DezsÅ‘ Boda

List of Publications by Year
in descending order

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128 papers	4,279 citations	116194 36 h-index	145109 60 g-index
130 all docs	130 docs citations	130 times ranked	2377 citing authors

#	Article	IF	Citations
1	Scaling for rectification of bipolar nanopores as a function of a modified Dukhin number: the case of 1:1 electrolytes. Molecular Simulation, 2022, 48, 43-56.	0.9	8
2	The Dukhin number as a scaling parameter for selectivity in the infinitely long nanopore limit: Extension to multivalent electrolytes. Journal of Molecular Liquids, 2022, 357, 119072.	2.3	2
3	A systematic study of the dynamics of chain formation in electrorheological fluids. AIP Advances, 2021, 11, 025243.	0.6	3
4	From nanotubes to nanoholes: Scaling of selectivity in uniformly charged nanopores through the Dukhin number for 1:1 electrolytes. Journal of Chemical Physics, 2021, 154, 154704.	1.2	9
5	Induced permittivity increment of electrorheological fluids in an applied electric field in association with chain formation: A Brownian dynamics simulation study. Physical Review E, 2021, 103, 062608.	0.8	4
6	Electrostatic correlations in electrolytes: Contribution of screening ion interactions to the excess chemical potential. Journal of Chemical Physics, 2021, 155, 221102.	1.2	8
7	Modeling the Device Behavior of Biological and Synthetic Nanopores with Reduced Models. Entropy, 2020, 22, 1259.	1.1	7
8	Rectification of bipolar nanopores in multivalent electrolytes: effect of charge inversion and strong ionic correlations. Physical Chemistry Chemical Physics, 2020, 22, 19033-19045.	1.3	15
9	Modeling of a pHâ€“tunable dualâ€“response nanopore sensor. Journal of Molecular Liquids, 2020, 310, 112946.	2.3	3
10	Brownian dynamics simulation of chain formation in electrorheological fluids. Hungarian Journal of Industrial Chemistry, 2020, 48, .	0.1	2
11	Application of a bipolar nanopore as a sensor: rectification as an additional device function. Physical Chemistry Chemical Physics, 2019, 21, 19772-19784.	1.3	10
12	Scaling Behavior of Bipolar Nanopore Rectification with Multivalent Ions. Journal of Physical Chemistry C, 2019, 123, 28985-28996.	1.5	20
13	The effect of the charge pattern on the applicability of a nanopore as a sensor. Journal of Molecular Liquids, 2019, 283, 391-398.	2.3	12
14	Multiscale analysis of the effect of surface charge pattern on a nanoporeâ€™s rectification and selectivity properties: From all-atom model to Poisson-Nernst-Planck. Journal of Chemical Physics, 2019, 150, 144703.	1.2	26
15	Controlling ionic current through a nanopore by tuning pH: a local equilibrium Monte Carlo study. Molecular Physics, 2019, 117, 2793-2801.	0.8	7
16	A systematic Monte Carlo simulation study of the primitive model planar electrical double layer over an extended range of concentrations, electrode charges, cation diameters and valences. AIP Advances, 2018, 8, .	0.6	25
17	Controlling ion transport through nanopores: modeling transistor behavior. Physical Chemistry Chemical Physics, 2018, 20, 24156-24167.	1.3	24
18	Activity coefficients of individual ions in LaCl₃from the II+IW theory. Molecular Physics, 2017, 115, 1245-1252.	0.8	19

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19	Multiscale modeling of a rectifying bipolar nanopore: Comparing Poisson-Nernst-Planck to Monte Carlo. Journal of Chemical Physics, 2017, 146, 124125.	1.2	22
20	Multiscale modeling of a rectifying bipolar nanopore: explicit-water versus implicit-water simulations. Physical Chemistry Chemical Physics, 2017, 19, 17816-17826.	1.3	23
21	Simulation of a model nanopore sensor: Ion competition underlies device behavior. Journal of Chemical Physics, 2017, 147, 244702.	1.2	17
22	Simulating Ion Transport with the NP+LEMC Method. Applications to Ion Channels and Nanopores.. Hungarian Journal of Industrial Chemistry, 2017, 45, 73-84.	0.1	7
23	Simulation study of a rectifying bipolar ion channel: Detailed model versus reduced model. Condensed Matter Physics, 2016, 19, 13802.	0.3	10
24	Unraveling the Behavior of the Individual Ionic Activity Coefficients on the Basis of the Balance of Ionâ€“Ion and Ionâ€“Water Interactions. Journal of Physical Chemistry B, 2015, 119, 1546-1557.	1.2	38
25	Comment on â€œThe Role of Concentration Dependent Static Permittivity of Electrolyte Solutions in the Debyeâ€“HÃ¼ckel Theoryâ€. Journal of Physical Chemistry B, 2015, 119, 14332-14336.	1.2	22
26	Energetics of ion competition in the DEKA selectivity filter of neuronal sodium channels. Condensed Matter Physics, 2015, 18, 13601.	0.3	3
27	Monte Carlo Simulation of Electrolyte Solutions in Biology. Annual Reports in Computational Chemistry, 2014, 10, 127-163.	0.9	19
28	The effect of concentration- and temperature-dependent dielectric constant on the activity coefficient of NaCl electrolyte solutions. Journal of Chemical Physics, 2014, 140, 234508.	1.2	58
29	Selective transport through a model calcium channel studied by Local Equilibrium Monte Carlo simulations coupled to the Nernstâ€“Planck equation. Journal of Molecular Liquids, 2014, 189, 100-112.	2.3	23
30	Three-Dimensional Brownian Dynamics Simulator for the Study of Ion Permeation through Membrane Pores. Journal of Chemical Theory and Computation, 2014, 10, 2911-2926.	2.3	33
31	Dynamic Monte Carlo Simulation of Coupled Transport through a Narrow Multiply-Occupied Pore. Journal of Physical Chemistry C, 2014, 118, 700-707.	1.5	9
32	The role of solvation in the binding selectivity of the L-type calcium channel. Journal of Chemical Physics, 2013, 139, 055103.	1.2	24
33	Selective adsorption of ions in charged slit-systems. Condensed Matter Physics, 2013, 16, 43601.	0.3	3
34	The origin of the interparticle potential of electrorheological fluids. Condensed Matter Physics, 2013, 16, 43002.	0.3	0
35	Simulation of steady-state diffusion: Driving force ensured by dual control volumes or local equilibrium Monte Carlo. Journal of Chemical Physics, 2012, 137, 054109.	1.2	22
36	Steady-State Electrodiffusion from the Nernstâ€“Planck Equation Coupled to Local Equilibrium Monte Carlo Simulations. Journal of Chemical Theory and Computation, 2012, 8, 824-829.	2.3	43

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37	Current and selectivity in a model sodium channel under physiological conditions: Dynamic Monte Carlo simulations. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 592-600.	1.4	33
38	An analytic solution for the magnetization of two-dimensional ferrofluids based on the mean spherical approximation. Journal of Physics Condensed Matter, 2012, 24, 336002.	0.7	1
39	Monte Carlo simulation of the electrical properties of electrolytes adsorbed in charged slit-systems. Condensed Matter Physics, 2012, 15, 23803.	0.3	5
40	Mean spherical approximation for the Yukawa fluid radial distribution function. Molecular Physics, 2011, 109, 1009-1013.	0.8	9
41	Behavior of 2:1 and 3:1 Electrolytes at Polarizable Interfaces. Journal of Chemical & Engineering Data, 2011, 56, 1316-1322.	1.0	6
42	Heat capacities of the dipolar Yukawa model polar fluid. Molecular Physics, 2011, 109, 203-208.	0.8	7
43	Simulation of an Electrical Double Layer Model with a Low Dielectric Layer between the Electrode and the Electrolyte. Journal of Physical Chemistry B, 2011, 115, 11409-11419.	1.2	37
44	Analyzing the components of the free-energy landscape in a calcium selective ion channel by Widom's particle insertion method. Journal of Chemical Physics, 2011, 134, 055102.	1.2	37
45	Response to â€œComment on â€˜The nonmonotonic concentration dependence of the mean activity coefficient of electrolytes is a result of a balance between solvation and ionâ€“ion correlationsâ€™â€•[J. Chem. Phys. 134, 157101 (2011)]. Journal of Chemical Physics, 2011, 134, .	1.2	10
46	A method for treating the passage of a charged hard sphere ion as it passes through a sharp dielectric boundary. Journal of Chemical Physics, 2011, 135, 064105.	1.2	17
47	Self-organized models of selectivity in calcium channels. Physical Biology, 2011, 8, 026004.	0.8	23
48	The structure of strongly dipolar hard sphere fluids with extended dipoles by Monte Carlo simulations. Molecular Physics, 2010, 108, 87-96.	0.8	9
49	An efficient iterative grand canonical Monte Carlo algorithm to determine individual ionic chemical potentials in electrolytes. Journal of Chemical Physics, 2010, 132, 244103.	1.2	44
50	The nonmonotonic concentration dependence of the mean activity coefficient of electrolytes is a result of a balance between solvation and ion-ion correlations. Journal of Chemical Physics, 2010, 133, 154507.	1.2	83
51	Simulations of calcium channel block by trivalent cations: Gd3+ competes with permeant ions for the selectivity filter. Biochimica Et Biophysica Acta - Biomembranes, 2010, 1798, 2013-2021.	1.4	31
52	Relating Binding Affinity to Dynamical Selectivity from Dynamic Monte Carlo Simulations of a Model Calcium Channel. Journal of Physical Chemistry Letters, 2010, 1, 2179-2184.	2.1	21
53	Ionic selectivity in L-type calcium channels by electrostatics and hard-core repulsion. Journal of General Physiology, 2009, 133, 497-509.	0.9	76
54	Protein structure and ionic selectivity in calcium channels: Selectivity filter size, not shape, matters. Biochimica Et Biophysica Acta - Biomembranes, 2009, 1788, 2471-2480.	1.4	42

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55	Ions and Inhibitors in the Binding Site of HIV Protease: Comparison ofÂMonte Carlo Simulations and the Linearized Poisson-Boltzmann Theory. Biophysical Journal, 2009, 96, 1293-1306.	0.2	15
56	Tuning Transport Properties of Nanofluidic Devices with Local Charge Inversion. Journal of the American Chemical Society, 2009, 131, 5194-5202.	6.6	246
57	Correction to the Clausiusâ€“Mosotti equation: The dielectric constant of nonpolar fluids from Monte Carlo simulations. Journal of Chemical Physics, 2009, 131, 164120.	1.2	8
58	Insights from theory and simulation on the electrical double layer. Physical Chemistry Chemical Physics, 2009, 11, 3822.	1.3	116
59	Volume Exclusion in Calcium Selective Channels. Biophysical Journal, 2008, 94, 3486-3496.	0.2	58
60	The Anomalous Mole Fraction Effect in Calcium Channels: A Measure of Preferential Selectivity. Biophysical Journal, 2008, 95, 2658-2672.	0.2	71
61	Synthetic Nanopores as a Test Case for Ion Channel Theories: The Anomalous Mole Fraction Effect without Single Filing. Biophysical Journal, 2008, 95, 609-619.	0.2	72
62	Simulating prescribed particle densities in the grand canonical ensemble using iterative algorithms. Journal of Chemical Physics, 2008, 128, 124102.	1.2	45
63	The effects of deviations from Lorentzâ€“Berthelot rules on the properties of a simple mixture. Molecular Physics, 2008, 106, 2367-2370.	0.8	117
64	Combined Effect of Pore Radius and Protein Dielectric Coefficient on the Selectivity of a Calcium Channel. Physical Review Letters, 2007, 98, 168102.	2.9	78
65	Selective Adsorption of Ions with Different Diameter and Valence at Highly Charged Interfaces. Journal of Physical Chemistry C, 2007, 111, 15575-15585.	1.5	89
66	Simple Extension of a Field Theory Approach for the Description of the Double Layer Accounting for Excluded Volume Effects. Journal of Physical Chemistry C, 2007, 111, 15700-15705.	1.5	11
67	Steric Selectivity in Na Channels Arising from Protein Polarization and Mobile Side Chains. Biophysical Journal, 2007, 93, 1960-1980.	0.2	111
68	The capacitance of the electrical double layer of valence-asymmetric salts at low reduced temperatures. Journal of Molecular Liquids, 2007, 131-132, 179-184.	2.3	14
69	The effect of protein dielectric coefficient on the ionic selectivity of a calcium channel. Journal of Chemical Physics, 2006, 125, 034901.	1.2	93
70	Anomalous temperature dependence of the differential capacitance in valence asymmetric electrolytes. Comparison of Monte Carlo simulation results and the field theoretical approach. Molecular Physics, 2006, 104, 3777-3786.	0.8	20
71	Monte Carlo simulation and renormalized perturbation theory study of the dielectric properties of mixtures of polarizable hard spheres and polarizable dipolar hard spheres. Molecular Physics, 2006, 104, 3821-3830.	0.8	2
72	On a conjecture of Fawcett. Journal of Electroanalytical Chemistry, 2005, 582, 16-20.	1.9	24

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73	Density functional theory of the electrical double layer: the RFD functional. Journal of Physics Condensed Matter, 2005, 17, 6609-6626.	0.7	94
74	Relative Permittivity of Polar Liquids. Comparison of Theory, Experiment, and Simulation. Journal of Physical Chemistry B, 2005, 109, 6355-6365.	1.2	18
75	Temperature dependence of the double layer capacitance for the restricted primitive model of an electrolyte solution from a density functional approach. Journal of Chemical Physics, 2005, 122, 084504.	1.2	78
76	Monte Carlo simulation of the electric double layer: dielectric boundaries and the effects of induced charge. Molecular Physics, 2005, 103, 2851-2861.	0.8	29
77	Dielectric constant of the polarizable dipolar hard sphere fluid studied by Monte Carlo simulation and theories. Condensed Matter Physics, 2005, 8, 357.	0.3	15
78	Computing induced charges in inhomogeneous dielectric media: Application in a Monte Carlo simulation of complex ionic systems. Physical Review E, 2004, 69, 046702.	0.8	138
79	Monte Carlo Simulation Study of a System with a Dielectric Boundary: Application to Calcium Channel Selectivity. Molecular Simulation, 2004, 30, 89-96.	0.9	35
80	Monte Carlo and Density Functional Theory Study of the Electrical Double Layer: The Dependence of the Charge/Voltage Relation on the Diameter of the Ions. Molecular Simulation, 2004, 30, 137-141.	0.9	27
81	Competition between the Effects of Asymmetries in Ion Diameters and Charges in an Electrical Double Layer Studied by Monte Carlo Simulations and Theories. Journal of Physical Chemistry B, 2004, 108, 16548-16555.	1.2	62
82	Phase separation in mixtures of Yukawa and charged Yukawa particles from Gibbs ensemble Monte Carlo simulations and the mean spherical approximation. Journal of Chemical Physics, 2004, 120, 2846-2850.	1.2	3
83	A systematic Monte Carlo simulation and renormalized perturbation theoretical study of the dielectric constant of the polarizable Stockmayer fluid. Molecular Physics, 2003, 101, 2309-2313.	0.8	9
84	Vapour-liquid equilibrium of the charged Yukawa fluid from Gibbs ensemble Monte Carlo simulations and the mean spherical approximation. Molecular Physics, 2003, 101, 1611-1616.	0.8	15
85	Monte Carlo study of the selectivity of calcium channels: improved geometrical model. Molecular Physics, 2002, 100, 2361-2368.	0.8	43
86	The dielectric constant of polarizable fluids from the renormalized perturbation theory. Molecular Physics, 2002, 100, 3239-3243.	0.8	7
87	The application of density functional theory and the generalized mean spherical approximation to double layers containing strongly coupled ions. Journal of Physics Condensed Matter, 2002, 14, 11945-11954.	0.7	24
88	Computer simulation of the selectivity of a model calcium channel. Journal of Physics Condensed Matter, 2002, 14, 9485-9488.	0.7	2
89	Monte Carlo, density functional theory, and Poissonâ€“Boltzmann theory study of the structure of an electrolyte near an electrode. Journal of Chemical Physics, 2002, 116, 7170-7176.	1.2	139
90	Monte Carlo simulations of ion selectivity in a biological Na channel: Chargeâ€“space competition. Physical Chemistry Chemical Physics, 2002, 4, 5154-5160.	1.3	83

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91	The extrapolation of phase equilibrium curves of mixtures in the isobaricâ€”isothermal Gibbs ensemble. Molecular Physics, 2002, 100, 3429-3441.	0.8	8
92	The extrapolation of the vapourâ€”liquid equilibrium curves of pure fluids in the isothermal Gibbs ensemble. Molecular Physics, 2002, 100, 1989-2000.	0.8	7
93	Simulation of the selectivity of a calcium channel. Applied Surface Science, 2002, 196, 154-156.	3.1	0
94	Computer Simulation Studies of the Selectivity and Conductance of A Model Calcium Channel. Journal of Computational Electronics, 2002, 1, 353-357.	1.3	2
95	Relative permittivity of dipolar liquids and their mixtures. Comparison of theory and experiment. Physical Chemistry Chemical Physics, 2001, 3, 2995-3000.	1.3	27
96	Monte Carlo Study of the Effect of Ion and Channel Size on the Selectivity of a Model Calcium Channelâ€. Journal of Physical Chemistry B, 2001, 105, 11574-11577.	1.2	65
97	A new simulation method for the determination of phase equilibria in mixtures in the grand canonical ensemble. Molecular Physics, 2001, 99, 2011-2022.	0.8	15
98	On the low temperature anomalies in the properties of the electrochemical interface. A non-local free-energy density functional approach. Molecular Physics, 2001, 99, 1323-1328.	0.8	14
99	Density Functional Study of a Simple Membrane Using the Solvent Primitive Model. Journal of Colloid and Interface Science, 2001, 239, 432-439.	5.0	10
100	On the influence of ionic association on the capacitance of an electrical double layer. Chemical Physics Letters, 2001, 341, 363-368.	1.2	69
101	Density Functional Theory and the Capillary Evaporation of a Liquid in a Slit. Journal of Colloid and Interface Science, 2000, 227, 223-226.	5.0	27
102	A corrected 3D Ewald calculation of the low effective temperature properties of the electrochemical interface. Chemical Physics Letters, 2000, 325, 675-677.	1.2	10
103	A generalized mean spherical approximation of the anomalies in the electrochemical double layer for strong ionic interactions. Chemical Physics Letters, 2000, 325, 655-660.	1.2	14
104	Simulation and density functional study of a simple membrane. II. Solvent effects using the solvent primitive model. Journal of Chemical Physics, 2000, 113, 802-806.	1.2	22
105	Structure of charged colloids under a wedge confinement. Physical Review E, 2000, 62, 3875-3881.	0.8	26
106	The capacitance of the solvent primitive model double layer at low effective temperatures. Journal of Chemical Physics, 2000, 112, 8934-8938.	1.2	37
107	A Gibbs ensemble Monte Carlo study of phase coexistence in the solvent primitive model. Journal of Chemical Physics, 2000, 113, 7488-7491.	1.2	16
108	Ions at membranes: a density functional approach. Physical Chemistry Chemical Physics, 2000, 2, 269-276.	1.3	2

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109	Monte Carlo Simulations of the Mechanism for Channel Selectivity:Â The Competition between Volume Exclusion and Charge Neutrality. Journal of Physical Chemistry B, 2000, 104, 8903-8910.	1.2	115
110	Simulation and density functional study of a simple membrane separating two restricted primitive model electrolytes. Journal of Chemical Physics, 1999, 111, 9382-9388.	1.2	41
111	Thermodynamics and structural properties of the dipolar Yukawa fluid. Journal of Chemical Physics, 1999, 111, 337-344.	1.2	32
112	Monte Carlo study of the capacitance of the double layer in a model molten salt. Journal of Chemical Physics, 1999, 110, 5346-5350.	1.2	114
113	The mean spherical approximation for a dipolar Yukawa fluid. Journal of Chemical Physics, 1999, 110, 7348-7353.	1.2	30
114	Low temperature anomalies in the properties of the electrochemical interface. Chemical Physics Letters, 1999, 308, 473-478.	1.2	78
115	Structure and Pressure of a Hard Sphere Fluid in a Wedge-Shaped Cell or Meniscus. Langmuir, 1999, 15, 4311-4313.	1.6	32
116	Monte Carlo simulation of an ion-dipole mixture as a model of an electrical double layer. Journal of Chemical Physics, 1998, 109, 7362-7371.	1.2	140
117	Phase separation in fluid additive hard sphere mixtures?. Molecular Physics, 1998, 95, 131-135.	0.8	21
118	Phase separation in fluid additive hard sphere mixtures?. Molecular Physics, 1998, 95, 131-135.	0.8	6
119	Determination of vapour-liquid equilibrium using cavity-biased grand canonical Monte Carlo method. Molecular Physics, 1997, 92, 1067-1072.	0.8	19
120	Fluidâ€“fluid equilibrium of a mixture of non-polar and dipolar hard spheres in an applied field. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 2709-2714.	1.7	9
121	Vapour-liquid equilibrium of Stockmayer fluids in applied field. Molecular Physics, 1996, 87, 601-624.	0.8	19
122	The isochoric-, isobaric- and saturation-heat capacities of the Lennard-Jones fluid from equations of state and Monte Carlo simulations. Fluid Phase Equilibria, 1996, 119, 1-16.	1.4	18
123	A new simulation method for the determination of the vapour-liquid equilibria in the grand canonical ensemble. Chemical Physics Letters, 1996, 256, 474-482.	1.2	18
124	Vapour-liquid equilibrium of Stockmayer fluids in applied field Application of the NpTE plus test particle method and perturbation theory. Molecular Physics, 1996, 87, 601-624.	0.8	19
125	An extension of the NpT plus test particle method for the determination of the vapour-liquid equilibria of pure fluids. Chemical Physics Letters, 1995, 235, 140-145.	1.2	43
126	The NVT plus test particle method for the determination of the vapour-liquid equilibria of pure fluids. Chemical Physics Letters, 1995, 246, 214-220.	1.2	26

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127	Influence of static electric field on the vapourâ€“liquid coexistence of dipolar soft-sphere fluids. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 889-894.	1.7	22
128	Dielectric constant of a Stockmayer fluid along the vapour-liquid coexistence curve. Molecular Physics, 1995, 85, 429-434.	0.8	22