

Andrey G Kalinichev

List of Publications by Year in descending order

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94
papers

7,825
citations

57758

44
h-index

51608

86
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97
all docs

97
docs citations

97
times ranked

5124
citing authors

#	ARTICLE	IF	CITATIONS
1	Deciphering the non-linear impact of Al on chemical durability of silicate glass. <i>Acta Materialia</i> , 2022, 225, 117478.	7.9	17
2	Atomistic simulations of ettringite and its aqueous interfaces: Structure and properties revisited with the modified ClayFF force field. <i>Cement and Concrete Research</i> , 2022, 156, 106759.	11.0	19
3	Atomistic Computer Modeling of Hydrocalumite As an Adsorbent for Radioactive Anions from Aqueous Solutions. <i>Russian Journal of Physical Chemistry A</i> , 2022, 96, 748-750.	0.6	1
4	Atomistic Modeling of the Structural and Dynamic Properties of Aqueous NaCl and Na ₂ SO ₄ Solutions in the Interlayer Space of Ettringite. <i>Russian Journal of Physical Chemistry A</i> , 2022, 96, 818-823.	0.6	0
5	Molecular-level understanding of metal ion retention in clay-rich materials. <i>Nature Reviews Earth & Environment</i> , 2022, 3, 461-476.	29.7	39
6	Direct Experimental Evidence of the Effects of Clay Particles' Basal-to-Lateral Surface Ratio on Methane and Carbon Dioxide Adsorption. <i>Journal of Physical Chemistry C</i> , 2021, 125, 11499-11507.	3.1	4
7	Carbonation Reaction Mechanisms of Portlandite Predicted from Enhanced Ab Initio Molecular Dynamics Simulations. <i>Minerals (Basel, Switzerland)</i> , 2021, 11, 509.	2.0	8
8	Advances in Clayff Molecular Simulation of Layered and Nanoporous Materials and Their Aqueous Interfaces. <i>Journal of Physical Chemistry C</i> , 2021, 125, 17573-17589.	3.1	95
9	Atomistic computer simulations of the cement degradation mechanisms in the context of geological carbon sequestration. , 2021, , .		0
10	Layered double hydroxide-borate composites supported on magnetic nanoparticles: preparation, characterization and molecular dynamics simulations. <i>Journal of Porous Materials</i> , 2020, 27, 735-743.	2.6	3
11	Molecular dynamics simulation of the interaction of uranium (VI) with the Ca-S-H phase of cement in the presence of gluconate. <i>Applied Geochemistry</i> , 2020, 113, 104496.	3.0	21
12	Intrinsic hydrophobicity of smectite basal surfaces quantitatively probed by molecular dynamics simulations. <i>Applied Clay Science</i> , 2020, 188, 105497.	5.2	29
13	Thermodynamic data of adsorption reveal the entry of CH ₄ and CO ₂ in a smectite clay interlayer. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16727-16733.	2.8	11
14	Role of Cations in the Methane/Carbon Dioxide Partitioning in Nano- and Mesopores of Illite Using Constant Reservoir Composition Molecular Dynamics Simulation. <i>Journal of Physical Chemistry C</i> , 2020, 124, 2490-2500.	3.1	20
15	Identification of montmorillonite particle edge orientations by atomic-force microscopy. <i>Applied Clay Science</i> , 2020, 186, 105442.	5.2	15
16	Structure of Hydrated Kaolinite Edge Surfaces: DFT Results and Further Development of the ClayFF Classical Force Field with Metal-O-H Angle Bending Terms. <i>Journal of Physical Chemistry C</i> , 2019, 123, 11628-11638.	3.1	61
17	Understanding methane/carbon dioxide partitioning in clay nano- and meso-pores with constant reservoir composition molecular dynamics modeling. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 6917-6924.	2.8	21
18	Clay Swelling in Dry Supercritical Carbon Dioxide: Effects of Interlayer Cations on the Structure, Dynamics, and Energetics of CO ₂ Intercalation Probed by XRD, NMR, and GCMD Simulations. <i>Journal of Physical Chemistry C</i> , 2018, 122, 4391-4402.	3.1	42

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19	Competitive Adsorption of H ₂ O and CO ₂ in 2-Dimensional Nanoconfinement: GCMC Simulations of Cs- and Ca-Hectorites. <i>Journal of Physical Chemistry C</i> , 2018, 122, 23460-23469.	3.1	17
20	Interaction of Ions with Hydrated Clay Surfaces: Computational Molecular Modeling for Nuclear Waste Disposal Applications. <i>Procedia Earth and Planetary Science</i> , 2017, 17, 566-569.	0.6	12
21	Introduction to the special issue of the <i>Journal of Molecular Liquids</i> "Supercritical fluids. Theory and applications" dedicated to Prof. Yu. E. Gorbaty. <i>Journal of Molecular Liquids</i> , 2017, 239, 1-2.	4.9	0
22	Adsorption of gluconate and uranyl on C-S-H phases: Combination of wet chemistry experiments and molecular dynamics simulations for the binary systems. <i>Physics and Chemistry of the Earth</i> , 2017, 99, 194-203.	2.9	31
23	Quantifying the Mechanisms of Site-Specific Ion Exchange at an Inhomogeneously Charged Surface: Case of Cs ⁺ /K ⁺ on Hydrated Muscovite Mica. <i>Journal of Physical Chemistry C</i> , 2017, 121, 7829-7836.	3.1	40
24	: A force field database for cementitious materials including validations, applications and opportunities. <i>Cement and Concrete Research</i> , 2017, 102, 68-89.	11.0	186
25	Molecular Dynamics Study of CO ₂ and H ₂ O Intercalation in Smectite Clays: Effect of Temperature and Pressure on Interlayer Structure and Dynamics in Hectorite. <i>Journal of Physical Chemistry C</i> , 2017, 121, 24527-24540.	3.1	34
26	Structure of Hydrated Gibbsite and Brucite Edge Surfaces: DFT Results and Further Development of the ClayFF Classical Force Field with Metal-O-H Angle Bending Terms. <i>Journal of Physical Chemistry C</i> , 2017, 121, 14757-14771.	3.1	91
27	Universality of hydrogen bond distributions in liquid and supercritical water. <i>Journal of Molecular Liquids</i> , 2017, 241, 1038-1043.	4.9	27
28	Introduction to a Special Issue on Molecular Computer Simulations of Clays and Clay-Water Interfaces: Recent Progress, Challenges, and Opportunities. <i>Clays and Clay Minerals</i> , 2016, 64, 335-336.	1.3	13
29	Intercalation of Ethylene Glycol in Smectites: Several Molecular Simulation Models Verified by X-Ray Diffraction Data. <i>Clays and Clay Minerals</i> , 2016, 64, 488-502.	1.3	28
30	Structure and Dynamics of Water-Smectite Interfaces: Hydrogen Bonding and the Origin of the Sharp O-D _w /O ¹⁸ H _w Infrared Band From Molecular Simulations. <i>Clays and Clay Minerals</i> , 2016, 64, 452-471.	1.3	32
31	Structure, Energetics, and Dynamics of Cs ⁺ and H ₂ O in Hectorite: Molecular Dynamics Simulations with an Unconstrained Substrate Surface. <i>Journal of Physical Chemistry C</i> , 2016, 120, 10298-10310.	3.1	60
32	Cation and Water Structure, Dynamics, and Energetics in Smectite Clays: A Molecular Dynamics Study of Ca ²⁺ -Hectorite. <i>Journal of Physical Chemistry C</i> , 2016, 120, 12429-12439.	3.1	48
33	NMR and computational molecular modeling studies of mineral surfaces and interlayer galleries: A review. <i>American Mineralogist</i> , 2015, 100, 1341-1354.	1.9	32
34	Molecular modeling of the effects of ⁴⁰ Ar recoil in illite particles on their ⁴⁰ Ar isotope dating. <i>Geochimica Et Cosmochimica Acta</i> , 2015, 159, 162-176.	3.9	24
35	Ethylene glycol intercalation in smectites. <i>Molecular dynamics simulation studies. Applied Clay Science</i> , 2014, 91-92, 87-97.	5.2	28
36	Structural Arrangements of Isomorphic Substitutions in Smectites: Molecular Simulation of the Swelling Properties, Interlayer Structure, and Dynamics of Hydrated Cs ⁺ -Montmorillonite Revisited with New Clay Models. <i>Journal of Physical Chemistry C</i> , 2014, 118, 12758-12773.	3.1	118

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37	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.	0.2	2
38	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.	3.1	102
39	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.	1.5	17
40	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.	1.9	14
41	Effects of Ca ²⁺ on supramolecular aggregation of natural organic matter in aqueous solutions: A comparison of molecular modeling approaches. Geoderma, 2011, 169, 27-32.	5.1	74
42	Metal Cation Complexation with Natural Organic Matter in Aqueous Solutions: Molecular Dynamics Simulations and Potentials of Mean Force. Langmuir, 2010, 26, 15909-15919.	3.5	155
43	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.	1.6	52
44	A multistate empirical valence bond model for solvation and transport simulations of OH ⁻ in aqueous solutions. Physical Chemistry Chemical Physics, 2009, 11, 9420.	2.8	45
45	Hydrogen-Bonding Structure and Dynamics of Aqueous Carbonate Species from CaráˆParrinello Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 794-802.	2.6	86
46	Molecular models and simulations of layered materials. Journal of Materials Chemistry, 2009, 19, 2470.	6.7	244
47	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.	3.1	90
48	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.	8.2	169
49	Dissociation of carbonic acid: Gas phase energetics and mechanism from ab initio metadynamics simulations. Journal of Chemical Physics, 2007, 126, 204315.	3.0	58
50	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.	3.1	74
51	A charged ring model for classical OH ⁻ (aq) simulations. Chemical Physics Letters, 2007, 442, 128-133.	2.6	46
52	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.	11.0	63
53	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.	11.0	226
54	Molecular dynamics simulation of cationic complexation with natural organic matter. European Journal of Soil Science, 2007, 58, 909-917.	3.9	151

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55	Structure and Hydrogen Bonding in Liquid and Supercritical Aqueous NaCl Solutions at a Pressure of 1000 bar and Temperatures up to 500 Å°C:â€‰ A Comprehensive Experimental and Computational Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4042-4052.	2.5	66
56	Hydration, Swelling, Interlayer Structure, and Hydrogen Bonding in Organolayered Double Hydroxides:Â Insights from Molecular Dynamics Simulation of Citrate-Intercalated Hydrotalcite. <i>Journal of Physical Chemistry B</i> , 2006, 110, 3841-3844.	2.6	95
57	Effects of substrate structure and composition on the structure, dynamics, and energetics of water at mineral surfaces: A molecular dynamics modeling study. <i>Geochimica Et Cosmochimica Acta</i> , 2006, 70, 562-582.	3.9	250
58	¹³³ Cs and ³⁵ Cl NMR spectroscopy and molecular dynamics modeling of Cs ⁺ and Cl ^{âˆ’} complexation with natural organic matter. <i>Geochimica Et Cosmochimica Acta</i> , 2006, 70, 4319-4331.	3.9	48
59	Structure, Energetics, and Dynamics of Water Adsorbed on the Muscovite (001) Surface:Â A Molecular Dynamics Simulation. <i>Journal of Physical Chemistry B</i> , 2005, 109, 15893-15905.	2.6	202
60	Structure and Decompression Melting of a Novel, High-Pressure Nanoconfined 2-D Ice. <i>Journal of Physical Chemistry B</i> , 2005, 109, 14308-14313.	2.6	32
61	Molecular dynamics modelling of hydrated mineral interlayers and surfaces: structure and dynamics. <i>Mineralogical Magazine</i> , 2005, 69, 289-308.	1.4	63
62	Molecular Modeling of the Vibrational Spectra of Interlayer and Surface Species of Layered Double Hydroxides. , 2005, , .		9
63	Experimental and molecular dynamics modeling studies of interlayer swelling: water incorporation in kanemite and ASR gel. <i>Materials and Structures/Materiaux Et Constructions</i> , 2005, 38, 449-458.	3.1	24
64	Molecular Models of Hydroxide, Oxyhydroxide, and Clay Phases and the Development of a General Force Field. <i>Journal of Physical Chemistry B</i> , 2004, 108, 1255-1266.	2.6	2,281
65	Molecular modeling of water structure in nano-pores between brucite (001) surfaces. <i>Geochimica Et Cosmochimica Acta</i> , 2004, 68, 3351-3365.	3.9	148
66	Molecular modeling of the 10-Å... phase at subduction zone conditions. <i>Earth and Planetary Science Letters</i> , 2004, 222, 517-527.	4.4	40
67	Molecular Modeling of Confined Fluids and Solid-Fluid Interfaces in Portland Cement and Related Materials. <i>Special Publication - Royal Society of Chemistry</i> , 2004, , 183-184.	0.0	1
68	Interlayer structure and dynamics of Cl-bearing hydrotalcite: far infrared spectroscopy and molecular dynamics modeling. <i>American Mineralogist</i> , 2003, 88, 398-409.	1.9	73
69	Molecular Dynamics Modeling of Chloride Binding to the Surfaces of Calcium Hydroxide, Hydrated Calcium Aluminate, and Calcium Silicate Phases. <i>Chemistry of Materials</i> , 2002, 14, 3539-3549.	6.7	249
70	Interlayer Structure and Dynamics of Cl-âˆ’LiAl ₂ -Layered Double Hydroxide:Â ³⁵ Cl NMR Observations and Molecular Dynamics Modeling. <i>Chemistry of Materials</i> , 2002, 14, 2078-2085.	6.7	54
71	Molecular Modeling of the Structure and Energetics of Hydrotalcite Hydration. <i>Chemistry of Materials</i> , 2001, 13, 145-150.	6.7	126
72	Molecular Simulations of Liquid and Supercritical Water: Thermodynamics, Structure, and Hydrogen Bonding. <i>Reviews in Mineralogy and Geochemistry</i> , 2001, 42, 83-129.	4.8	92

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73	4. Molecular Simulations of Liquid and Supercritical Water: Thermodynamics, Structure, and Hydrogen Bonding. , 2001, , 83-130.		13
74	Thermodynamics and structure of molecular clusters in supercritical water. Fluid Phase Equilibria, 2001, 183-184, 271-278.	2.5	59
75	Molecular modeling of the structure and dynamics of the interlayer and surface species of mixed-metal layered hydroxides: Chloride and water in hydrocalumite (Friedel's salt). American Mineralogist, 2000, 85, 1046-1052.	1.9	101
76	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.	4.9	45
77	Size and topology of molecular clusters in supercritical water: a molecular dynamics simulation. Chemical Physics Letters, 1999, 302, 411-417.	2.6	92
78	Size and structure of molecular clusters in supercritical water. Journal of Structural Chemistry, 1999, 40, 548-553.	1.0	4
79	Silica transfer and β -quartz growth from supercritical aqueous fluids. Journal of Supercritical Fluids, 1998, 13, 357-362.	3.2	4
80	Hydrogen Bonding in Supercritical Water. 2. Computer Simulations. Journal of Physical Chemistry A, 1997, 101, 9720-9727.	2.5	189
81	Elastic properties of tetragonal PbTiO_3 single crystals by Brillouin scattering. Journal of Materials Research, 1997, 12, 2623-2627.	2.6	60
82	Growth of high temperature β -quartz from supercritical aqueous fluids. Journal of Crystal Growth, 1996, 162, 142-146.	1.5	4
83	Molecular dynamics of supercritical water: A computer simulation of vibrational spectra with the flexible BJH potential. Geochimica Et Cosmochimica Acta, 1995, 59, 641-650.	3.9	53
84	Hydrogen Bonding in Supercritical Water. 1. Experimental Results. The Journal of Physical Chemistry, 1995, 99, 5336-5340.	2.9	189
85	Hydrogen bonding in supercritical water: a Monte Carlo simulation. Chemical Physics Letters, 1994, 231, 301-307.	2.6	112
86	Elastic properties of orthorhombic KNbO_3 single crystals by Brillouin scattering. Journal of Applied Physics, 1993, 74, 6603-6608.	2.5	40
87	Pressure dependence of optical absorption in PbTiO_3 to 35 GPa: Observation of the tetragonal to cubic phase transition. Journal of Applied Physics, 1992, 72, 3705-3707.	2.5	17
88	Computer Simulations of Aqueous Fluids at High Temperatures and Pressures. , 1992, , 1-59.		8
89	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.	1.5	4
90	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.	1.5	38

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91	Theoretical modeling of geochemical fluids under high-pressure, high-temperature conditions. High Pressure Research, 1991, 7, 378-380.	1.2	7
92	Monte Carlo study of the thermodynamics and structure of dense supercritical water. International Journal of Thermophysics, 1986, 7, 887-900.	2.1	27
93	Deciphering the Non-Linear Impact of Al on Chemical Durability of Silicate Glass. SSRN Electronic Journal, 0, , .	0.4	1
94	Diffusion Behavior of Methane in 3D Kerogen Models. Energy & Fuels, 0, , .	5.1	10