

Sebastien Kerisit

List of Publications by Year in descending order

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Version: 2024-02-01

97
papers

4,303
citations

117571

34
h-index

118793

62
g-index

98
all docs

98
docs citations

98
times ranked

4398
citing authors

#	ARTICLE	IF	CITATIONS
1	Cobalt hydroxide-cobalt carbonate competitive growth on carbonate surfaces. <i>Chemical Geology</i> , 2022, 605, 120951.	1.4	6
2	Patchy particle model of hydrated amorphous silica. <i>Journal of Non-Crystalline Solids</i> , 2021, 556, 120555.	1.5	3
3	Ab Initio Molecular Dynamics Simulations of Amorphous Calcium Carbonate: Interpretation of Pair Distribution Function and X-ray Absorption Spectroscopy Data. <i>Crystal Growth and Design</i> , 2021, 21, 2212-2221.	1.4	10
4	Monte Carlo simulation of the passage of β -rays and α -particles in CsI. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2021, 490, 25-33.	0.6	5
5	Seeded Stage III glass dissolution behavior of a statistically designed glass matrix. <i>Journal of the American Ceramic Society</i> , 2021, 104, 4145-4162.	1.9	9
6	Effect of Cd on the Nucleation and Transformation of Amorphous Calcium Carbonate. <i>Crystal Growth and Design</i> , 2021, 21, 3384-3393.	1.4	7
7	Thin Water Films Enable Low-Temperature Magnesite Growth Under Conditions Relevant to Geologic Carbon Sequestration. <i>Environmental Science & Technology</i> , 2021, 55, 12539-12548.	4.6	17
8	Moving beyond the Solvent-Tip Approximation to Determine Site-Specific Variations of Interfacial Water Structure through 3D Force Microscopy. <i>Journal of Physical Chemistry C</i> , 2021, 125, 1282-1291.	1.5	31
9	Acceleration of glass alteration rates induced by zeolite seeds at controlled pH. <i>Applied Geochemistry</i> , 2020, 113, 104515.	1.4	16
10	Ab initio molecular dynamics simulation of Nd ³⁺ incorporation in calcite. <i>Chemical Geology</i> , 2020, 534, 119460.	1.4	2
11	Low temperature and limited water activity reveal a pathway to magnesite via amorphous magnesium carbonate. <i>Chemical Communications</i> , 2020, 56, 12154-12157.	2.2	17
12	Immobilizing Pertechetate in Ettringite via Sulfate Substitution. <i>Environmental Science & Technology</i> , 2020, 54, 13610-13618.	4.6	20
13	Insights into the mechanisms controlling the residual corrosion rate of borosilicate glasses. <i>Npj Materials Degradation</i> , 2020, 4, .	2.6	26
14	Critical Water Coverage during Forsterite Carbonation in Thin Water Films: Activating Dissolution and Mass Transport. <i>Environmental Science & Technology</i> , 2020, 54, 6888-6899.	4.6	22
15	Emerging investigator series: ion diffusivities in nanoconfined interfacial water films contribute to mineral carbonation thresholds. <i>Environmental Science: Nano</i> , 2020, 7, 1068-1081.	2.2	19
16	A General Mechanism for Gel Layer Formation on Borosilicate Glass under Aqueous Corrosion. <i>Journal of Physical Chemistry C</i> , 2020, 124, 5132-5144.	1.5	43
17	Effect of Hydrophilicity and Interfacial Water Structure on Particle Attachment. <i>Journal of Physical Chemistry C</i> , 2020, 124, 5480-5488.	1.5	18
18	Ab initio calculations of the rate of carrier trapping and release at dopant sites in NaI: Tl beyond the harmonic approximation. <i>Physical Review B</i> , 2020, 101, .	1.1	2

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19	Can mineral growth by oriented attachment lead to incorporation of uranium(vi) into the structure of goethite?. <i>Environmental Science: Nano</i> , 2019, 6, 3000-3009.	2.2	10
20	Monte Carlo simulation of borosilicate glass dissolution using molecular dynamics-generated glass structures. <i>Journal of Non-Crystalline Solids</i> , 2019, 522, 119601.	1.5	18
21	Chromate Effect on Iodate Incorporation into Calcite. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 1624-1630.	1.2	16
22	Monte Carlo simulation of the corrosion of irradiated simplified nuclear waste glasses. <i>Journal of Non-Crystalline Solids</i> , 2019, 519, 119449.	1.5	13
23	Separation of Radiolytic Species at the Boehmite–Water Interface. <i>Journal of Physical Chemistry C</i> , 2019, 123, 15534-15539.	1.5	8
24	Ab Initio Molecular Dynamics Simulation of Divalent Metal Cation Incorporation in Calcite: Implications for Interpreting X-ray Absorption Spectroscopy Data. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 2582-2592.	1.2	11
25	Molecular dynamics simulation of ballistic effects in simplified nuclear waste glasses. <i>Journal of Non-Crystalline Solids</i> , 2019, 505, 188-201.	1.5	16
26	Radiocesium interaction with clay minerals: Theory and simulation advances Post–Fukushima. <i>Journal of Environmental Radioactivity</i> , 2019, 210, 105809.	0.9	7
27	Predicting Surface Energies and Particle Morphologies of Boehmite ($\text{I}^3\text{-AlOOH}$) from Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2018, 122, 10400-10412.	1.5	26
28	Radiocesium interaction with clay minerals: Theory and simulation advances Post–Fukushima. <i>Journal of Environmental Radioactivity</i> , 2018, 189, 135-145.	0.9	60
29	Anisotropic Growth of Otavite on Calcite: Implications for Heteroepitaxial Growth Mechanisms. <i>Crystal Growth and Design</i> , 2018, 18, 159-170.	1.4	11
30	Size and Morphology Controlled Synthesis of Boehmite Nanoplates and Crystal Growth Mechanisms. <i>Crystal Growth and Design</i> , 2018, 18, 3596-3606.	1.4	82
31	Incorporation Modes of Iodate in Calcite. <i>Environmental Science & Technology</i> , 2018, 52, 5902-5910.	4.6	31
32	Free-Energy Landscape of the Dissolution of Gibbsite at High pH. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1809-1814.	2.1	25
33	Boehmite and Gibbsite Nanoplates for the Synthesis of Advanced Alumina Products. <i>ACS Applied Nano Materials</i> , 2018, 1, 7115-7128.	2.4	79
34	Diffusion Mechanisms of Radiolytic Species in Irradiated Al (Oxy-)Hydroxides. <i>Journal of Physical Chemistry C</i> , 2018, 122, 28990-28997.	1.5	12
35	Adaptation of the GRAAL model of Glass Reactivity to accommodate non-linear diffusivity. <i>Journal of Nuclear Materials</i> , 2018, 512, 79-93.	1.3	11
36	Iron Vacancies Accommodate Uranyl Incorporation into Hematite. <i>Environmental Science & Technology</i> , 2018, 52, 6282-6290.	4.6	44

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37	Dynamics of self-reorganization explains passivation of silicate glasses. <i>Nature Communications</i> , 2018, 9, 2169.	5.8	94
38	Electronic response of aluminum-bearing minerals. <i>Journal of Chemical Physics</i> , 2018, 149, 024502.	1.2	11
39	Impacts of glass composition, pH, and temperature on glass forward dissolution rate. <i>Npj Materials Degradation</i> , 2018, 2, .	2.6	46
40	Trace Uranium Partitioning in a Multiphase Nano-FeOOH System. <i>Environmental Science & Technology</i> , 2017, 51, 4970-4977.	4.6	44
41	Molecular Dynamics Simulations of the Interfacial Region between Boehmite and Gibbsite Basal Surfaces and High Ionic Strength Aqueous Solutions. <i>Journal of Physical Chemistry C</i> , 2017, 121, 13692-13700.	1.5	18
42	Nucleation and Epitaxy-Mediated Phase Transformation of a Precursor Cadmium Carbonate Phase at the Calcite/Water Interface. <i>Journal of Physical Chemistry C</i> , 2017, 121, 5012-5019.	1.5	14
43	Manganese-calcium intermixing facilitates heteroepitaxial growth at the calcite-water interface. <i>Chemical Geology</i> , 2017, 470, 152-163.	1.4	17
44	Electron-phonon scattering rates in complex polar crystals. <i>Physical Review B</i> , 2017, 96, .	1.1	7
45	Fast Synthesis of Gibbsite Nanoplates and Process Optimization using Box-Behnken Experimental Design. <i>Crystal Growth and Design</i> , 2017, 17, 6801-6808.	1.4	47
46	Monte Carlo simulation of electron thermalization in scintillator materials: Implications for scintillator nonproportionality. <i>Journal of Applied Physics</i> , 2017, 122, .	1.1	16
47	Molecular Simulation of Cesium Adsorption at the Basal Surface of Phyllosilicate Minerals. <i>Clays and Clay Minerals</i> , 2016, 64, 389-400.	0.6	30
48	Ion-Exchange Interdiffusion Model with Potential Application to Long-Term Nuclear Waste Glass Performance. <i>Journal of Physical Chemistry C</i> , 2016, 120, 9374-9384.	1.5	30
49	Ab Initio Molecular Dynamics of Uranium Incorporated in Goethite (FeOOH): Interpretation of X-ray Absorption Spectroscopy of Trace Polyvalent Metals. <i>Inorganic Chemistry</i> , 2016, 55, 11736-11746.	1.9	42
50	Internal Domains of Natural Porous Media Revealed: Critical Locations for Transport, Storage, and Chemical Reaction. <i>Environmental Science & Technology</i> , 2016, 50, 2811-2829.	4.6	76
51	XPS determination of Mn oxidation states in Mn (hydr)oxides. <i>Applied Surface Science</i> , 2016, 366, 475-485.	3.1	654
52	6. Pore-Scale Process Coupling and Effective Surface Reaction Rates in Heterogeneous Subsurface Materials. , 2015, , 191-216.		1
53	Heterogeneous growth of cadmium and cobalt carbonate phases at the calcite surface. <i>Chemical Geology</i> , 2015, 397, 24-36.	1.4	18
54	Monte Carlo simulations of coupled diffusion and surface reactions during the aqueous corrosion of borosilicate glasses. <i>Journal of Non-Crystalline Solids</i> , 2015, 408, 142-149.	1.5	18

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55	Solvation structure and transport properties of alkali cations in dimethyl sulfoxide under exogenous static electric fields. <i>Journal of Chemical Physics</i> , 2015, 142, 224502.	1.2	12
56	Calculation of energy relaxation rates of fast particles by phonons in crystals. <i>Physical Review B</i> , 2015, 91, .	1.1	12
57	Pore-Scale Process Coupling and Effective Surface Reaction Rates in Heterogeneous Subsurface Materials. <i>Reviews in Mineralogy and Geochemistry</i> , 2015, 80, 191-216.	2.2	31
58	Modeling Interfacial Glass-Water Reactions: Recent Advances and Current Limitations. <i>International Journal of Applied Glass Science</i> , 2014, 5, 421-435.	1.0	34
59	Kinetics and Mechanisms of Cadmium Carbonate Heteroepitaxial Growth at the Calcite-Water Interface. <i>Journal of Physical Chemistry C</i> , 2014, 118, 24231-24239.	1.7	26
60	Kinetic Monte Carlo Simulations of Scintillation Processes in NaI(Tl). <i>IEEE Transactions on Nuclear Science</i> , 2014, 61, 860-869.	1.2	12
61	Anion pairs in room temperature ionic liquids predicted by molecular dynamics simulation, verified by spectroscopic characterization. <i>RSC Advances</i> , 2014, 4, 5457.	1.7	26
62	Shell Model for Atomistic Simulation of Lithium Diffusion in Mixed Mn/Ti Oxides. <i>Journal of Physical Chemistry C</i> , 2014, 118, 24231-24239.	1.5	11
63	Molecular Dynamics Simulations of Uranyl and Uranyl Carbonate Adsorption at Aluminosilicate Surfaces. <i>Environmental Science & Technology</i> , 2014, 48, 3899-3907.	4.6	65
64	Low-temperature lithium diffusion in simulated high-level borosilicate nuclear waste glasses. <i>Journal of Non-Crystalline Solids</i> , 2014, 405, 83-90.	1.5	18
65	Effects of Oxygen-Containing Functional Groups on Supercapacitor Performance. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2330-2334.	2.1	85
66	Structure, Kinetics, and Thermodynamics of the Aqueous Uranyl(VI) Cation. <i>Journal of Physical Chemistry A</i> , 2013, 117, 6421-6432.	1.1	52
67	Water and carbon dioxide adsorption at olivine surfaces. <i>Chemical Geology</i> , 2013, 359, 81-89.	1.4	60
68	Monte Carlo simulations of the corrosion of aluminoborosilicate glasses. <i>Journal of Non-Crystalline Solids</i> , 2013, 378, 273-281.	1.5	26
69	Scale-dependent rates of uranyl surface complexation reaction in sediments. <i>Geochimica Et Cosmochimica Acta</i> , 2013, 105, 326-341.	1.6	54
70	Kinetic Monte Carlo simulations of excitation density dependent scintillation in CsI. <i>Physica Status Solidi (B): Basic Research</i> , 2013, 250, 1532-1540.	0.7	31
71	Is the Calcite-Water Interface Understood? Direct Comparisons of Molecular Dynamics Simulations with Specular X-ray Reflectivity Data. <i>Journal of Physical Chemistry C</i> , 2013, 117, 5028-5042.	1.5	148
72	Monte Carlo simulation of gamma-ray response of BaF2 and CaF2. <i>Journal of Applied Physics</i> , 2013, 114, .	1.1	19

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73	Diffusion and Adsorption of Uranyl Carbonate Species in Nanosized Mineral Fractures. <i>Environmental Science & Technology</i> , 2012, 46, 1632-1640.	4.6	55
74	Monte Carlo simulations of electron thermalization in alkali iodide and alkaline-earth fluoride scintillators. <i>Journal of Applied Physics</i> , 2012, 112, .	1.1	32
75	Monte Carlo simulations of the dissolution of borosilicate glasses in near-equilibrium conditions. <i>Journal of Non-Crystalline Solids</i> , 2012, 358, 1324-1332.	1.5	20
76	Structure and dynamics of forsterite- $\text{scCO}_2/\text{H}_2\text{O}$ interfaces as a function of water content. <i>Geochimica Et Cosmochimica Acta</i> , 2012, 84, 137-151.	1.6	67
77	Atomistic Simulations of Uranium Incorporation into Iron (Hydr)Oxides. <i>Environmental Science & Technology</i> , 2011, 45, 2770-2776.	4.6	58
78	Water structure at hematite-water interfaces. <i>Geochimica Et Cosmochimica Acta</i> , 2011, 75, 2043-2061.	1.6	92
79	Monte Carlo simulations of the dissolution of borosilicate and aluminoborosilicate glasses in dilute aqueous solutions. <i>Geochimica Et Cosmochimica Acta</i> , 2011, 75, 5296-5309.	1.6	25
80	Yield, variance and spatial distribution of electron-hole pairs in CsI. <i>Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment</i> , 2011, 652, 564-567.	0.7	23
81	Computer simulation of electron thermalization in CsI and CsI(Tl). <i>Journal of Applied Physics</i> , 2011, 110, .	1.1	47
82	Molecular simulation of the diffusion of uranyl carbonate species in aqueous solution. <i>Geochimica Et Cosmochimica Acta</i> , 2010, 74, 4937-4952.	1.6	109
83	Transition path sampling of water exchange rates and mechanisms around aqueous ions. <i>Journal of Chemical Physics</i> , 2009, 131, 114512.	1.2	30
84	Computer simulation of the light yield nonlinearity of inorganic scintillators. <i>Journal of Applied Physics</i> , 2009, 105, .	1.1	43
85	Molecular Simulations of Water and Ion Diffusion in Nanosized Mineral Fractures. <i>Environmental Science & Technology</i> , 2009, 43, 777-782.	4.6	135
86	Kinetic Monte Carlo Model of Scintillation Mechanisms in CsI and CsI(Tl). <i>IEEE Transactions on Nuclear Science</i> , 2008, 55, 1251-1258.	1.2	31
87	Molecular dynamics simulations of the orthoclase (001)- and (010)-water interfaces. <i>Geochimica Et Cosmochimica Acta</i> , 2008, 72, 1481-1497.	1.6	68
88	Molecular Dynamics Simulations of Electrolyte Solutions at the (100) Goethite Surface. <i>Journal of Physical Chemistry B</i> , 2006, 110, 20491-20501.	1.2	54
89	Atomistic simulation of the free energies of dissolution of ions from flat and stepped calcite surfaces. <i>Journal of Crystal Growth</i> , 2006, 294, 103-110.	0.7	60
90	Kinetics of Triscarbonate Uranyl Reduction by Aqueous Ferrous Iron: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9691-9701.	1.1	34

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91	Atomistic simulation of charged iron oxyhydroxide surfaces in contact with aqueous solution. Chemical Communications, 2005, , 3027.	2.2	33
92	Self diffusion of argon in flexible, single wall, carbon nanotubes. Molecular Simulation, 2005, 31, 385-389.	0.9	11
93	Molecular dynamics simulations of the interactions between water and inorganic solids. Journal of Materials Chemistry, 2005, 15, 1454.	6.7	95
94	Ab Initio Surface Phase Diagram of the {101̄,4} Calcite Surface. Journal of Physical Chemistry B, 2005, 109, 18211-18213.	1.2	34
95	Free energy of adsorption of water and calcium on the {10 1? 4} calcite surfaceElectronic supplementary information (ESI) available: free energy calculations. See http://www.rsc.org/suppdata/cc/b3/b311928a/ . Chemical Communications, 2004, , 52.	2.2	67
96	Free Energy of Adsorption of Water and Metal Ions on the {101̄,4} Calcite Surface. Journal of the American Chemical Society, 2004, 126, 10152-10161.	6.6	276
97	Atomistic Simulation of the Dissociative Adsorption of Water on Calcite Surfaces. Journal of Physical Chemistry B, 2003, 107, 7676-7682.	1.2	141