Roland J-M Pellenq

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/9575138/publications.pdf

Version: 2024-02-01

94 papers	6,050 citations	100601 38 h-index	81351 76 g-index
95 all docs	95 docs citations	95 times ranked	4213 citing authors

#	Article	IF	Citations
1	Alkali silica reaction: A view from the nanoscale. Cement and Concrete Research, 2022, 152, 106652.	4.6	13
2	Condensation and growth of amorphous aluminosilicate nanoparticles via an aggregation process. Physical Chemistry Chemical Physics, 2022, 24, 9229-9235.	1.3	2
3	Binary CoOxâ€“SiO₂ Porous Nanostructures for Catalytic CO Oxidation. ACS Applied Nano Materials, 2022, 5, 7331-7343.	2.4	5
4	Atomic-scale mechanism of carbon nucleation from a deep crustal fluid by replica exchange reactive molecular dynamics simulation. Geochimica Et Cosmochimica Acta, 2022, 329, 106-118.	1.6	4
5	Ion Specificity of Confined Ionâ€“Water Structuring and Nanoscale Surface Forces in Clays. Journal of Physical Chemistry B, 2022, 126, 4977-4989.	1.2	3
6	Phase diagram of brittle fracture in the semi-grand-canonical ensemble. Physical Review E, 2021, 103, 013003.	0.8	2
7	Nanoscale Accessible Porosity as a Key Parameter Depicting the Topological Evolution of Organic Porous Networks. Langmuir, 2021, 37, 5464-5474.	1.6	7
8	The physics of cement cohesion. Science Advances, 2021, 7, .	4.7	28
9	Theory of freezing point depression in charged porous media. Physical Review E, 2021, 104, 045102.	0.8	4
10	Creep in reactive colloidal gels: A nanomechanical study of cement hydrates. Physical Review Research, 2021, 3, .	1.3	14
11	Hydrocarbon Diffusion in Mesoporous Carbon Materials: Implications for Unconventional Gas Recovery. ACS Applied Nano Materials, 2020, 3, 7604-7610.	2.4	7
12	¹³C NMR Parameters of Disordered Carbons: Atomistic Simulations, DFT Calculations, and Experimental Results. Journal of Physical Chemistry C, 2020, 124, 12784-12793.	1.5	6
13	Dissociation Mechanisms of Dissolved Alkali Silicates in Sodium Hydroxide. Journal of Physical Chemistry C, 2020, 124, 8288-8294.	1.5	20
14	Heterogeneous Surface Growth and Gelation of Cement Hydrates. Journal of Physical Chemistry C, 2020, 124, 15500-15510.	1.5	15
15	Time resolved alkali silicate decondensation by sodium hydroxide solution. JPhys Materials, 2020, 3, 014012.	1.8	6
16	Simulating the Geological Fate of Terrestrial Organic Matter: Lignin vs Cellulose. Energy & Fuels, 2020, 34, 1537-1547.	2.5	15
17	Freezing point depression and freeze-thaw damage by nanofluidic salt trapping. Physical Review Fluids, 2020, 5, .	1.0	15
18	Effect of Confinement on Capillary Phase Transition in Granular Aggregates. Physical Review Letters, 2020, 125, 255501.	2.9	9

#	Article	IF	Citations
19	Nanoscale Composition-Texture-Property Relation in Calcium-Silicate-Hydrates. , 2020, , 1761-1792.		3
20	Effects of size polydispersity on random close-packed configurations of spherical particles. Physical Review E, 2019, 100, 042906.	0.8	26
21	Mesoscale simulation of aggregation of imogolite nanotubes from potential of mean force interactions. Molecular Physics, 2019, 117, 3445-3455.	0.8	3
22	Agglomeration of wet particles in dense granular flows. European Physical Journal E, 2019, 42, 127.	0.7	16
23	Multiscale poromechanics of wet cement paste. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 10652-10657.	3.3	38
24	Methane Diffusion in a Flexible Kerogen Matrix. Journal of Physical Chemistry B, 2019, 123, 5635-5640.	1.2	30
25	Capillary Stress and Structural Relaxation in Moist Granular Materials. Langmuir, 2019, 35, 4397-4402.	1.6	17
26	Analyzing the Raman Spectra of Graphenic Carbon Materials from Kerogens to Nanotubes: What Type of Information Can Be Extracted from Defect Bands?. Journal of Carbon Research, 2019, 5, 69.	1.4	91
27	Molecular simulation of silica gels: Formation, dilution, and drying. Physical Review Materials, 2019, 3, .	0.9	8
28	Role of City Texture in Urban Heat Islands at Nighttime. Physical Review Letters, 2018, 120, 108701.	2.9	65
29	Impact of Nanoporosity on Hydrocarbon Transport in Shalesâ€™ Organic Matter. Nano Letters, 2018, 18, 832-837.	4.5	55
30	Le ChÃ¢telierâ€™s conjecture: Measurement of colloidal eigenstresses in chemically reactive materials. Journal of the Mechanics and Physics of Solids, 2018, 112, 334-344.	2.3	25
31	Mesoscale structure, mechanics, and transport properties of source rocksâ€™ organic pore networks. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 12365-12370.	3.3	41
32	Poroelasticity of Methane-Loaded Mature and Immature Kerogen from Molecular Simulations. Langmuir, 2018, 34, 13766-13780.	1.6	35
33	Thermalizing and Damping in Structural Dynamics. Journal of Applied Mechanics, Transactions ASME, 2018, 85, .	1.1	7
34	A reaction model for cement solidification: Evolving the Câ€“Sâ€“H packing density at the micrometer-scale. Journal of the Mechanics and Physics of Solids, 2018, 118, 58-73.	2.3	27
35	A methodology to calibrate and to validate effective solid potentials of heterogeneous porous media from computed tomography scans and laboratory-measured nanoindentation data. Acta Geotechnica, 2018, 13, 1369-1394.	2.9	6
36	Atomistic and mesoscale simulation of sodium and potassium adsorption in cement paste. Journal of Chemical Physics, 2018, 149, 074705.	1.2	16

#	Article	IF	Citations
37	Griffithâ€™s postulate: Grand Canonical Monte Carlo approach for fracture mechanics of solids. Engineering Fracture Mechanics, 2018, 199, 544-554.	2.0	4
38	Thermodynamics, kinetics, and mechanics of cesium sorption in cement paste: A multiscale assessment. Physical Review Materials, 2018, 2, .	0.9	13
39	Inhomogeneity in Cement Hydrates: Linking Local Packing to Local Pressure. Journal of Nanomechanics & Micromechanics, 2017, 7, .	1.4	26
40	A potential-of-mean-force approach for fracture mechanics of heterogeneous materials using the lattice element method. Journal of the Mechanics and Physics of Solids, 2017, 105, 116-130.	2.3	16
41	Disorder-induced stiffness degradation of highly disordered porous materials. Journal of the Mechanics and Physics of Solids, 2017, 106, 207-228.	2.3	41
42	From cellulose to kerogen: molecular simulation of a geological process. Chemical Science, 2017, 8, 8325-8335.	3.7	37
43	: A force field database for cementitious materials including validations, applications and opportunities. Cement and Concrete Research, 2017, 102, 68-89.	4.6	186
44	Topological Control on the Structural Relaxation of Atomic Networks under Stress. Physical Review Letters, 2017, 119, 035502.	2.9	51
45	Role of Interfaces in Elasticity and Failure of Clayâ€“Organic Nanocomposites: Toughening upon Interface Weakening?. Langmuir, 2017, 33, 11457-11466.	1.6	17
46	Nano-granular texture of cement hydrates. EPJ Web of Conferences, 2017, 140, 15027.	0.1	1
47	Model representations of kerogen structures: An insight from density functional theory calculations and spectroscopic measurements. Scientific Reports, 2017, 7, 7068.	1.6	19
48	Stress Transmission and Failure in Disordered Porous Media. Physical Review Letters, 2017, 119, 075501.	2.9	54
49	Mesoscale Poroelasticity of Heterogeneous Media. Journal of Nanomechanics & Micromechanics, 2017, 7, 04017016.	1.4	6
50	Effective Potentials and Elastic Properties in the Lattice-Element Method: Isotropy and Transverse Isotropy. Journal of Nanomechanics & Micromechanics, 2017, 7, .	1.4	15
51	The Potential of Mean Force concept for bridging (length and time) scales in the modeling of complex porous materials. EPJ Web of Conferences, 2017, 140, 01009.	0.1	11
52	Effect of Polydispersity of Clay Platelets on the Aggregation and Mechanical Properties of Clay at the Mesoscale. Clays and Clay Minerals, 2016, 64, 425-437.	0.6	14
53	Data analytics for simplifying thermal efficiency planning in cities. Journal of the Royal Society Interface, 2016, 13, 20150971.	1.5	24
54	Free Volume Theory of Hydrocarbon Mixture Transport in Nanoporous Materials. Journal of Physical Chemistry Letters, 2016, 7, 3712-3717.	2.1	74

#	Article	IF	Citations
55	Evolution of organo-clay composites with respect to thermal maturity in type II organic-rich source rocks. Geochimica Et Cosmochimica Acta, 2016, 195, 68-83.	1.6	54
56	Fracture toughness anomalies: Viewpoint of topological constraint theory. Acta Materialia, 2016, 121, 234-239.	3.8	84
57	Mesoscale simulation of clay aggregate formation and mechanical properties. Granular Matter, 2016, 18, 1.	1.1	33
58	Effect of Water on Elastic and Creep Properties of Self-Standing Clay Films. Langmuir, 2016, 32, 1370-1379.	1.6	17
59	Mesoscale texture of cement hydrates. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 2029-2034.	3.3	193
60	Realistic molecular model of kerogenâ€™s nanostructure. Nature Materials, 2016, 15, 576-582.	13.3	300
61	Bottom-up model of adsorption and transport in multiscale porous media. Physical Review E, 2015, 91, 032133.	0.8	39
62	Subcontinuum mass transport of condensed hydrocarbons in nanoporous media. Nature Communications, 2015, 6, 6949.	5.8	239
63	Optimized molecular reconstruction procedure combining hybrid reverse Monte Carlo and molecular dynamics. Journal of Chemical Physics, 2015, 142, 114112.	1.2	24
64	Rigidity Transition in Materials: Hardness is Driven by Weak Atomic Constraints. Physical Review Letters, 2015, 114, 125502.	2.9	93
65	Organicâ€“Clay Interfacial Chemical Bonds Probed by ab Initio Calculations. Journal of Physical Chemistry C, 2015, 119, 6511-6517.	1.5	9
66	Cement As a Waste Form for Nuclear Fission Products: The Case of ⁹⁰Sr and Its Daughters. Environmental Science & Technology, 2015, 49, 13676-13683.	4.6	19
67	Effect of Chain Length and Pore Accessibility on Alkane Adsorption in Kerogen. Energy & Fuels, 2015, 29, 7889-7896.	2.5	65
68	Anomalous composition-dependent dynamics of nanoconfined water in the interlayer of disordered calcium-silicates. Journal of Chemical Physics, 2014, 140, 054515.	1.2	121
69	Order and disorder in calciumâ€“silicateâ€“hydrate. Journal of Chemical Physics, 2014, 140, 214503.	1.2	99
70	Mesoscale properties of clay aggregates from potential of mean force representation of interactions between nanoplatelets. Journal of Chemical Physics, 2014, 140, .	1.2	73
71	Effect of temperature on adsorption of mixtures in porous materials. Molecular Simulation, 2014, 40, 45-51.	0.9	2
72	Nano-scale mechanics of colloidal Câ€“Sâ€“H gels. Soft Matter, 2014, 10, 491-499.	1.2	65

#	Article	IF	Citations
73	Combinatorial molecular optimization of cement hydrates. Nature Communications, 2014, 5, 4960.	5.8	358
74	Atomic-scale modelling of elastic and failure properties of clays. Molecular Physics, 2014, 112, 1294-1305.	0.8	61
75	Controlling local packing and growth in calciumâ€“silicateâ€“hydrate gels. Soft Matter, 2014, 10, 1121-1133.	1.2	94
76	Nanoscale Structure of Cement: Viewpoint of Rigidity Theory. Journal of Physical Chemistry C, 2014, 118, 12485-12493.	1.5	80
77	Docking 90Sr radionuclide in cement: An atomistic modeling study. Physics and Chemistry of the Earth, 2014, 70-71, 39-44.	1.2	13
78	Elastic Properties of Swelling Clay Particles at Finite Temperature upon Hydration. Journal of Physical Chemistry C, 2014, 118, 8933-8943.	1.5	83
79	Molecular intermittent dynamics of interfacial water: probing adsorption and bulk confinement. Soft Matter, 2013, 9, 8654.	1.2	20
80	Nanoscale Elastic Properties of Montmorillonite upon Water Adsorption. Langmuir, 2012, 28, 16855-16863.	1.6	104
81	Confined Water Dissociation in Microporous Defective Silicates: Mechanism, Dipole Distribution, and Impact on Substrate Properties. Journal of the American Chemical Society, 2012, 134, 2208-2215.	6.6	264
82	Nanostructure and Nanomechanics of Cement: Polydisperse Colloidal Packing. Physical Review Letters, 2012, 109, 155503.	2.9	161
83	Thermodynamics of Water Confined in Porous Calcium-Silicate-Hydrates. Langmuir, 2012, 28, 11422-11432.	1.6	157
84	Evidence on the Dual Nature of Aluminum in the Calciumâ€Silicateâ€Hydrates Based on Atomistic Simulations. Journal of the American Ceramic Society, 2012, 95, 1128-1137.	1.9	66
85	Glassy Nature of Water in an Ultraconfining Disordered Material: The Case of Calciumâ€Silicateâ€Hydrate. Journal of the American Chemical Society, 2011, 133, 2499-2510.	6.6	232
86	NANOSCALE SIMULATIONS FOR ENERGY STORAGE RELATED ENGINEERING PROBLEMS: THE CASE STUDY OF NANOPOROUS CARBONS UNDER THE NANOSCOPE. , 2011, , .		0
87	Molecular simulation of water confined in nanoporous silica. Journal of Physics Condensed Matter, 2010, 22, 284110.	0.7	111
88	Firstâ€Principles Study of Elastic Constants and Interlayer Interactions of Complex Hydrated Oxides: Case Study of Tobermorite and Jennite. Journal of the American Ceramic Society, 2009, 92, 2323-2330.	1.9	190
89	A realistic molecular model of cement hydrates. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 16102-16107.	3.3	734
90	Simple Phenomenological Model for Phase Transitions in Confined Geometry. 2. Capillary Condensation/Evaporation in Cylindrical Mesopores. Langmuir, 2009, 25, 1393-1402.	1.6	62

#	Article	IF	Citations
91	Argon and Nitrogen Adsorption in Disordered Nanoporous Carbons:Â Simulation and Experiment. Langmuir, 2005, 21, 4431-4440.	1.6	56
92	Why Does Concrete Set?: The Nature of Cohesion Forces in Hardened Cement-Based Materials. MRS Bulletin, 2004, 29, 319-323.	1.7	137
93	Capillary condensation in a disordered mesoporous medium: a grand canonical Monte Carlo study. Molecular Physics, 2002, 100, 2059-2077.	0.8	100
94	Electrostatic Attraction between Two Charged Surfaces:â€‰ A (N,V,T) Monte Carlo Simulation. Journal of Physical Chemistry B, 1997, 101, 8584-8594.	1.2	143