Andrey G Kalinichev

List of Publications by Citations

90 papers	6,232 citations	41 h-index	78 g-index
97 ext. papers	6,970 ext. citations	4.3 avg, IF	6.05 L-index

#	Paper	IF	Citations
90	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	3.4	1662
89	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	5.5	227
88	Molecular models and simulations of layered materials. *Journal of Materials Chemistry*, **2009**, 19, 2470		210
87	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	9.6	208
86	Molecular dynamics modeling of the structure, dynamics and energetics of mineral□water interfaces: Application to cement materials. *Cement and Concrete Research*, **2007**, 37, 337-347	10.3	190
85	Structure, energetics, and dynamics of water adsorbed on the muscovite (001) surface: a molecular dynamics simulation. *Journal of Physical Chemistry B*, **2005**, 109, 15893-905	3.4	183
84	Hydrogen Bonding in Supercritical Water. 2. Computer Simulations. *Journal of Physical Chemistry A*, **1997**, 101, 9720-9727	2.8	178
83	Hydrogen Bonding in Supercritical Water. 1. Experimental Results. *The Journal of Physical Chemistry* , **1995**, 99, 5336-5340		169
82	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	9.6	133
81	Molecular modeling of water structure in nano-pores between brucite (001) surfaces. *Geochimica Et Cosmochimica Acta*, **2004**, 68, 3351-3365	5.5	126
80	Molecular dynamics simulation of cationic complexation with natural organic matter. *European Journal of Soil Science*, **2007**, 58, 909-917	3.4	123
79	: A force field database for cementitious materials including validations, applications and opportunities. *Cement and Concrete Research*, **2017**, 102, 68-89	10.3	122
78	Metal cation complexation with natural organic matter in aqueous solutions: molecular dynamics simulations and potentials of mean force. *Langmuir*, **2010**, 26, 15909-19	4	120
77	Molecular Modeling of the Structure and Energetics of Hydrotalcite Hydration. *Chemistry of Materials*, **2001**, 13, 145-150	9.6	116
76	Hydrogen bonding in supercritical water: a Monte Carlo simulation. *Chemical Physics Letters*, **1994**, 231, 301-307	2.5	99
75	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. *Journal of Physical Chemistry C*, **2014**, 118, 12758-12773	3.8	95
74	Hydration, swelling, interlayer structure, and hydrogen bonding in organolayered double hydroxides: insights from molecular dynamics simulation of citrate-intercalated hydrotalcite. *Journal of Physical Chemistry B*, **2006**, 110, 3841-4	3.4	87

73	Molecular modeling of the structure and dynamics of the interlayer and surface species of mixed-metal layered hydroxides: Chloride and water in hydrocalumite (Friedel salt). *American Mineralogist*, **2000**, 85, 1046-1052	2.9	86
72	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	3.8	85
71	Size and topology of molecular clusters in supercritical water: a molecular dynamics simulation. *Chemical Physics Letters*, **1999**, 302, 411-417	2.5	83
70	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	3.8	81
69	Hydrogen-bonding structure and dynamics of aqueous carbonate species from car-parrinello molecular dynamics simulations. *Journal of Physical Chemistry B*, **2009**, 113, 794-802	3.4	77
68	Molecular Simulations of Liquid and Supercritical Water: Thermodynamics, Structure, and Hydrogen Bonding. *Reviews in Mineralogy and Geochemistry*, **2001**, 42, 83-129	7.1	74
67	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	3.8	69
66	Interlayer structure and dynamics of Cl-bearing hydrotalcite: far infrared spectroscopy and molecular dynamics modeling. *American Mineralogist*, **2003**, 88, 398-409	2.9	67
65	Effects of Ca2+ on supramolecular aggregation of natural organic matter in aqueous solutions: A comparison of molecular modeling approaches. *Geoderma*, **2011**, 169, 27-32	6.7	64
64	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. *Journal of Physical Chemistry C*, **2017**, 121, 14757-14771	3.8	60
63	Comparison of proton field-cycling relaxometry and molecular dynamics simulations for proton–water surface dynamics in cement-based materials. *Cement and Concrete Research*, **2007**, 37, 348-350	10.3	60
62	Structure and hydrogen bonding in liquid and supercritical aqueous NaCl solutions at a pressure of 1000 bar and temperatures up to 500 degrees C: A comprehensive experimental and computational study. *Journal of Physical Chemistry A*, **2006**, 110, 4042-52	2.8	60
61	Thermodynamics and structure of molecular clusters in supercritical water. *Fluid Phase Equilibria*, **2001**, 183-184, 271-278	2.5	57
60	Molecular dynamics modelling of hydrated mineral interlayers and surfaces: structure and dynamics. *Mineralogical Magazine*, **2005**, 69, 289-308	1.7	56
59	Elastic properties of tetragonal PbTiO3 single crystals by Brillouin scattering. *Journal of Materials Research*, **1997**, 12, 2623-2627	2.5	52
58	Dissociation of carbonic acid: gas phase energetics and mechanism from ab initio metadynamics simulations. *Journal of Chemical Physics*, **2007**, 126, 204315	3.9	51
57	Interlayer Structure and Dynamics of Cl-LiAl2-Layered Double Hydroxide: 35Cl NMR Observations and Molecular Dynamics Modeling. *Chemistry of Materials*, **2002**, 14, 2078-2085	9.6	50
56	Molecular dynamics of supercritical water: A computer simulation of vibrational spectra with the flexible BJH potential. *Geochimica Et Cosmochimica Acta*, **1995**, 59, 641-650	5.5	50

55	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	3.8	50
54	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	47
53	133Cs and 35Cl NMR spectroscopy and molecular dynamics modeling of Cs+ and Cl□ complexation with natural organic matter. *Geochimica Et Cosmochimica Acta*, **2006**, 70, 4319-4331	5.5	46
52	A multistate empirical valence bond model for solvation and transport simulations of OH- in aqueous solutions. *Physical Chemistry Chemical Physics*, **2009**, 11, 9420-30	3.6	43
51	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	6	43
50	A charged ring model for classical OH□(aq) simulations. *Chemical Physics Letters*, **2007**, 442, 128-133	2.5	42
49	Cation and Water Structure, Dynamics, and Energetics in Smectite Clays: A Molecular Dynamics Study of Ca□Hectorite. *Journal of Physical Chemistry C*, **2016**, 120, 12429-12439	3.8	40
48	Structure of Hydrated Kaolinite Edge Surfaces: DFT Results and Further Development of the ClayFF Classical Force Field with Metal□OH□ Angle Bending Terms. *Journal of Physical Chemistry C*, **2019**, 123, 11628-11638	3.8	37
47	Molecular modeling of the 10-□phase at subduction zone conditions. *Earth and Planetary Science Letters*, **2004**, 222, 517-527	5.3	37
46	Elastic properties of orthorhombic KNbO3 single crystals by Brillouin scattering. *Journal of Applied Physics*, **1993**, 74, 6603-6608	2.5	36
45	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	1.4	36
44	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	3.8	35
43	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	3.8	30
42	Structure and decompression melting of a novel, high-pressure nanoconfined 2-D ice. *Journal of Physical Chemistry B*, **2005**, 109, 14308-13	3.4	30
41	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	3.8	26
40	Structure and Dynamics of Water-Smectite Interfaces: Hydrogen Bonding and the Origin of the Sharp O-Dw/O-Hw Infrared Band From Molecular Simulations. *Clays and Clay Minerals*, **2016**, 64, 452-471	2.1	26
39	Review. NMR and computational molecular modeling studies of mineral surfaces and interlayer galleries: A review. *American Mineralogist*, **2015**, 100, 1341-1354	2.9	25
38	Advances in Clayff Molecular Simulation of Layered and Nanoporous Materials and Their Aqueous Interfaces. *Journal of Physical Chemistry C*, **2021**, 125, 17573-17589	3.8	25

37	Universality of hydrogen bond distributions in liquid and supercritical water. *Journal of Molecular Liquids*, **2017**, 241, 1038-1043	6	24
36	Monte Carlo study of the thermodynamics and structure of dense supercritical water. *International Journal of Thermophysics*, **1986**, 7, 887-900	2.1	24
35	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	3.4	23
34	Ethylene glycol intercalation in smectites. Molecular dynamics simulation studies. *Applied Clay Science*, **2014**, 91-92, 87-97	5.2	21
33	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	3	20
32	Intercalation of Ethylene Glycol in Smectites: Several Molecular Simulation Models Verified by X-Ray Diffraction Data. *Clays and Clay Minerals*, **2016**, 64, 488-502	2.1	20
31	Molecular modeling of the effects of 40Ar recoil in illite particles on their K-Ar isotope dating. *Geochimica Et Cosmochimica Acta*, **2015**, 159, 162-176	5.5	19
30	Pressure dependence of optical absorption in PbTiO3 to 35 GPa: Observation of the tetragonal-to-cubic phase transition. *Journal of Applied Physics*, **1992**, 72, 3705-3707	2.5	17
29	Intrinsic hydrophobicity of smectite basal surfaces quantitatively probed by molecular dynamics simulations. *Applied Clay Science*, **2020**, 188, 105497	5.2	16
28	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	3.6	15
27	4. Molecular Simulations of Liquid and Supercritical Water: Thermodynamics, Structure, and Hydrogen Bonding **2001**, 83-130		13
26	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	1.4	12
25	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	2.1	12
24	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	3.8	12
23	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	3.8	11
22	Molecular dynamics simulation of the interaction of uranium (VI) with the C-S-H phase of cement in the presence of gluconate. *Applied Geochemistry*, **2020**, 113, 104496	3.5	10
21	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	2.1	9
20	Identification of montmorillonite particle edge orientations by atomic-force microscopy. *Applied Clay Science*, **2020**, 186, 105442	5.2	8

19	Interaction of Ions with Hydrated Clay Surfaces: Computational Molecular Modeling for Nuclear Waste Disposal Applications. *Procedia Earth and Planetary Science*, **2017**, 17, 566-569		7
18	Theoretical modeling of geochemical fluids under high-pressure, high-temperature conditions. *High Pressure Research*, **1991**, 7, 378-380	1.6	7
17	Thermodynamic data of adsorption reveal the entry of CH and CO in a smectite clay interlayer. *Physical Chemistry Chemical Physics*, **2020**, 22, 16727-16733	3.6	6
16	Computer Simulations of Aqueous Fluids at High Temperatures and Pressures **1992**, 1-59		5
15	Molecular Modeling of the Vibrational Spectra of Interlayer and Surface Species of Layered Double Hydroxides **2005**,		5
14	Molecular-level understanding of metal ion retention in clay-rich materials. *Nature Reviews Earth & Environment*,	30.2	5
13	Size and structure of molecular clusters in supercritical water. *Journal of Structural Chemistry*, **1999**, 40, 548-553	0.9	4
12	Silica transfer and α-quartz growth from supercritical aqueous fluids. *Journal of Supercritical Fluids*, **1998**, 13, 357-362	4.2	3
11	Growth of high temperature α-quartz from supercritical aqueous fluids. *Journal of Crystal Growth*, **1996**, 162, 142-146	1.6	3
10	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	1.4	3
9	Deciphering the non-linear impact of Al on chemical durability of silicate glass. *Acta Materialia*, **2022**, 225, 117478	8.4	2
8	Layered double hydroxide–borate composites supported on magnetic nanoparticles: preparation, characterization and molecular dynamics simulations. *Journal of Porous Materials*, **2020**, 27, 735-743	2.4	2
7	Carbonation Reaction Mechanisms of Portlandite Predicted from Enhanced Ab Initio Molecular Dynamics Simulations. *Minerals (Basel, Switzerland)*, **2021**, 11, 509	2.4	2
6	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	0.3	1
5	Direct Experimental Evidence of the Effects of Clay Particles' Basal-to-Lateral Surface Ratio on Methane and Carbon Dioxide Adsorption. *Journal of Physical Chemistry C*, **2021**, 125, 11499-11507	3.8	1
4	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	10.3	1
3	Introduction to the special issue of the Journal of Molecular Liquids "Supercritical fluids. Theory and applications" dedicated to Prof. Yu. E. Gorbaty. *Journal of Molecular Liquids*, **2017**, 239, 1-2	6	
2	Atomistic Computer Modeling of Hydrocalumite As an Adsorbent for Radioactive Anions from Aqueous Solutions. *Russian Journal of Physical Chemistry A*, **2022**, 96, 748-750	0.7	

1 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 0.7