Sebastien Kerisit

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5970588/publications.pdf

Version: 2024-02-01

97	4,303	117571	118793
papers	citations	34 h-index	62 g-index

98	98	98	4398
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	XPS determination of Mn oxidation states in Mn (hydr)oxides. Applied Surface Science, 2016, 366, 475-485.	3.1	654
2	Free Energy of Adsorption of Water and Metal Ions on the {101Ì„4} Calcite Surface. Journal of the American Chemical Society, 2004, 126, 10152-10161.	6.6	276
3	Is the Calciteâ€“Water Interface Understood? Direct Comparisons of Molecular Dynamics Simulations with Specular X-ray Reflectivity Data. Journal of Physical Chemistry C, 2013, 117, 5028-5042.	1.5	148
4	Atomistic Simulation of the Dissociative Adsorption of Water on Calcite Surfaces. Journal of Physical Chemistry B, 2003, 107, 7676-7682.	1.2	141
5	Molecular Simulations of Water and Ion Diffusion in Nanosized Mineral Fractures. Environmental Science & Technology, 2009, 43, 777-782.	4.6	135
6	Molecular simulation of the diffusion of uranyl carbonate species in aqueous solution. Geochimica Et Cosmochimica Acta, 2010, 74, 4937-4952.	1.6	109
7	Molecular dynamics simulations of the interactions between water and inorganic solids. Journal of Materials Chemistry, 2005, 15, 1454.	6.7	95
8	Dynamics of self-reorganization explains passivation of silicate glasses. Nature Communications, 2018, 9, 2169.	5.8	94
9	Water structure at hematiteâ€“water interfaces. Geochimica Et Cosmochimica Acta, 2011, 75, 2043-2061.	1.6	92
10	Effects of Oxygen-Containing Functional Groups on Supercapacitor Performance. Journal of Physical Chemistry Letters, 2014, 5, 2330-2334.	2.1	85
11	Size and Morphology Controlled Synthesis of Boehmite Nanoplates and Crystal Growth Mechanisms. Crystal Growth and Design, 2018, 18, 3596-3606.	1.4	82
12	Boehmite and Gibbsite Nanoplates for the Synthesis of Advanced Alumina Products. ACS Applied Nano Materials, 2018, 1, 7115-7128.	2.4	79
13	Internal Domains of Natural Porous Media Revealed: Critical Locations for Transport, Storage, and Chemical Reaction. Environmental Science & Technology, 2016, 50, 2811-2829.	4.6	76
14	Molecular dynamics simulations of the orthoclase (001)- and (010)-water interfaces. Geochimica Et Cosmochimica Acta, 2008, 72, 1481-1497.	1.6	68
15	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
16	Structure and dynamics of forsteriteâ€“scCO2/H2O interfaces as a function of water content. Geochimica Et Cosmochimica Acta, 2012, 84, 137-151.	1.6	67
17	Molecular Dynamics Simulations of Uranyl and Uranyl Carbonate Adsorption at Aluminosilicate Surfaces. Environmental Science & Technology, 2014, 48, 3899-3907.	4.6	65
18	Atomistic simulation of the free energies of dissolution of ions from flat and stepped calcite surfaces. Journal of Crystal Growth, 2006, 294, 103-110.	0.7	60

#	Article	IF	Citations
19	Water and carbon dioxide adsorption at olivine surfaces. Chemical Geology, 2013, 359, 81-89.	1.4	60
20	Radiocesium interaction with clay minerals: Theory and simulation advances Postâ€“Fukushima. Journal of Environmental Radioactivity, 2018, 189, 135-145.	0.9	60
21	Atomistic Simulations of Uranium Incorporation into Iron (Hydr)Oxides. Environmental Science & Technology, 2011, 45, 2770-2776.	4.6	58
22	Diffusion and Adsorption of Uranyl Carbonate Species in Nanosized Mineral Fractures. Environmental Science & Technology, 2012, 46, 1632-1640.	4.6	55
23	Molecular Dynamics Simulations of Electrolyte Solutions at the (100) Goethite Surface. Journal of Physical Chemistry B, 2006, 110, 20491-20501.	1.2	54
24	Scale-dependent rates of uranyl surface complexation reaction in sediments. Geochimica Et Cosmochimica Acta, 2013, 105, 326-341.	1.6	54
25	Structure, Kinetics, and Thermodynamics of the Aqueous Uranyl(VI) Cation. Journal of Physical Chemistry A, 2013, 117, 6421-6432.	1.1	52
26	Computer simulation of electron thermalization in CsI and CsI(Tl). Journal of Applied Physics, 2011, 110, .	1.1	47
27	Fast Synthesis of Gibbsite Nanoplates and Process Optimization using Box-Behnken Experimental Design. Crystal Growth and Design, 2017, 17, 6801-6808.	1.4	47
28	Impacts of glass composition, pH, and temperature on glass forward dissolution rate. Npj Materials Degradation, 2018, 2, .	2.6	46
29	Trace Uranium Partitioning in a Multiphase Nano-FeOOH System. Environmental Science & Technology, 2017, 51, 4970-4977.	4.6	44
30	Iron Vacancies Accommodate Uranyl Incorporation into Hematite. Environmental Science & Technology, 2018, 52, 6282-6290.	4.6	44
31	Computer simulation of the light yield nonlinearity of inorganic scintillators. Journal of Applied Physics, 2009, 105, .	1.1	43
32	A General Mechanism for Gel Layer Formation on Borosilicate Glass under Aqueous Corrosion. Journal of Physical Chemistry C, 2020, 124, 5132-5144.	1.5	43
33	Ab Initio Molecular Dynamics of Uranium Incorporated in Goethite (Î±-FeOOH): Interpretation of X-ray Absorption Spectroscopy of Trace Polyvalent Metals. Inorganic Chemistry, 2016, 55, 11736-11746.	1.9	42
34	Ab Initio Surface Phase Diagram of the {101Ì„4} Calcite Surface. Journal of Physical Chemistry B, 2005, 109, 18211-18213.	1.2	34
35	Kinetics of Triscarbonato Uranyl Reduction by Aqueous Ferrous Iron:Â A Theoretical Study. Journal of Physical Chemistry A, 2006, 110, 9691-9701.	1.1	34
36	Modeling Interfacial Glassâ€“Water Reactions: Recent Advances and Current Limitations. International Journal of Applied Glass Science, 2014, 5, 421-435.	1.0	34

#	Article	IF	Citations
37	Atomistic simulation of charged iron oxyhydroxide surfaces in contact with aqueous solution. Chemical Communications, 2005, , 3027.	2.2	33
38	Monte Carlo simulations of electron thermalization in alkali iodide and alkaline-earth fluoride scintillators. Journal of Applied Physics, 2012, 112, .	1.1	32
39	Kinetic Monte Carlo Model of Scintillation Mechanisms in CsI and CsI(Tl). IEEE Transactions on Nuclear Science, 2008, 55, 1251-1258.	1.2	31
40	Kinetic Monte Carlo simulations of excitation density dependent scintillation in Cs<scp>I</scp> and Cs<scp>I</scp>(<scp>T</scp>l). Physica Status Solidi (B): Basic Research, 2013, 250, 1532-1540.	0.7	31
41	Pore-Scale Process Coupling and Effective Surface Reaction Rates in Heterogeneous Subsurface Materials. Reviews in Mineralogy and Geochemistry, 2015, 80, 191-216.	2.2	31
42	Incorporation Modes of Iodate in Calcite. Environmental Science & Technology, 2018, 52, 5902-5910.	4.6	31
43	Moving beyond the Solvent-Tip Approximation to Determine Site-Specific Variations of Interfacial Water Structure through 3D Force Microscopy. Journal of Physical Chemistry C, 2021, 125, 1282-1291.	1.5	31
44	Transition path sampling of water exchange rates and mechanisms around aqueous ions. Journal of Chemical Physics, 2009, 131, 114512.	1.2	30
45	Molecular Simulation of Cesium Adsorption at the Basal Surface of Phyllosilicate Minerals. Clays and Clay Minerals, 2016, 64, 389-400.	0.6	30
46	Ion-Exchange Interdiffusion Model with Potential Application to Long-Term Nuclear Waste Glass Performance. Journal of Physical Chemistry C, 2016, 120, 9374-9384.	1.5	30
47	Monte Carlo simulations of the corrosion of aluminoborosilicate glasses. Journal of Non-Crystalline Solids, 2013, 378, 273-281.	1.5	26
48	Kinetics and mechanisms of cadmium carbonate heteroepitaxial growth at the calcite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:mo stretchy="false">(</mml:mo><mml:mn>10</mml:mn><mml:mspace width="0.12em" /><mml:mover) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.6	26
49	Anion pairs in room temperature ionic liquids predicted by molecular dynamics simulation, verified by spectroscopic characterization. RSC Advances, 2014, 4, 5457.	1.7	26
50	Predicting Surface Energies and Particle Morphologies of Boehmite (Î³-AlOOH) from Density Functional Theory. Journal of Physical Chemistry C, 2018, 122, 10400-10412.	1.5	26
51	Insights into the mechanisms controlling the residual corrosion rate of borosilicate glasses. Npj Materials Degradation, 2020, 4, .	2.6	26
52	Monte Carlo simulations of the dissolution of borosilicate and aluminoborosilicate glasses in dilute aqueous solutions. Geochimica Et Cosmochimica Acta, 2011, 75, 5296-5309.	1.6	25
53	Free-Energy Landscape of the Dissolution of Gibbsite at High pH. Journal of Physical Chemistry Letters, 2018, 9, 1809-1814.	2.1	25
54	Yield, variance and spatial distribution of electronâ€“hole pairs in CsI. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2011, 652, 564-567.	0.7	23

#	Article	IF	Citations
55	Critical Water Coverage during Forsterite Carbonation in Thin Water Films: Activating Dissolution and Mass Transport. Environmental Science & Technology, 2020, 54, 6888-6899.	4.6	22
56	Monte Carlo simulations of the dissolution of borosilicate glasses in near-equilibrium conditions. Journal of Non-Crystalline Solids, 2012, 358, 1324-1332.	1.5	20
57	Immobilizing Pertechnetate in Ettringite via Sulfate Substitution. Environmental Science & Technology, 2020, 54, 13610-13618.	4.6	20
58	Monte Carlo simulation of gamma-ray response of BaF2 and CaF2. Journal of Applied Physics, 2013, 114, .	1.1	19
59	Emerging investigator series: ion diffusivities in nanoconfined interfacial water films contribute to mineral carbonation thresholds. Environmental Science: Nano, 2020, 7, 1068-1081.	2.2	19
60	Low-temperature lithium diffusion in simulated high-level boroaluminosilicate nuclear waste glasses. Journal of Non-Crystalline Solids, 2014, 405, 83-90.	1.5	18
61	Heterogeneous growth of cadmium and cobalt carbonate phases at the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mfenced open="(" close=")"><mml:mrow><mml:mn>10</mml:mn><mml:mover accent="true"><mml:mn>1</mml:mn><mml:mo stretchy="true">Â¯</mml:mo></mml:mover><mml:mn>4</mml:mn></mml:mrow></mml:mfenced></mml:math> calcite surface. Chemical Geology, 2015, 397, 24-36.	1.4	18
62	Monte Carlo simulations of coupled diffusion and surface reactions during the aqueous corrosion of borosilicate glasses. Journal of Non-Crystalline Solids, 2015, 408, 142-149.	1.5	18
63	Molecular Dynamics Simulations of the Interfacial Region between Boehmite and Gibbsite Basal Surfaces and High Ionic Strength Aqueous Solutions. Journal of Physical Chemistry C, 2017, 121, 13692-13700.	1.5	18
64	Monte Carlo simulation of borosilicate glass dissolution using molecular dynamics-generated glass structures. Journal of Non-Crystalline Solids, 2019, 522, 119601.	1.5	18
65	Effect of Hydrophilicity and Interfacial Water Structure on Particle Attachment. Journal of Physical Chemistry C, 2020, 124, 5480-5488.	1.5	18
66	Manganese-calcium intermixing facilitates heteroepitaxial growth at the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si3.gif" overflow="scroll"><mml:mfenced open="(" close=")"><mml:mrow><mml:mn>10</mml:mn><mml:mover accent="false"><mml:mn>1</mml:mn><mml:mo>Â¯</mml:mo></mml:mover><mml:mn>4</mml:mn></mml:mrow></mml:mfenced></r calcite-water interface. Chemical Geology, 2017, 470, 152-163.	1.4	17
67	Low temperature and limited water activity reveal a pathway to magnesiteviaamorphous magnesium carbonate. Chemical Communications, 2020, 56, 12154-12157.	2.2	17
68	Thin Water Films Enable Low-Temperature Magnesite Growth Under Conditions Relevant to Geologic Carbon Sequestration. Environmental Science & Technology, 2021, 55, 12539-12548.	4.6	17
69	Monte Carlo simulation of electron thermalization in scintillator materials: Implications for scintillator nonproportionality. Journal of Applied Physics, 2017, 122, .	1.1	16
70	Chromate Effect on Iodate Incorporation into Calcite. ACS Earth and Space Chemistry, 2019, 3, 1624-1630.	1.2	16
71	Molecular dynamics simulation of ballistic effects in simplified nuclear waste glasses. Journal of Non-Crystalline Solids, 2019, 505, 188-201.	1.5	16
72	Acceleration of glass alteration rates induced by zeolite seeds at controlled pH. Applied Geochemistry, 2020, 113, 104515.	1.4	16

#	Article	IF	Citations
73	Nucleation and Epitaxy-Mediated Phase Transformation of a Precursor Cadmium Carbonate Phase at the Calcite/Water Interface. Journal of Physical Chemistry C, 2017, 121, 5012-5019.	1.5	14
74	Monte Carlo simulation of the corrosion of irradiated simplified nuclear waste glasses. Journal of Non-Crystalline Solids, 2019, 519, 119449.	1.5	13
75	Kinetic Monte Carlo Simulations of Scintillation Processes in NaI(Tl). IEEE Transactions on Nuclear Science, 2014, 61, 860-869.	1.2	12
76	Solvation structure and transport properties of alkali cations in dimethyl sulfoxide under exogenous static electric fields. Journal of Chemical Physics, 2015, 142, 224502.	1.2	12
77	Calculation of energy relaxation rates of fast particles by phonons in crystals. Physical Review B, 2015, 91, .	1.1	12
78	Diffusion Mechanisms of Radiolytic Species in Irradiated Al (Oxy-)Hydroxides. Journal of Physical Chemistry C, 2018, 122, 28990-28997.	1.5	12
79	Self diffusion of argon in flexible, single wall, carbon nanotubes. Molecular Simulation, 2005, 31, 385-389.	0.9	11
80	Shell Model for Atomistic Simulation of Lithium Diffusion in Mixed Mn/Ti Oxides. Journal of Physical Chemistry C, 2014, 118, 24231-24239.	1.5	11
81	Anisotropic Growth of Otavite on Calcite: Implications for Heteroepitaxial Growth Mechanisms. Crystal Growth and Design, 2018, 18, 159-170.	1.4	11
82	Adaptation of the GRAAL model of Glass Reactivity to accommodate non-linear diffusivity. Journal of Nuclear Materials, 2018, 512, 79-93.	1.3	11
83	Electronic response of aluminum-bearing minerals. Journal of Chemical Physics, 2018, 149, 024502.	1.2	11
84	Ab Initio Molecular Dynamics Simulation of Divalent Metal Cation Incorporation in Calcite: Implications for Interpreting X-ray Absorption Spectroscopy Data. ACS Earth and Space Chemistry, 2019, 3, 2582-2592.	1.2	11
85	Can mineral growth by oriented attachment lead to incorporation of uranium(vi) into the structure of goethite?. Environmental Science: Nano, 2019, 6, 3000-3009.	2.2	10
86	Ab Initio Molecular Dynamics Simulations of Amorphous Calcium Carbonate: Interpretation of Pair Distribution Function and X-ray Absorption Spectroscopy Data. Crystal Growth and Design, 2021, 21, 2212-2221.	1.4	10
87	Seeded Stage III glass dissolution behavior of a statistically designed glass matrix. Journal of the American Ceramic Society, 2021, 104, 4145-4162.	1.9	9
88	Separation of Radiolytic Species at the Boehmiteâ€“Water Interface. Journal of Physical Chemistry C, 2019, 123, 15534-15539.	1.5	8
89	Electron-phonon scattering rates in complex polar crystals. Physical Review B, 2017, 96, .	1.1	7
90	Radiocesium interaction with clay minerals: Theory and simulation advances Postâ€“Fukushima. Journal of Environmental Radioactivity, 2019, 210, 105809.	0.9	7

#	Article	IF	Citations
91	Effect of Cd on the Nucleation and Transformation of Amorphous Calcium Carbonate. Crystal Growth and Design, 2021, 21, 3384-3393.	1.4	7
92	Cobalt hydroxideâ€“cobalt carbonate competitive growth on carbonate surfaces. Chemical Geology, 2022, 605, 120951.	1.4	6
93	Monte Carlo simulation of the passage of Î³-rays and Î±-particles in CsI. Nuclear Instruments & Methods in Physics Research B, 2021, 490, 25-33.	0.6	5
94	Patchy particle model of hydrated amorphous silica. Journal of Non-Crystalline Solids, 2021, 556, 120555.	1.5	3
95	Ab initio molecular dynamics simulation of Nd3+ incorporation in calcite. Chemical Geology, 2020, 534, 119460.	1.4	2
96	Ab initio calculations of the rate of carrier trapping and release at dopant sites in NaI: Tl beyond the harmonic approximation. Physical Review B, 2020, 101, .	1.1	2
97	6. Pore-Scale Process Coupling and Effective Surface Reaction Rates in Heterogeneous Subsurface Materials. , 2015, , 191-216.		1