

# Benjamin Rotenberg

## List of Publications by Year in descending order

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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	Efficient storage mechanisms for building better supercapacitors. <i>Nature Energy</i> , 2016, 1, .	39.5	1,655
2	On the molecular origin of supercapacitance in nanoporous carbon electrodes. <i>Nature Materials</i> , 2012, 11, 306-310.	27.5	861
3	Highly confined ions store charge more efficiently in supercapacitors. <i>Nature Communications</i> , 2013, 4, 2701.	12.8	570
4	Simulating Supercapacitors: Can We Model Electrodes As Constant Charge Surfaces?. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 264-268.	4.6	220
5	Structure and dynamics of water at a clay surface from molecular dynamics simulation. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 4802.	2.8	207
6	On the Dynamics of Charging in Nanoporous Carbon-Based Supercapacitors. <i>ACS Nano</i> , 2014, 8, 1576-1583.	14.6	201
7	The Electric Double Layer Has a Life of Its Own. <i>Journal of Physical Chemistry C</i> , 2014, 118, 18291-18298.	3.1	195
8	Hydrodynamics in Clay Nanopores. <i>Journal of Physical Chemistry C</i> , 2011, 115, 16109-16115.	3.1	168
9	Molecular Explanation for Why Talc Surfaces Can Be Both Hydrophilic and Hydrophobic. <i>Journal of the American Chemical Society</i> , 2011, 133, 20521-20527.	13.7	152
10	Confinement, Desolvation, And Electrosorption Effects on the Diffusion of Ions in Nanoporous Carbon Electrodes. <i>Journal of the American Chemical Society</i> , 2015, 137, 12627-12632.	13.7	152
11	Computer simulations of ionic liquids at electrochemical interfaces. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 15781.	2.8	148
12	Carbon Dioxide in Montmorillonite Clay Hydrates: Thermodynamics, Structure, and Transport from Molecular Simulation. <i>Journal of Physical Chemistry C</i> , 2010, 114, 14962-14969.	3.1	143
13	Imidazolium Ionic Liquid Interfaces with Vapor and Graphite: Interfacial Tension and Capacitance from Coarse-Grained Molecular Simulations. <i>Journal of Physical Chemistry C</i> , 2011, 115, 16613-16618.	3.1	139
14	Water and ions in clays: Unraveling the interlayer/micropore exchange using molecular dynamics. <i>Geochimica Et Cosmochimica Acta</i> , 2007, 71, 5089-5101.	3.9	135
15	Charge Fluctuations in Nanoscale Capacitors. <i>Physical Review Letters</i> , 2013, 111, 106102.	7.8	129
16	New Coarse-Grained Models of Imidazolium Ionic Liquids for Bulk and Interfacial Molecular Simulations. <i>Journal of Physical Chemistry C</i> , 2012, 116, 7687-7693.	3.1	126
17	Including many-body effects in models for ionic liquids. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	117
18	Influence of solvation on the structural and capacitive properties of electrical double layer capacitors. <i>Electrochimica Acta</i> , 2013, 101, 262-271.	5.2	96

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19	Absolute acidity of clay edge sites from ab-initio simulations. <i>Geochimica Et Cosmochimica Acta</i> , 2012, 94, 1-11.	3.9	89
20	On the driving force of cation exchange in clays: Insights from combined microcalorimetry experiments and molecular simulation. <i>Geochimica Et Cosmochimica Acta</i> , 2009, 73, 4034-4044.	3.9	88
21	Encapsulation of Magnetic and Fluorescent Nanoparticles in Emulsion Droplets. <i>Langmuir</i> , 2005, 21, 4175-4179.	3.5	86
22	Diffusion coefficient and shear viscosity of rigid water models. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 284117.	1.8	86
23	Preparation of Doublet, Triangular, and Tetrahedral Colloidal Clusters by Controlled Emulsification. <i>Langmuir</i> , 2006, 22, 57-62.	3.5	83
24	Structural Transitions at Ionic Liquid Interfaces. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4978-4985.	4.6	81
25	Diffusion under Confinement: Hydrodynamic Finite-Size Effects in Simulation. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2881-2889.	5.3	81
26	Microscopic Simulations of Electrochemical Double-Layer Capacitors. <i>Chemical Reviews</i> , 2022, 122, 10860-10898.	47.7	81
27	Recent advances in the modelling and simulation of electrokinetic effects: bridging the gap between atomistic and macroscopic descriptions. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 9566.	2.8	75
28	Molecular Hydrodynamics from Memory Kernels. <i>Physical Review Letters</i> , 2016, 116, 147804.	7.8	68
29	Molecular Simulation of Electrode-Solution Interfaces. <i>Annual Review of Physical Chemistry</i> , 2021, 72, 189-212.	10.8	64
30	Multi-scale modelling of supercapacitors: From molecular simulations to a transmission line model. <i>Journal of Power Sources</i> , 2016, 326, 680-685.	7.8	62
31	Transport Properties of Li-TFSI Water-in-Salt Electrolytes. <i>Journal of Physical Chemistry B</i> , 2019, 123, 10514-10521.	2.6	60
32	How Electrostatics Influences Hydrodynamic Boundary Conditions: Poiseuille and Electro-osmotic Flows in Clay Nanopores.. <i>Journal of Physical Chemistry C</i> , 2013, 117, 978-985.	3.1	59
33	A transferable <i>ab initio</i> based force field for aqueous ions. <i>Journal of Chemical Physics</i> , 2012, 136, 114507.	3.0	58
34	MetalWalls: A classical molecular dynamics software dedicated to the simulation of electrochemical systems. <i>Journal of Open Source Software</i> , 2020, 5, 2373.	4.6	56
35	Charge fluctuations from molecular simulations in the constant-potential ensemble. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 10480-10489.	2.8	53
36	Competitive Salt Precipitation/Dissolution During Free-Water Reduction in Water-in-Salt Electrolyte. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 15913-15917.	13.8	52

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37	Performance of microporous carbon electrodes for supercapacitors: Comparing graphene with disordered materials. <i>Energy Storage Materials</i> , 2019, 17, 88-92.	18.0	51
38	Electrokinetics: insights from simulation on the microscopic scale. <i>Molecular Physics</i> , 2013, 111, 827-842.	1.7	50
39	Driplons as localized and superfast ripples of water confined between graphene sheets. <i>Nature Communications</i> , 2018, 9, 1496.	12.8	50
40	Coarse-grained simulations of charge, current and flow in heterogeneous media. <i>Faraday Discussions</i> , 2010, 144, 223-243.	3.2	49
41	Capacitive Performance of Water-in-Salt Electrolytes in Supercapacitors: A Simulation Study. <i>Journal of Physical Chemistry C</i> , 2018, 122, 23917-23924.	3.1	49
42	A semiclassical Thomas-Fermi model to tune the metallicity of electrodes in molecular simulations. <i>Journal of Chemical Physics</i> , 2020, 153, 174704.	3.0	49
43	Simulating Electrochemical Systems by Combining the Finite Field Method with a Constant Potential Electrode. <i>Physical Review Letters</i> , 2019, 123, 195501.	7.8	48
44	Effect of the carbon microporous structure on the capacitance of aqueous supercapacitors. <i>Energy Storage Materials</i> , 2019, 21, 190-195.	18.0	48
45	An Analytical Model for Probing Ion Dynamics in Clays with Broadband Dielectric Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2005, 109, 15548-15557.	2.6	47
46	Molecular simulation of aqueous solutions at clay surfaces. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 284114.	1.8	47
47	Salt exclusion in charged porous media: a coarse-graining strategy in the case of montmorillonite clays. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 2023.	2.8	45
48	Modelling water and ion diffusion in clays: A multiscale approach. <i>Comptes Rendus Chimie</i> , 2007, 10, 1108-1116.	0.5	43
49	Two algorithms to compute projected correlation functions in molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2014, 140, 124103.	3.0	43
50	Underscreening in ionic liquids: a first principles analysis. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 054005.	1.8	42
51	Pore network model of electrokinetic transport through charged porous media. <i>Physical Review E</i> , 2014, 89, 043013.	2.1	40
52	Computation of pair distribution functions and three-dimensional densities with a reduced variance principle. <i>Molecular Physics</i> , 2013, 111, 3486-3492.	1.7	39
53	Accounting for adsorption and desorption in lattice Boltzmann simulations. <i>Physical Review E</i> , 2013, 88, 013308.	2.1	39
54	Invited article: Thermodynamic perturbation theory of the phase behaviour of colloid/interacting polymer mixtures. <i>Molecular Physics</i> , 2004, 102, 1-11.	1.7	37

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55	From Localized Orbitals to Material Properties: Building Classical Force Fields for Nonmetallic Condensed Matter Systems. <i>Physical Review Letters</i> , 2010, 104, 138301.	7.8	36
56	Molecular Simulation of CO <sub>2</sub> - and CO <sub>3</sub> -Brine-Mineral Systems. <i>Reviews in Mineralogy and Geochemistry</i> , 2013, 77, 189-228.	4.8	36
57	Mineral- and Ion-Specific Effects at Clay-Water Interfaces: Structure, Diffusion, and Hydrodynamics. <i>Journal of Physical Chemistry C</i> , 2018, 122, 18484-18492.	3.1	34
58	Correlation Length in Concentrated Electrolytes: Insights from All-Atom Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2020, 124, 1778-1786.	2.6	34
59	Dynamics in Clays - Combining Neutron Scattering and Microscopic Simulation. <i>Zeitschrift Fur Physikalische Chemie</i> , 2010, 224, 153-181.	2.8	33
60	Single Electrode Capacitances of Porous Carbons in Neat Ionic Liquid Electrolyte at 100°C: A Combined Experimental and Modeling Approach. <i>Journal of the Electrochemical Society</i> , 2015, 162, A5091-A5095.	2.9	32
61	A multiscale approach to ion diffusion in clays: Building a two-state diffusion reaction scheme from microscopic dynamics. <i>Journal of Colloid and Interface Science</i> , 2007, 309, 289-295.	9.4	31
62	Classical Polarizable Force Field for Clays: Pyrophyllite and Talc. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3749-3758.	3.1	31
63	Study of a water-graphene capacitor with molecular density functional theory. <i>Journal of Chemical Physics</i> , 2019, 151, 124111.	3.0	31
64	Chasing Aqueous Biphasic Systems from Simple Salts by Exploring the LiTFSI/LiCl/H <sub>2</sub> O Phase Diagram. <i>ACS Central Science</i> , 2019, 5, 640-643.	11.3	31
65	H <sub>2</sub> in intense laser field pulses: ionization versus dissociation within moving nucleus simulations. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2002, 35, L397-L402.	1.5	29
66	Solving the Fokker-Planck kinetic equation on a lattice. <i>Physical Review E</i> , 2006, 73, 066707.	2.1	28
67	Dispersion of charged tracers in charged porous media. <i>Europhysics Letters</i> , 2008, 83, 34004.	2.0	28
68	Ion-ion correlations across and between electrified graphene layers. <i>Journal of Chemical Physics</i> , 2018, 148, 193812.	3.0	28
69	Unexpected coupling between flow and adsorption in porous media. <i>Soft Matter</i> , 2015, 11, 6125-6133.	2.7	27
70	Effect of the metallicity on the capacitance of gold-aqueous sodium chloride interfaces. <i>Journal of Chemical Physics</i> , 2021, 155, 044703.	3.0	26
71	Diffusion in bulk liquids: finite-size effects in anisotropic systems. <i>Molecular Physics</i> , 2015, 113, 2674-2679.	1.7	25
72	A molecular density functional theory approach to electron transfer reactions. <i>Chemical Science</i> , 2019, 10, 2130-2143.	7.4	24

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73	Taylor dispersion with adsorption and desorption. <i>Physical Review E</i> , 2012, 86, 036316.	2.1	23
74	Solvation of complex surfaces via molecular density functional theory. <i>Journal of Chemical Physics</i> , 2012, 137, 224107.	3.0	23
75	Blue Energy and Desalination with Nanoporous Carbon Electrodes: Capacitance from Molecular Simulations to Continuous Models. <i>Physical Review X</i> , 2018, 8, .	8.9	23
76	Use the force! Reduced variance estimators for densities, radial distribution functions, and local mobilities in molecular simulations. <i>Journal of Chemical Physics</i> , 2020, 153, 150902.	3.0	23
77	Competitive Salt Precipitation/Dissolution During Free-Water Reduction in Water-in-Salt Electrolyte. <i>Angewandte Chemie</i> , 2020, 132, 16047-16051.	2.0	23
78	Dielectric spectroscopy as a probe for dynamic properties of compacted smectites. <i>Physics and Chemistry of the Earth</i> , 2006, 31, 505-510.	2.9	22
79	Understanding the different (dis)charging steps of supercapacitors: influence of potential and solvation. <i>Electrochimica Acta</i> , 2016, 206, 504-512.	5.2	22
80	On the Gibbs-Thomson equation for the crystallization of confined fluids. <i>Journal of Chemical Physics</i> , 2021, 154, 114711.	3.0	22
81	Numerical homogenization of electrokinetic equations in porous media using lattice-Boltzmann simulations. <i>Physical Review E</i> , 2013, 88, 013019.	2.1	21
82	Likelihood-based non-Markovian models from molecular dynamics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, e2117586119.	7.1	21
83	Water in clay nanopores. <i>MRS Bulletin</i> , 2014, 39, 1074-1081.	3.5	18
84	On the microscopic fluctuations driving the NMR relaxation of quadrupolar ions in water. <i>Journal of Chemical Physics</i> , 2015, 143, 194504.	3.0	18
85	Field-Dependent Ionic Conductivities from Generalized Fluctuation-Dissipation Relations. <i>Physical Review Letters</i> , 2020, 124, 206001.	7.8	18
86	Effect of polymer-polymer interactions on the surface tension of colloid-polymer mixtures. <i>Journal of Chemical Physics</i> , 2003, 119, 12667-12672.	3.0	17
87	Lattice Boltzmann electrokinetics simulation of nanocapacitors. <i>Journal of Chemical Physics</i> , 2019, 151, 114104.	3.0	17
88	Accurate Quadrupolar NMR Relaxation Rates of Aqueous Cations from Classical Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2014, 118, 13252-13257.	2.6	16
89	Classical Polarizable Force Field To Study Hydrated Charged Clays and Zeolites. <i>Journal of Physical Chemistry C</i> , 2018, 122, 24690-24704.	3.1	16
90	Mass-zero constrained molecular dynamics for electrode charges in simulations of electrochemical systems. <i>Journal of Chemical Physics</i> , 2020, 152, 194701.	3.0	16

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91	Coarse graining the dynamics of nano-confined solutes: the case of ions in clays. <i>Molecular Simulation</i> , 2014, 40, 237-244.	2.0	15
92	Ca <sup>2+</sup> ⋯Cl <sup>-</sup> Association in Water Revisited: the Role of Cation Hydration. <i>ChemPhysChem</i> , 2017, 18, 2807-2811.	2.1	15
93	Modeling the transport of water and ionic tracers in a micrometric clay sample. <i>Applied Clay Science</i> , 2016, 123, 18-28.	5.2	14
94	An Integral Equation Approach to Effective Interactions between Polymers in Solution. <i>Journal of Physical Chemistry B</i> , 2004, 108, 6697-6706.	2.6	13
95	Collective water dynamics in the first solvation shell drive the NMR relaxation of aqueous quadrupolar cations. <i>Journal of Chemical Physics</i> , 2016, 145, 124508.	3.0	13
96	Ion dynamics in compacted clays: Derivation of a two-state diffusion-reaction scheme from the lattice Fokker-Planck equation. <i>Journal of Chemical Physics</i> , 2006, 124, 154701.	3.0	12
97	Molecular diffusion between walls with adsorption and desorption. <i>Journal of Chemical Physics</i> , 2013, 138, 034107.	3.0	12
98	Multiscale modelling of transport in clays from the molecular to the sample scale. <i>Comptes Rendus - Geoscience</i> , 2014, 346, 298-306.	1.2	12
99	Computing three-dimensional densities from force densities improves statistical efficiency. <i>Journal of Chemical Physics</i> , 2019, 151, 064124.	3.0	12
100	On the molecular correlations that result in field-dependent conductivities in electrolyte solutions. <i>Journal of Chemical Physics</i> , 2021, 155, 014507.	3.0	12
101	Hydration of clays at the molecular scale: the promising perspective of classical density functional theory. <i>Molecular Physics</i> , 2014, 112, 1320-1329.	1.7	11
102	Cation Migration and Structural Deformations upon Dehydration of Nickel-Exchanged NaY Zeolite: A Combined Neutron Diffraction and Monte Carlo Study. <i>Journal of Physical Chemistry C</i> , 2016, 120, 18115-18125.	3.1	11
103	Classical Polarizable Force Field To Study Dry Charged Clays and Zeolites. <i>Journal of Physical Chemistry C</i> , 2017, 121, 9833-9846.	3.1	11
104	Sampling mobility profiles of confined fluids with equilibrium molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2020, 153, 044125.	3.0	11
105	Structure and position-dependent properties of inhomogeneous suspensions of responsive colloids. <i>Physical Review E</i> , 2020, 102, 042602.	2.1	11
106	Frequency-dependent dielectric permittivity of salt-free charged lamellar systems. <i>Journal of Chemical Physics</i> , 2005, 123, 154902.	3.0	10
107	Classical Polarizable Force Field to Study Hydrated Hectorite: Optimization on DFT Calculations and Validation against XRD Data. <i>Minerals (Basel, Switzerland)</i> , 2018, 8, 205.	2.0	10
108	A molecular perspective on induced charges on a metallic surface. <i>Journal of Chemical Physics</i> , 2021, 155, 204705.	3.0	10

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109	Chemisorbed vs physisorbed surface charge and its impact on electrokinetic transport: Carbon vs boron nitride surface. <i>Journal of Chemical Physics</i> , 2022, 156, 044703.	3.0	10
110	Cation redistribution upon dehydration of Na <sub>58</sub> Y faujasite zeolite: a joint neutron diffraction and molecular simulation study. <i>Molecular Simulation</i> , 2015, 41, 1371-1378.	2.0	9
111	Bridging molecular and continuous descriptions: the case of dynamics in clays. <i>Anais Da Academia Brasileira De Ciencias</i> , 2010, 82, 61-68.	0.8	8
112	Transient hydrodynamic finite-size effects in simulations under periodic boundary conditions. <i>Physical Review E</i> , 2017, 95, 061301.	2.1	8
113	Casimir force in dense confined electrolytes. <i>Molecular Physics</i> , 2018, 116, 3147-3153.	1.7	8
114	Upscaling Strategies for Modeling Clay-Rock Properties. <i>Developments in Clay Science</i> , 2015, 6, 399-417.	0.5	7
115	Stochastic rotation dynamics simulation of electro-osmosis. <i>Molecular Physics</i> , 2015, 113, 2476-2486.	1.7	7
116	Structure of tetraalkylammonium ionic liquids in the interlayer of modified montmorillonite. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 284107.	1.8	6
117	Printed Dielectrophoretic Electrode-Based Continuous Flow Microfluidic Systems for Particles 3D-Trapping. <i>Particle and Particle Systems Characterization</i> , 2021, 38, 2000235.	2.3	6
118	Reduced variance analysis of molecular dynamics simulations by linear combination of estimators. <i>Journal of Chemical Physics</i> , 2021, 154, 191101.	3.0	6
119	Second-order lattice Fokker-Planck algorithm from the trapezoidal rule. <i>Physical Review E</i> , 2006, 74, 037701.	2.1	5
120	Moment propagation method for the dynamics of charged adsorbing/desorbing species at solid-liquid interfaces. <i>Molecular Physics</i> , 2018, 116, 2965-2976.	1.7	5
121	Lattice Boltzmann method for adsorption under stationary and transient conditions: Interplay between transport and adsorption kinetics in porous media. <i>Physical Review E</i> , 2021, 104, 015314.	2.1	5
122	NMR Relaxation Rates of Quadrupolar Aqueous Ions from Classical Molecular Dynamics Using Force-Field Specific Sternheimer Factors. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6006-6017.	5.3	5
123	Microscopic origin of the effect of substrate metallicity on interfacial free energies. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	4
124	Salt-induced effective interactions and phase separation of an ultrasoft model of polyelectrolytes. <i>Molecular Physics</i> , 2014, 112, 1313-1319.	1.7	1
125	Numerical study of density functional theory with mean spherical approximation for ionic condensation in highly charged confined electrolytes. <i>Physical Review E</i> , 2014, 89, 062302.	2.1	1
126	Jean-Pierre Hansen "a stimulating history of simulating fluids. <i>Molecular Physics</i> , 2015, 113, 2363-2375.	1.7	1



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127	Experiments “ Simulations “ Theories: Multiscale approaches for solutions. <i>École Thématique De La Sociétés Française De La Neutronique</i> , 2011, 12, 263-283.	0.2	1
128	Solvation in atomic liquids: connection between Gaussian field theory and density functional theory. <i>Condensed Matter Physics</i> , 2017, 20, 33005.	0.7	1
129	Pierre Turq, an inspirational scientist in charge and at interfaces. <i>Molecular Physics</i> , 2014, 112, 1213-1221.	1.7	0
130	Daan Frenkel “ An entropic career. <i>Molecular Physics</i> , 2018, 116, 2737-2741.	1.7	0
131	Ions in Clays. , 2014, , 1140-1144.		0