Benjamin Rotenberg

List of Publications by Year
in descending order

131 papers	8,739 citations	53794 45 h-index	46799 89 g-index
137 all docs	137 docs citations	137 times ranked	9134 citing authors

#	Article	IF	Citations
1	Chemisorbed vs physisorbed surface charge and its impact on electrokinetic transport: Carbon vs boron nitride surface. Journal of Chemical Physics, 2022, 156, 044703.	3.0	10
2	Likelihood-based non-Markovian models from molecular dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2117586119.	7.1	21
3	Microscopic Simulations of Electrochemical Double-Layer Capacitors. Chemical Reviews, 2022, 122, 10860-10898.	47.7	81
4	Printed Dielectrophoretic Electrodeâ€Based Continuous Flow Microfluidic Systems for Particles 3Dâ€Trapping. Particle and Particle Systems Characterization, 2021, 38, 2000235.	2.3	6
5	On the Gibbsâ€“Thomson equation for the crystallization of confined fluids. Journal of Chemical Physics, 2021, 154, 114711.	3.0	22
6	Molecular Simulation of Electrode-Solution Interfaces. Annual Review of Physical Chemistry, 2021, 72, 189-212.	10.8	64
7	Reduced variance analysis of molecular dynamics simulations by linear combination of estimators. Journal of Chemical Physics, 2021, 154, 191101.	3.0	6
8	On the molecular correlations that result in field-dependent conductivities in electrolyte solutions. Journal of Chemical Physics, 2021, 155, 014507.	3.0	12
9	Lattice Boltzmann method for adsorption under stationary and transient conditions: Interplay between transport and adsorption kinetics in porous media. Physical Review E, 2021, 104, 015314.	2.1	5
10	Effect of the metallicity on the capacitance of goldâ€“aqueous sodium chloride interfaces. Journal of Chemical Physics, 2021, 155, 044703.	3.0	26
11	NMR Relaxation Rates of Quadrupolar Aqueous Ions from Classical Molecular Dynamics Using Force-Field Specific Sternheimer Factors. Journal of Chemical Theory and Computation, 2021, 17, 6006-6017.	5.3	5
12	A molecular perspective on induced charges on a metallic surface. Journal of Chemical Physics, 2021, 155, 204705.	3.0	10
13	Microscopic origin of the effect of substrate metallicity on interfacial free energies. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	4
14	Charge fluctuations from molecular simulations in the constant-potential ensemble. Physical Chemistry Chemical Physics, 2020, 22, 10480-10489.	2.8	53
15	Sampling mobility profiles of confined fluids with equilibrium molecular dynamics simulations. Journal of Chemical Physics, 2020, 153, 044125.	3.0	11
16	Use the force! Reduced variance estimators for densities, radial distribution functions, and local mobilities in molecular simulations. Journal of Chemical Physics, 2020, 153, 150902.	3.0	23
17	Structure and position-dependent properties of inhomogeneous suspensions of responsive colloids. Physical Review E, 2020, 102, 042602.	2.1	11
18	A semiclassical Thomasâ€“Fermi model to tune the metallicity of electrodes in molecular simulations. Journal of Chemical Physics, 2020, 153, 174704.	3.0	49

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19	Mass-zero constrained molecular dynamics for electrode charges in simulations of electrochemical systems. Journal of Chemical Physics, 2020, 152, 194701.	3.0	16
20	Competitive Salt Precipitation/Dissolution During Freeâ€Water Reduction in Waterâ€inâ€Salt Electrolyte. Angewandte Chemie - International Edition, 2020, 59, 15913-15917.	13.8	52
21	Competitive Salt Precipitation/Dissolution During Freeâ€Water Reduction in Waterâ€inâ€Salt Electrolyte. Angewandte Chemie, 2020, 132, 16047-16051.	2.0	23
22	Correlation Length in Concentrated Electrolytes: Insights from All-Atom Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2020, 124, 1778-1786.	2.6	34
23	Field-Dependent Ionic Conductivities from Generalized Fluctuation-Dissipation Relations. Physical Review Letters, 2020, 124, 206001.	7.8	18
24	MetalWalls: A classical molecular dynamics software dedicated to the simulation of electrochemical systems. Journal of Open Source Software, 2020, 5, 2373.	4.6	56
25	Simulating Electrochemical Systems by Combining the Finite Field Method with a Constant Potential Electrode. Physical Review Letters, 2019, 123, 195501.	7.8	48
26	Transport Properties of Li-TFSI Water-in-Salt Electrolytes. Journal of Physical Chemistry B, 2019, 123, 10514-10521.	2.6	60
27	Computing three-dimensional densities from force densities improves statistical efficiency. Journal of Chemical Physics, 2019, 151, 064124.	3.0	12
28	Lattice Boltzmann electrokinetics simulation of nanocapacitors. Journal of Chemical Physics, 2019, 151, 114104.	3.0	17
29	Study of a water-graphene capacitor with molecular density functional theory. Journal of Chemical Physics, 2019, 151, 124111.	3.0	31
30	A molecular density functional theory approach to electron transfer reactions. Chemical Science, 2019, 10, 2130-2143.	7.4	24
31	Effect of the carbon microporous structure on the capacitance of aqueous supercapacitors. Energy Storage Materials, 2019, 21, 190-195.	18.0	48
32	Chasing Aqueous Biphasic Systems from Simple Salts by Exploring the LiTFSI/LiCl/H₂O Phase Diagram. ACS Central Science, 2019, 5, 640-643.	11.3	31
33	Performance of microporous carbon electrodes for supercapacitors: Comparing graphene with disordered materials. Energy Storage Materials, 2019, 17, 88-92.	18.0	51
34	Dripplons as localized and superfast ripples of water confined between graphene sheets. Nature Communications, 2018, 9, 1496.	12.8	50
35	Moment propagation method for the dynamics of charged adsorbing/desorbing species at solid-liquid interfaces. Molecular Physics, 2018, 116, 2965-2976.	1.7	5
36	Blue Energy and Desalination with Nanoporous Carbon Electrodes: Capacitance from Molecular Simulations to Continuous Models. Physical Review X, 2018, 8, .	8.9	23

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37	Ion-ion correlations across and between electrified graphene layers. Journal of Chemical Physics, 2018, 148, 193812.	3.0	28
38	Underscreening in ionic liquids: a first principles analysis. Journal of Physics Condensed Matter, 2018, 30, 054005.	1.8	42
39	Classical Polarizable Force Field To Study Hydrated Charged Clays and Zeolites. Journal of Physical Chemistry C, 2018, 122, 24690-24704.	3.1	16
40	Capacitive Performance of Water-in-Salt Electrolytes in Supercapacitors: A Simulation Study. Journal of Physical Chemistry C, 2018, 122, 23917-23924.	3.1	49
41	Daan Frenkel â€" An entropic career. Molecular Physics, 2018, 116, 2737-2741.	1.7	0
42	Casimir force in dense confined electrolytes. Molecular Physics, 2018, 116, 3147-3153.	1.7	8
43	Mineral- and Ion-Specific Effects at Clayâ€"Water Interfaces: Structure, Diffusion, and Hydrodynamics. Journal of Physical Chemistry C, 2018, 122, 18484-18492.	3.1	34
44	Classical Polarizable Force Field to Study Hydrated Hectorite: Optimization on DFT Calculations and Validation against XRD Data. Minerals (Basel, Switzerland), 2018, 8, 205.	2.0	10
45	Classical Polarizable Force Field To Study Dry Charged Clays and Zeolites. Journal of Physical Chemistry C, 2017, 121, 9833-9846.	3.1	11
46	Ca²⁺â€Cl^{â^'} Association in Water Revisited: the Role of Cation Hydration. ChemPhysChem, 2017, 18, 2807-2811.	2.1	15
47	Diffusion under Confinement: Hydrodynamic Finite-Size Effects in Simulation. Journal of Chemical Theory and Computation, 2017, 13, 2881-2889.	5.3	81
48	Transient hydrodynamic finite-size effects in simulations under periodic boundary conditions. Physical Review E, 2017, 95, 061301.	2.1	8
49	Solvation in atomic liquids: connection between Gaussian field theory and density functional theory. Condensed Matter Physics, 2017, 20, 33005.	0.7	1
50	Multi-scale modelling of supercapacitors: From molecular simulations to a transmission line model. Journal of Power Sources, 2016, 326, 680-685.	7.8	62
51	Efficient storage mechanisms for building better supercapacitors. Nature Energy, 2016, 1, .	39.5	1,655
52	Molecular Hydrodynamics from Memory Kernels. Physical Review Letters, 2016, 116, 147804.	7.8	68
53	Cation Migration and Structural Deformations upon Dehydration of Nickel-Exchanged NaY Zeolite: A Combined Neutron Diffraction and Monte Carlo Study. Journal of Physical Chemistry C, 2016, 120, 18115-18125.	3.1	11
54	Collective water dynamics in the first solvation shell drive the NMR relaxation of aqueous quadrupolar cations. Journal of Chemical Physics, 2016, 145, 124508.	3.0	13

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55	Modeling the transport of water and ionic tracers in a micrometric clay sample. Applied Clay Science, 2016, 123, 18-28.	5.2	14
56	Understanding the different (dis)charging steps of supercapacitors: influence of potential and solvation. Electrochimica Acta, 2016, 206, 504-512.	5.2	22
57	Classical Polarizable Force Field for Clays: Pyrophyllite and Talc. Journal of Physical Chemistry C, 2016, 120, 3749-3758.	3.1	31
58	On the microscopic fluctuations driving the NMR relaxation of quadrupolar ions in water. Journal of Chemical Physics, 2015, 143, 194504.	3.0	18
59	Upscaling Strategies for Modeling Clay-Rock Properties. Developments in Clay Science, 2015, 6, 399-417.	0.5	7
60	Single Electrode Capacitances of Porous Carbons in Neat Ionic Liquid Electrolyte at 100Â°C: A Combined Experimental and Modeling Approach. Journal of the Electrochemical Society, 2015, 162, A5091-A5095.	2.9	32
61	Diffusion in bulk liquids: finite-size effects in anisotropic systems. Molecular Physics, 2015, 113, 2674-2679.	1.7	25
62	Unexpected coupling between flow and adsorption in porous media. Soft Matter, 2015, 11, 6125-6133.	2.7	27
63	Cation redistribution upon dehydration of Na₅₈Y faujasite zeolite: a joint neutron diffraction and molecular simulation study. Molecular Simulation, 2015, 41, 1371-1378.	2.0	9
64	Jean-Pierre Hansen â€“ a stimulating history of simulating fluids. Molecular Physics, 2015, 113, 2363-2375.	1.7	1
65	Stochastic rotation dynamics simulation of electro-osmosis. Molecular Physics, 2015, 113, 2476-2486.	1.7	7
66	Confinement, Desolvation, And Electrosorption Effects on the Diffusion of Ions in Nanoporous Carbon Electrodes. Journal of the American Chemical Society, 2015, 137, 12627-12632.	13.7	152
67	Structural Transitions at Ionic Liquid Interfaces. Journal of Physical Chemistry Letters, 2015, 6, 4978-4985.	4.6	81
68	Water in clay nanopores. MRS Bulletin, 2014, 39, 1074-1081.	3.5	18
69	Pierre Turq, an inspirational scientist in charge and at interfaces. Molecular Physics, 2014, 112, 1213-1221.	1.7	0
70	Coarse graining the dynamics of nano-confined solutes: the case of ions in clays. Molecular Simulation, 2014, 40, 237-244.	2.0	15
71	Accurate Quadrupolar NMR Relaxation Rates of Aqueous Cations from Classical Molecular Dynamics. Journal of Physical Chemistry B, 2014, 118, 13252-13257.	2.6	16
72	Two algorithms to compute projected correlation functions in molecular dynamics simulations. Journal of Chemical Physics, 2014, 140, 124103.	3.0	43

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73	Pore network model of electrokinetic transport through charged porous media. Physical Review E, 2014, 89, 043013.	2.1	40
74	On the Dynamics of Charging in Nanoporous Carbon-Based Supercapacitors. ACS Nano, 2014, 8, 1576-1583.	14.6	201
75	Salt-induced effective interactions and phase separation of an ultrasoft model of polyelectrolytes. Molecular Physics, 2014, 112, 1313-1319.	1.7	1
76	Structure of tetraalkylammonium ionic liquids in the interlayer of modified montmorillonite. Journal of Physics Condensed Matter, 2014, 26, 284107.	1.8	6
77	Multiscale modelling of transport in clays from the molecular to the sample scale. Comptes Rendus - Geoscience, 2014, 346, 298-306.	1.2	12
78	Numerical study of density functional theory with mean spherical approximation for ionic condensation in highly charged confined electrolytes. Physical Review E, 2014, 89, 062302.	2.1	1
79	The Electric Double Layer Has a Life of Its Own. Journal of Physical Chemistry C, 2014, 118, 18291-18298.	3.1	195
80	Hydration of clays at the molecular scale: the promising perspective of classical density functional theory. Molecular Physics, 2014, 112, 1320-1329.	1.7	11
81	Ions in Clays. , 2014, , 1140-1144.		0
82	Computer simulations of ionic liquids at electrochemical interfaces. Physical Chemistry Chemical Physics, 2013, 15, 15781.	2.8	148
83	Charge Fluctuations in Nanoscale Capacitors. Physical Review Letters, 2013, 111, 106102.	7.8	129
84	Highly confined ions store charge more efficiently in supercapacitors. Nature Communications, 2013, 4, 2701.	12.8	570
85	Computation of pair distribution functions and three-dimensional densities with a reduced variance principle. Molecular Physics, 2013, 111, 3486-3492.	1.7	39
86	Simulating Supercapacitors: Can We Model Electrodes As Constant Charge Surfaces?. Journal of Physical Chemistry Letters, 2013, 4, 264-268.	4.6	220
87	How Electrostatics Influences Hydrodynamic Boundary Conditions: Poiseuille and Electro-osmostic Flows in Clay Nanopores.. Journal of Physical Chemistry C, 2013, 117, 978-985.	3.1	59
88	Electrokinetics: insights from simulation on the microscopic scale. Molecular Physics, 2013, 111, 827-842.	1.7	50
89	Influence of solvation on the structural and capacitive properties of electrical double layer capacitors. Electrochimica Acta, 2013, 101, 262-271.	5.2	96
90	Molecular diffusion between walls with adsorption and desorption. Journal of Chemical Physics, 2013, 138, 034107.	3.0	12

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91	Molecular Simulation of CO2- and CO3-Brine-Mineral Systems. Reviews in Mineralogy and Geochemistry, 2013, 77, 189-228.	4.8	36
92	Accounting for adsorption and desorption in lattice Boltzmann simulations. Physical Review E, 2013, 88, 013308.	2.1	39
93	Numerical homogenization of electrokinetic equations in porous media using lattice-Boltzmann simulations. Physical Review E, 2013, 88, 013019.	2.1	21
94	Taylor dispersion with adsorption and desorption. Physical Review E, 2012, 86, 036316.	2.1	23
95	A transferable ab initio based force field for aqueous ions. Journal of Chemical Physics, 2012, 136, 114507.	3.0	58
96	New Coarse-Grained Models of Imidazolium Ionic Liquids for Bulk and Interfacial Molecular Simulations. Journal of Physical Chemistry C, 2012, 116, 7687-7693.	3.1	126
97	Absolute acidity of clay edge sites from ab-initio simulations. Geochimica Et Cosmochimica Acta, 2012, 94, 1-11.	3.9	89
98	Solvation of complex surfaces via molecular density functional theory. Journal of Chemical Physics, 2012, 137, 224107.	3.0	23
99	Diffusion coefficient and shear viscosity of rigid water models. Journal of Physics Condensed Matter, 2012, 24, 284117.	1.8	86
100	On the molecular origin of supercapacitance in nanoporous carbon electrodes. Nature Materials, 2012, 11, 306-310.	27.5	861
101	Including many-body effects in models for ionic liquids. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	117
102	Molecular Explanation for Why Talc Surfaces Can Be Both Hydrophilic and Hydrophobic. Journal of the American Chemical Society, 2011, 133, 20521-20527.	13.7	152
103	Hydrodynamics in Clay Nanopores. Journal of Physical Chemistry C, 2011, 115, 16109-16115.	3.1	168
104	Imidazolium Ionic Liquid Interfaces with Vapor and Graphite: Interfacial Tension and Capacitance from Coarse-Grained Molecular Simulations. Journal of Physical Chemistry C, 2011, 115, 16613-16618.	3.1	139
105	Experiments â€“ Simulations â€“ Theories: Multiscale approaches for solutions. Ã‰cole ThÃ©matique De La SociÃ©tÃ© FranÃ§aise De La Neutronique, 2011, 12, 263-283.	0.2	1
106	Bridging molecular and continuous descriptions: the case of dynamics in clays. Anais Da Academia Brasileira De Ciencias, 2010, 82, 61-68.	0.8	8
107	From Localized Orbitals to Material Properties: Building Classical Force Fields for Nonmetallic Condensed Matter Systems. Physical Review Letters, 2010, 104, 138301.	7.8	36
108	Recent advances in the modelling and simulation of electrokinetic effects: bridging the gap between atomistic and macroscopic descriptions. Physical Chemistry Chemical Physics, 2010, 12, 9566.	2.8	75

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109	Coarse-grained simulations of charge, current and flow in heterogeneous media. Faraday Discussions, 2010, 144, 223-243.	3.2	49
110	Molecular simulation of aqueous solutions at clay surfaces. Journal of Physics Condensed Matter, 2010, 22, 284114.	1.8	47
111	Dynamics in Clays - Combining Neutron Scattering and Microscopic Simulation. Zeitschrift Fur Physikalische Chemie, 2010, 224, 153-181.	2.8	33
112	Carbon Dioxide in Montmorillonite Clay Hydrates: Thermodynamics, Structure, and Transport from Molecular Simulation. Journal of Physical Chemistry C, 2010, 114, 14962-14969.	3.1	143
113	On the driving force of cation exchange in clays: Insights from combined microcalorimetry experiments and molecular simulation. Geochimica Et Cosmochimica Acta, 2009, 73, 4034-4044.	3.9	88
114	Salt exclusion in charged porous media: a coarse-graining strategy in the case of montmorillonite clays. Physical Chemistry Chemical Physics, 2009, 11, 2023.	2.8	45
115	Structure and dynamics of water at a clay surface from molecular dynamics simulation. Physical Chemistry Chemical Physics, 2008, 10, 4802.	2.8	207
116	Dispersion of charged tracers in charged porous media. Europhysics Letters, 2008, 83, 34004.	2.0	28
117	Water and ions in clays: Unraveling the interlayer/micropore exchange using molecular dynamics. Geochimica Et Cosmochimica Acta, 2007, 71, 5089-5101.	3.9	135
118	Modelling water and ion diffusion in clays: A multiscale approach. Comptes Rendus Chimie, 2007, 10, 1108-1116.	0.5	43
119	A multiscale approach to ion diffusion in clays: Building a two-state diffusionâ€“reaction scheme from microscopic dynamics. Journal of Colloid and Interface Science, 2007, 309, 289-295.	9.4	31
120	Solving the Fokker-Planck kinetic equation on a lattice. Physical Review E, 2006, 73, 066707.	2.1	28
121	Dielectric spectroscopy as a probe for dynamic properties of compacted smectites. Physics and Chemistry of the Earth, 2006, 31, 505-510.	2.9	22
122	Preparation of Doublet, Triangular, and Tetrahedral Colloidal Clusters by Controlled Emulsification. Langmuir, 2006, 22, 57-62.	3.5	83
123	Second-order lattice Fokker-Planck algorithm from the trapezoidal rule. Physical Review E, 2006, 74, 037701.	2.1	5
124	Ion dynamics in compacted clays: Derivation of a two-state diffusion-reaction scheme from the lattice Fokker-Planck equation. Journal of Chemical Physics, 2006, 124, 154701.	3.0	12
125	Frequency-dependent dielectric permittivity of salt-free charged lamellar systems. Journal of Chemical Physics, 2005, 123, 154902.	3.0	10
126	Encapsulation of Magnetic and Fluorescent Nanoparticles in Emulsion Droplets. Langmuir, 2005, 21, 4175-4179.	3.5	86

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127	An Analytical Model for Probing Ion Dynamics in Clays with Broadband Dielectric Spectroscopy. Journal of Physical Chemistry B, 2005, 109, 15548-15557.	2.6	47
128	Invited article: Thermodynamic perturbation theory of the phase behaviour of colloid/interacting polymer mixtures. Molecular Physics, 2004, 102, 1-11.	1.7	37
129	An Integral Equation Approach to Effective Interactions between Polymers in Solution. Journal of Physical Chemistry B, 2004, 108, 6697-6706.	2.6	13
130	Effect of polymerâ€“polymer interactions on the surface tension of colloidâ€“polymer mixtures. Journal of Chemical Physics, 2003, 119, 12667-12672.	3.0	17
131	H2Âin intense laser field pulses: ionization versus dissociation within moving nucleus simulations. Journal of Physics B: Atomic, Molecular and Optical Physics, 2002, 35, L397-L402.	1.5	29