organic matter. Geochimica Et Cosmochimica Acta, 2006, 70, 4319-4331.	1.6	48
41	Cation and Water Structure, Dynamics, and Energetics in Smectite Clays: A Molecular Dynamics Study of Caâ€“Hectorite. Journal of Physical Chemistry C, 2016, 120, 12429-12439.	1.5	48
42	A charged ring model for classical OHâ˜(aq) simulations. Chemical Physics Letters, 2007, 442, 128-133.	1.2	46
43	Structure and hydrogen bonding of liquid water at high hydrostatic pressures: Monte Carlo NPT-ensemble simulations up to 10 kbar. Journal of Molecular Liquids, 1999, 82, 57-72.	2.3	45
44	A multistate empirical valence bond model for solvation and transport simulations of OHâ˜ in aqueous solutions. Physical Chemistry Chemical Physics, 2009, 11, 9420.	1.3	45
45	Clay Swelling in Dry Supercritical Carbon Dioxide: Effects of Interlayer Cations on the Structure, Dynamics, and Energetics of CO₂ Intercalation Probed by XRD, NMR, and GCMD Simulations. Journal of Physical Chemistry C, 2018, 122, 4391-4402.	1.5	42
46	Elastic properties of orthorhombic KNbO3single crystals by Brillouin scattering. Journal of Applied Physics, 1993, 74, 6603-6608.	1.1	40
47	Molecular modeling of the 10-Ã... phase at subduction zone conditions. Earth and Planetary Science Letters, 2004, 222, 517-527.	1.8	40
48	Quantifying the Mechanisms of Site-Specific Ion Exchange at an Inhomogeneously Charged Surface: Case of Cs⁺/K⁺ on Hydrated Muscovite Mica. Journal of Physical Chemistry C, 2017, 121, 7829-7836.	1.5	40
49	Molecular-level understanding of metal ion retention in clay-rich materials. Nature Reviews Earth & Environment, 2022, 3, 461-476.	12.2	39
50	Monte Carlo Simulations of Water under Supercritical Conditions. I. Thermodynamic and Structural. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1991, 46, 433-444.	0.7	38
51	Molecular Dynamics Study of CO₂ and H₂O Intercalation in Smectite Clays: Effect of Temperature and Pressure on Interlayer Structure and Dynamics in Hectorite. Journal of Physical Chemistry C, 2017, 121, 24527-24540.	1.5	34
52	Structure and Decompression Melting of a Novel, High-Pressure Nanoconfined 2-D Ice. Journal of Physical Chemistry B, 2005, 109, 14308-14313.	1.2	32
53	NMR and computational molecular modeling studies of mineral surfaces and interlayer galleries: A review. American Mineralogist, 2015, 100, 1341-1354.	0.9	32
54	Structure and Dynamics of Waterâ€”Smectite Interfaces: Hydrogen Bonding and the Origin of the Sharp O-D_w/Oâ€”H_w Infrared Band From Molecular Simulations. Clays and Clay Minerals, 2016, 64, 452-471.	0.6	32

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55	Adsorption of gluconate and uranyl on C-S-H phases: Combination of wet chemistry experiments and molecular dynamics simulations for the binary systems. Physics and Chemistry of the Earth, 2017, 99, 194-203.	1.2	31
56	Intrinsic hydrophobicity of smectite basal surfaces quantitatively probed by molecular dynamics simulations. Applied Clay Science, 2020, 188, 105497.	2.6	29
57	Ethylene glycol intercalation in smectites. Molecular dynamics simulation studies. Applied Clay Science, 2014, 91-92, 87-97.	2.6	28
58	Intercalation of Ethylene Glycol in Smectites: Several Molecular Simulation Models Verified by X-Ray Diffraction Data. Clays and Clay Minerals, 2016, 64, 488-502.	0.6	28
59	Monte Carlo study of the thermodynamics and structure of dense supercritical water. International Journal of Thermophysics, 1986, 7, 887-900.	1.0	27
60	Universality of hydrogen bond distributions in liquid and supercritical water. Journal of Molecular Liquids, 2017, 241, 1038-1043.	2.3	27
61	Molecular modeling of the effects of 40Ar recoil in illite particles on their Kâ€“Ar isotope dating. Geochimica Et Cosmochimica Acta, 2015, 159, 162-176.	1.6	24
62	Experimental and molecular dynamics modeling studies of interlayer swelling: water incorporation in kanemite and ASR gel. Materials and Structures/Materiaux Et Constructions, 2005, 38, 449-458.	1.3	24
63	Understanding methane/carbon dioxide partitioning in clay nano- and meso-pores with constant reservoir composition molecular dynamics modeling. Physical Chemistry Chemical Physics, 2019, 21, 6917-6924.	1.3	21
64	Molecular dynamics simulation of the interaction of uranium (VI) with the Câ€“Sâ€“H phase of cement in the presence of gluconate. Applied Geochemistry, 2020, 113, 104496.	1.4	21
65	Role of Cations in the Methane/Carbon Dioxide Partitioning in Nano- and Mesopores of Illite Using Constant Reservoir Composition Molecular Dynamics Simulation. Journal of Physical Chemistry C, 2020, 124, 2490-2500.	1.5	20
66	Atomistic simulations of ettringite and its aqueous interfaces: Structure and properties revisited with the modified ClayFF force field. Cement and Concrete Research, 2022, 156, 106759.	4.6	19
67	Pressure dependence of optical absorption in PbTiO3to 35 GPa: Observation of the tetragonalâ€toâ€cubic phase transition. Journal of Applied Physics, 1992, 72, 3705-3707.	1.1	17
68	On the Hydrogen Bonding Structure at the Aqueous Interface of Ammonium-Substituted Mica: A Molecular Dynamics Simulation. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2013, 68, 91-100.	0.7	17
69	Competitive Adsorption of H₂O and CO₂ in 2-Dimensional Nanoconfinement: GCMD Simulations of Cs- and Ca-Hectorites. Journal of Physical Chemistry C, 2018, 122, 23460-23469.	1.5	17
70	Deciphering the non-linear impact of Al on chemical durability of silicate glass. Acta Materialia, 2022, 225, 117478.	3.8	17
71	Identification of montmorillonite particle edge orientations by atomic-force microscopy. Applied Clay Science, 2020, 186, 105442.	2.6	15
72	Molecular models of natural organic matter and its colloidal aggregation in aqueous solutions: Challenges and opportunities for computer simulations. Pure and Applied Chemistry, 2012, 85, 149-158.	0.9	14

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73	4. Molecular Simulations of Liquid and Supercritical Water: Thermodynamics, Structure, and Hydrogen Bonding. , 2001, , 83-130.		13
74	Introduction to a Special Issue on Molecular Computer Simulations of Clays and Clay-Water Interfaces: Recent Progress, Challenges, and Opportunities. Clays and Clay Minerals, 2016, 64, 335-336.	0.6	13
75	Interaction of Ions with Hydrated Clay Surfaces: Computational Molecular Modeling for Nuclear Waste Disposal Applications. Procedia Earth and Planetary Science, 2017, 17, 566-569.	0.6	12
76	Thermodynamic data of adsorption reveal the entry of CH₄ and CO₂ in a smectite clay interlayer. Physical Chemistry Chemical Physics, 2020, 22, 16727-16733.	1.3	11
77	Diffusion Behavior of Methane in 3D Kerogen Models. Energy & Fuels, 0, , .	2.5	10
78	Molecular Modeling of the Vibrational Spectra of Interlayer and Surface Species of Layered Double Hydroxides. , 2005, , .		9
79	Computer Simulations of Aqueous Fluids at High Temperatures and Pressures. , 1992, , 1-59.		8
80	Carbonation Reaction Mechanisms of Portlandite Predicted from Enhanced Ab Initio Molecular Dynamics Simulations. Minerals (Basel, Switzerland), 2021, 11, 509.	0.8	8
81	Theoretical modeling of geochemical fluids under high-pressure, high-temperature conditions. High Pressure Research, 1991, 7, 378-380.	0.4	7
82	Monte Carlo Simulations of Water under Supercritical Conditions. II. Convergence Characteristics and the System Size Effects. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1992, 47, 992-998.	0.7	4
83	Growth of high temperature Î²-quartz from supercritical aqueous fluids. Journal of Crystal Growth, 1996, 162, 142-146.	0.7	4
84	Silica transfer and Î²-quartz growth from supercritical aqueous fluids. Journal of Supercritical Fluids, 1998, 13, 357-362.	1.6	4
85	Size and structure of molecular clusters in supercritical water. Journal of Structural Chemistry, 1999, 40, 548-553.	0.3	4
86	Direct Experimental Evidence of the Effects of Clay Particlesâ€™ Basal-to-Lateral Surface Ratio on Methane and Carbon Dioxide Adsorption. Journal of Physical Chemistry C, 2021, 125, 11499-11507.	1.5	4
87	Layered double hydroxideâ€“borate composites supported on magnetic nanoparticles: preparation, characterization and molecular dynamics simulations. Journal of Porous Materials, 2020, 27, 735-743.	1.3	3
88	Molecular Structure and Dynamics of Nano-Confined Water: Computer Simulations of Aqueous Species in Clay, Cement, and Polymer Membranes. NATO Science for Peace and Security Series C: Environmental Security, 2014, , 103-115.	0.1	2
89	Deciphering the Non-Linear Impact of Al on Chemical Durability of Silicate Glass. SSRN Electronic Journal, 0, , .	0.4	1
90	Molecular Modeling of Confined Fluids and Solid-Fluid Interfaces in Portland Cement and Related Materials. Special Publication - Royal Society of Chemistry, 2004, , 183-184.	0.0	1

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91	Atomistic Computer Modeling of Hydrocalumite As an Adsorbent for Radioactive Anions from Aqueous Solutions. Russian Journal of Physical Chemistry A, 2022, 96, 748-750.	0.1	1
92	Introduction to the special issue of the Journal of Molecular Liquids â€œSupercritical fluids. Theory and applicationsâ€•dedicated to Prof. Yu. E. Gorbaty. Journal of Molecular Liquids, 2017, 239, 1-2.	2.3	0
93	Atomistic computer simulations of the cement degradation mechanisms in the context of geological carbon sequestration. , 2021, , .		0
94	Atomistic Modeling of the Structural and Dynamic Properties of Aqueous NaCl and Na2SO4 Solutions in the Interlayer Space of Ettringite. Russian Journal of Physical Chemistry A, 2022, 96, 818-823.	0.1	0