

Andrey G Kalinichev

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Deciphering the non-linear impact of Al on chemical durability of silicate glass. <i>Acta Materialia</i> , 2022 , 225, 117478	8.4	2
89	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	10.3	1
88	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	0.7	
87	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	0.7	
86	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	3.8	1
85	Carbonation Reaction Mechanisms of Portlandite Predicted from Enhanced Ab Initio Molecular Dynamics Simulations. <i>Minerals (Basel, Switzerland)</i> , 2021 , 11, 509	2.4	2
84	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	3.8	25
83	Intrinsic hydrophobicity of smectite basal surfaces quantitatively probed by molecular dynamics simulations. <i>Applied Clay Science</i> , 2020 , 188, 105497	5.2	16
82	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	3.6	6
81	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	3.8	11
80	Identification of montmorillonite particle edge orientations by atomic-force microscopy. <i>Applied Clay Science</i> , 2020 , 186, 105442	5.2	8
79	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	2.4	2
78	Molecular dynamics simulation of the interaction of uranium (VI) with the C ₃ S phase of cement in the presence of gluconate. <i>Applied Geochemistry</i> , 2020 , 113, 104496	3.5	10
77	Structure of Hydrated Kaolinite Edge Surfaces: DFT Results and Further Development of the ClayFF Classical Force Field with Metal-Clay Angle Bending Terms. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 11628-11638	3.8	37
76	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	3.6	15
75	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	3.8	30
74	Competitive Adsorption of H ₂ O and CO ₂ in 2-Dimensional Nanoconfinement: GCMD Simulations of Cs- and Ca-Hectorites. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 23460-23469	3.8	12

73	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		7
72	Introduction to the special issue of the Journal of Molecular Liquids Supercritical fluids. Theory and applications dedicated to Prof. Yu. E. Gorbaty. <i>Journal of Molecular Liquids</i> , 2017 , 239, 1-2	6	
71	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	3	20
70	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	3.8	35
69	: A force field database for cementitious materials including validations, applications and opportunities. <i>Cement and Concrete Research</i> , 2017 , 102, 68-89	10.3	122
68	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	3.8	26
67	Structure of Hydrated Gibbsite and Brucite Edge Surfaces: DFT Results and Further Development of the ClayFF Classical Force Field with Metal-DE Angle Bending Terms. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 14757-14771	3.8	60
66	Universality of hydrogen bond distributions in liquid and supercritical water. <i>Journal of Molecular Liquids</i> , 2017 , 241, 1038-1043	6	24
65	Cation and Water Structure, Dynamics, and Energetics in Smectite Clays: A Molecular Dynamics Study of Ca Hectorite. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 12429-12439	3.8	40
64	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	2.1	12
63	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	2.1	20
62	Structure and Dynamics of Water-Smectite Interfaces: Hydrogen Bonding and the Origin of the Sharp O-Dw/O-Hw Infrared Band From Molecular Simulations. <i>Clays and Clay Minerals</i> , 2016 , 64, 452-471	2.1	26
61	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	3.8	50
60	Review. NMR and computational molecular modeling studies of mineral surfaces and interlayer galleries: A review. <i>American Mineralogist</i> , 2015 , 100, 1341-1354	2.9	25
59	Molecular modeling of the effects of ⁴⁰ Ar recoil in illite particles on their K ⁴⁰ Ar isotope dating. <i>Geochimica Et Cosmochimica Acta</i> , 2015 , 159, 162-176	5.5	19
58	Structural Arrangements of Isomorphous 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	3.8	95
57	Ethylene glycol intercalation in smectites. Molecular dynamics simulation studies. <i>Applied Clay Science</i> , 2014 , 91-92, 87-97	5.2	21
56	Molecular Structure and Dynamics of Nano-Confined Water: Computer Simulations of Aqueous Species in Clay, Cement, and Polymer Membranes. <i>NATO Science for Peace and Security Series C: Environmental Security</i> , 2014 , 103-115	0.3	1

55	Structure, Energetics, and Dynamics of Smectite Clay Interlayer Hydration: Molecular Dynamics and Metadynamics Investigation of Na-Hectorite. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 5172-5187	3.8	85
54	On the Hydrogen Bonding Structure at the Aqueous Interface of Ammonium-Substituted Mica: A Molecular Dynamics Simulation. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2013 , 68, 91-100	1.4	12
53	Molecular models of natural organic matter and its colloidal aggregation in aqueous solutions: Challenges and opportunities for computer simulations. <i>Pure and Applied Chemistry</i> , 2012 , 85, 149-158	2.1	9
52	Effects of Ca ²⁺ on supramolecular aggregation of natural organic matter in aqueous solutions: A comparison of molecular modeling approaches. <i>Geoderma</i> , 2011 , 169, 27-32	6.7	64
51	Metal cation complexation with natural organic matter in aqueous solutions: molecular dynamics simulations and potentials of mean force. <i>Langmuir</i> , 2010 , 26, 15909-19	4	120
50	Molecular dynamics computer simulations of the effects of hydrogen bonding on the properties of layered double hydroxides intercalated with organic acids. <i>Philosophical Magazine</i> , 2010 , 90, 2475-2488	1.6	47
49	A multistate empirical valence bond model for solvation and transport simulations of OH ⁻ in aqueous solutions. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 9420-30	3.6	43
48	Hydrogen-bonding structure and dynamics of aqueous carbonate species from car-parrinello molecular dynamics simulations. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 794-802	3.4	77
47	Molecular models and simulations of layered materials. <i>Journal of Materials Chemistry</i> , 2009 , 19, 2470		210
46	Asymmetric Hydrogen Bonding and Orientational Ordering of Water at Hydrophobic and Hydrophilic Surfaces: A Comparison of Water/Vapor, Water/Talc, and Water/Mica Interfaces. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 11077-11085	3.8	81
45	Effects of background cations on the fouling of polyethersulfone membranes by natural organic matter: Experimental and molecular modeling study. <i>Journal of Membrane Science</i> , 2008 , 309, 128-140	9.6	133
44	Dissociation of carbonic acid: gas phase energetics and mechanism from ab initio metadynamics simulations. <i>Journal of Chemical Physics</i> , 2007 , 126, 204315	3.9	51
43	Molecular Dynamics Simulation of the Energetics and Structure of Layered Double Hydroxides Intercalated with Carboxylic Acids. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 13517-13523	3.8	69
42	A charged ring model for classical OH ⁻ (aq) simulations. <i>Chemical Physics Letters</i> , 2007 , 442, 128-133	2.5	42
41	Comparison of proton field-cycling relaxometry and molecular dynamics simulations for proton-water surface dynamics in cement-based materials. <i>Cement and Concrete Research</i> , 2007 , 37, 348-350	10.3	60
40	Molecular dynamics modeling of the structure, dynamics and energetics of mineral-water interfaces: Application to cement materials. <i>Cement and Concrete Research</i> , 2007 , 37, 337-347	10.3	190
39	Molecular dynamics simulation of cationic complexation with natural organic matter. <i>European Journal of Soil Science</i> , 2007 , 58, 909-917	3.4	123
38	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. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 4042-52	2.8	60

37	Hydration, swelling, interlayer structure, and hydrogen bonding in organolayered double hydroxides: insights from molecular dynamics simulation of citrate-intercalated hydrotalcite. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 3841-4	3.4	87
36	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	5.5	227
35	¹³³ Cs and ³⁵ Cl NMR spectroscopy and molecular dynamics modeling of Cs ⁺ and Cl ⁻ complexation with natural organic matter. <i>Geochimica Et Cosmochimica Acta</i> , 2006 , 70, 4319-4331	5.5	46
34	Structure and decompression melting of a novel, high-pressure nanoconfined 2-D ice. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 14308-13	3.4	30
33	Molecular dynamics modelling of hydrated mineral interlayers and surfaces: structure and dynamics. <i>Mineralogical Magazine</i> , 2005 , 69, 289-308	1.7	56
32	Structure, energetics, and dynamics of water adsorbed on the muscovite (001) surface: a molecular dynamics simulation. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 15893-905	3.4	183
31	Molecular Modeling of the Vibrational Spectra of Interlayer and Surface Species of Layered Double Hydroxides 2005 ,		5
30	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	3.4	23
29	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	3.4	1662
28	Molecular modeling of water structure in nano-pores between brucite (001) surfaces. <i>Geochimica Et Cosmochimica Acta</i> , 2004 , 68, 3351-3365	5.5	126
27	Molecular modeling of the 10- $\bar{1}$ phase at subduction zone conditions. <i>Earth and Planetary Science Letters</i> , 2004 , 222, 517-527	5.3	37
26	Interlayer structure and dynamics of Cl-bearing hydrotalcite: far infrared spectroscopy and molecular dynamics modeling. <i>American Mineralogist</i> , 2003 , 88, 398-409	2.9	67
25	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	9.6	208
24	Interlayer Structure and Dynamics of Cl- Π Al ₂ -Layered Double Hydroxide: ³⁵ Cl NMR Observations and Molecular Dynamics Modeling. <i>Chemistry of Materials</i> , 2002 , 14, 2078-2085	9.6	50
23	Thermodynamics and structure of molecular clusters in supercritical water. <i>Fluid Phase Equilibria</i> , 2001 , 183-184, 271-278	2.5	57
22	Molecular Modeling of the Structure and Energetics of Hydrotalcite Hydration. <i>Chemistry of Materials</i> , 2001 , 13, 145-150	9.6	116
21	Molecular Simulations of Liquid and Supercritical Water: Thermodynamics, Structure, and Hydrogen Bonding. <i>Reviews in Mineralogy and Geochemistry</i> , 2001 , 42, 83-129	7.1	74
20	4. Molecular Simulations of Liquid and Supercritical Water: Thermodynamics, Structure, and Hydrogen Bonding 2001 , 83-130		13

19	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). <i>American Mineralogist</i> , 2000 , 85, 1046-1052	2.9	86
18	Structure and hydrogen bonding of liquid water at high hydrostatic pressures: Monte Carlo NPT-ensemble simulations up to 10 kbar. <i>Journal of Molecular Liquids</i> , 1999 , 82, 57-72	6	43
17	Size and topology of molecular clusters in supercritical water: a molecular dynamics simulation. <i>Chemical Physics Letters</i> , 1999 , 302, 411-417	2.5	83
16	Size and structure of molecular clusters in supercritical water. <i>Journal of Structural Chemistry</i> , 1999 , 40, 548-553	0.9	4
15	Silica transfer and quartz growth from supercritical aqueous fluids. <i>Journal of Supercritical Fluids</i> , 1998 , 13, 357-362	4.2	3
14	Hydrogen Bonding in Supercritical Water. 2. Computer Simulations. <i>Journal of Physical Chemistry A</i> , 1997 , 101, 9720-9727	2.8	178
13	Elastic properties of tetragonal PbTiO ₃ single crystals by Brillouin scattering. <i>Journal of Materials Research</i> , 1997 , 12, 2623-2627	2.5	52
12	Growth of high temperature quartz from supercritical aqueous fluids. <i>Journal of Crystal Growth</i> , 1996 , 162, 142-146	1.6	3
11	Molecular dynamics of supercritical water: A computer simulation of vibrational spectra with the flexible BJH potential. <i>Geochimica Et Cosmochimica Acta</i> , 1995 , 59, 641-650	5.5	50
10	Hydrogen Bonding in Supercritical Water. 1. Experimental Results. <i>The Journal of Physical Chemistry</i> , 1995 , 99, 5336-5340		169
9	Hydrogen bonding in supercritical water: a Monte Carlo simulation. <i>Chemical Physics Letters</i> , 1994 , 231, 301-307	2.5	99
8	Elastic properties of orthorhombic KNbO ₃ single crystals by Brillouin scattering. <i>Journal of Applied Physics</i> , 1993 , 74, 6603-6608	2.5	36
7	Pressure dependence of optical absorption in PbTiO ₃ to 35 GPa: Observation of the tetragonal-to-cubic phase transition. <i>Journal of Applied Physics</i> , 1992 , 72, 3705-3707	2.5	17
6	Computer Simulations of Aqueous Fluids at High Temperatures and Pressures 1992 , 1-59		5
5	Monte Carlo Simulations of Water under Supercritical Conditions. II. Convergence Characteristics and the System Size Effects. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 1992 , 47, 992-998	1.4	3
4	Monte Carlo Simulations of Water under Supercritical Conditions. I. Thermodynamic and Structural. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 1991 , 46, 433-444	1.4	36
3	Theoretical modeling of geochemical fluids under high-pressure, high-temperature conditions. <i>High Pressure Research</i> , 1991 , 7, 378-380	1.6	7
2	Monte Carlo study of the thermodynamics and structure of dense supercritical water. <i>International Journal of Thermophysics</i> , 1986 , 7, 887-900	2.1	24

- 1 Molecular-level understanding of metal ion retention in clay-rich materials. *Nature Reviews Earth & Environment*, 30.2 5