Amalendu Chandra

List of Publications by Year
in descending order

173 papers	6,484 citations	87723 38 h-index	76769 74 g-index
174 all docs	174 docs citations	174 times ranked	4199 citing authors

#	Article	IF	Citations
1	Effects of Ion Atmosphere on Hydrogen-Bond Dynamics in Aqueous Electrolyte Solutions. Physical Review Letters, 2000, 85, 768-771.	2.9	509
2	Aqueous Basic Solutions: Hydroxide Solvation, Structural Diffusion, and Comparison to the Hydrated Proton. Chemical Reviews, 2010, 110, 2174-2216.	23.0	414
3	Molecular dynamics simulations of aqueous NaCl and KCl solutions: Effects of ion concentration on the single-particle, pair, and collective dynamical properties of ions and water molecules. Journal of Chemical Physics, 2001, 115, 3732-3741.	1.2	301
4	Dielectric Constant of Water Confined in a Nanocavity. Journal of Physical Chemistry B, 2001, 105, 5106-5109.	1.2	264
5	Structure and Dynamics of OH-(aq). Accounts of Chemical Research, 2006, 39, 151-158.	7.6	254
6	Dynamical Behavior of Anionâ^'Water and Waterâ^'Water Hydrogen Bonds in Aqueous Electrolyte Solutions:Â A Molecular Dynamics Study. Journal of Physical Chemistry B, 2003, 107, 3899-3906.	1.2	168
7	Collective Orientational Relaxation in Dense Dipolar Liquids. Advances in Chemical Physics, 2007, , 1-126.	0.3	165
8	Connecting Solvation Shell Structure to Proton Transport Kinetics in Hydrogenâ€“Bonded Networks via Population Correlation Functions. Physical Review Letters, 2007, 99, 145901.	2.9	157
9	Dynamics of Halide Ionâ^'Water Hydrogen Bonds in Aqueous Solutions:Â Dependence on Ion Size and Temperature. Journal of Physical Chemistry B, 2006, 110, 9674-9680.	1.2	156
10	From ab initio quantum chemistry to molecular dynamics: The delicate case of hydrogen bonding in ammonia. Journal of Chemical Physics, 2003, 119, 5965-5980.	1.2	153
11	Structure, Dynamics, and Spectral Diffusion of Water from First-Principles Molecular Dynamics. Journal of Physical Chemistry C, 2014, 118, 29401-29411.	1.5	139
12	Vibrational Spectral Diffusion and Hydrogen Bond Dynamics in Heavy Water from First Principles. Journal of Physical Chemistry A, 2008, 112, 5104-5112.	1.1	129
13	A first principles theoretical study of vibrational spectral diffusion and hydrogen bond dynamics in aqueous ionic solutions: D2O in hydration shells of Clâ^ ions. Journal of Chemical Physics, 2008, 129, 194512.	1.2	102
14	Hydrogen bond dynamics at vapourâ€“water and metalâ€“water interfaces. Chemical Physics Letters, 2004, 386, 218-224.	1.2	99
15	Hydration structure and diffusion of ions in supercooled water: Ion size effects. Journal of Chemical Physics, 2003, 118, 9719-9725.	1.2	95
16	Frequency dependence of ionic conductivity of electrolyte solutions. Journal of Chemical Physics, 2000, 112, 1876-1886.	1.2	92
17	Static dielectric constant of aqueous electrolyte solutions: Is there any dynamic contribution?. Journal of Chemical Physics, 2000, 113, 903-905.	1.2	89
18	Hydrogen bonds in aqueous electrolyte solutions: Statistics and dynamics based on both geometric and energetic criteria. Physical Review E, 2002, 66, 041203.	0.8	85

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19	Microscopic expression for frequency and wave vector dependent dielectric constant of a dipolar liquid. Journal of Chemical Physics, 1989, 90, 1832-1840.	1.2	81
20	Ion conductance in electrolyte solutions. Journal of Chemical Physics, 1999, 110, 10024-10034.	1.2	75
21	A molecular theory of collective orientational relaxation in pure and binary dipolar liquids. Journal of Chemical Physics, 1989, 91, 1829-1842.	1.2	74
22	Polarization relaxation, dielectric dispersion, and solvation dynamics in dense dipolar liquid. Journal of Chemical Physics, 1989, 90, 7338-7345.	1.2	73
23	Beyond the Classical Transport Laws of Electrochemistry:Â New Microscopic Approach to Ionic Conductance and Viscosity. Journal of Physical Chemistry B, 2000, 104, 9067-9080.	1.2	73
24	The role of translational diffusion in the polarization relaxation in dense polar liquids. Chemical Physics Letters, 1988, 151, 47-53.	1.2	70
25	Hydrogen Bond Properties and Dynamics of Liquidâ^'Vapor Interfaces of Aqueous Methanol Solutions. Journal of Chemical Theory and Computation, 2005, 1, 1221-1231.	2.3	70
26	Hydrogen bond and residence dynamics of ionâ€“water and waterâ€“water pairs in supercritical aqueous ionic solutions: Dependence on ion size and density. Journal of Chemical Physics, 2006, 125, 234502.	1.2	70
27	A statistical mechanical theory of proton transport kinetics in hydrogen-bonded networks based on population correlation functions with applications to acids and bases. Journal of Chemical Physics, 2010, 133, 124108.	1.2	69
28	Pressure Effects on the Dynamics and Hydrogen Bond Properties of Aqueous Electrolyte Solutions:â€‰ The Role of Ion Screening. Journal of Physical Chemistry B, 2002, 106, 6779-6783.	1.2	66
29	Ionic contribution to the viscosity of dilute electrolyte solutions: Towards a microscopic theory. Journal of Chemical Physics, 2000, 113, 3226-3232.	1.2	64
30	Liquid-vapor interfaces of water-acetonitrile mixtures of varying composition. Journal of Chemical Physics, 2005, 123, 184706.	1.2	64
31	Ab initio and classical molecular dynamics studies of the structural and dynamical behavior of water near a hydrophobic graphene sheet. Journal of Chemical Physics, 2013, 138, 204702.	1.2	64
32	Molecular dynamics simulations of simple dipolar liquids in spherical cavity: Effects of confinement on structural, dielectric, and dynamical properties. Journal of Chemical Physics, 1999, 111, 1223-1230.	1.2	59
33	Dynamics of water molecules at liquidâ€“vapour interfaces of aqueous ionic solutions: effects of ion concentration. Chemical Physics Letters, 2003, 373, 87-93.	1.2	54
34	Relationship between microscopic and macroscopic orientational relaxation times in polar liquids. The Journal of Physical Chemistry, 1990, 94, 3152-3156.	2.9	47
35	Dynamical properties of the soft sticky dipole model of water: Molecular dynamics simulations. Journal of Chemical Physics, 1999, 111, 2701-2709.	1.2	47
36	Exotic dielectric behavior of polar liquids. Journal of Chemical Physics, 1989, 91, 3056-3060.	1.2	45

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37	Ion solvation dynamics in binary dipolar liquids: theoretical and simulation results for mixtures of Stockmayer liquids. Chemical Physics Letters, 1995, 235, 133-139.	1.2	41
38	Liquid-vapor interfacial properties of water-ammonia mixtures: Dependence on ammonia concentration. Journal of Chemical Physics, 2005, 123, 174712.	1.2	39
39	A first principles simulation study of fluctuations of hydrogen bonds and vibrational frequencies of water at liquidâ€“vapor interface. Chemical Physics, 2012, 392, 96-104.	0.9	39
40	Solvation of an ion and of a dipole in a dipolar liquid: How different are the dynamics?. Chemical Physics Letters, 1989, 155, 533-538.	1.2	38
41	Hydrogen bonded structure and dynamics of liquid-vapor interface of water-ammonia mixture: An ab initio molecular dynamics study. Journal of Chemical Physics, 2011, 135, 114510.	1.2	38
42	Hydroxide Ion Can Move Faster Than an Excess Proton through One-Dimensional Water Chains in Hydrophobic Narrow Pores. Journal of Physical Chemistry B, 2012, 116, 9744-9757.	1.2	37
43	Water in Hydration Shell of an Iodide Ion: Structure and Dynamics of Solute-Water Hydrogen Bonds and Vibrational Spectral Diffusion from First-Principles Simulations. Journal of Physical Chemistry B, 2015, 119, 8561-8572.	1.2	36
44	Vibrational Spectral Diffusion in Supercritical D₂O from First Principles: An Interplay between the Dynamics of Hydrogen Bonds, Dangling OD Groups, and Inertial Rotation. Journal of Physical Chemistry A, 2008, 112, 13518-13527.	1.1	35
45	A temperature of maximum density in soft sticky dipole water. Chemical Physics Letters, 2003, 376, 646-652.	1.2	34
46	Structural and Dynamical Nature of Hydration Shells of the Carbonate Ion in Water: An Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry B, 2018, 122, 1495-1504.	1.2	34
47	Tracer diffusion of ionic and hydrophobic solutes in waterâ€“dimethyl sulfoxide mixtures: Effects of varying composition. Journal of Chemical Physics, 2003, 119, 4360-4366.	1.2	33
48	Filled and empty states of carbon nanotubes in water: Dependence on nanotube diameter, wall thickness and dispersion interactions. Journal of Chemical Sciences, 2007, 119, 367-376.	0.7	33
49	A First-Principles Molecular Dynamics Study of the Solvation Shell Structure, Vibrational Spectra, Polarity, and Dynamics around a Nitrate Ion in Aqueous Solution. Journal of Physical Chemistry B, 2017, 121, 9032-9044.	1.2	32
50	First-Principles Simulation Study of Vibrational Spectral Diffusion and Hydrogen Bond Fluctuations in Aqueous Solution of N-Methylacetamide. Journal of Physical Chemistry B, 2015, 119, 9858-9867.	1.2	31
51	Breakdown of Onsagerâ€™s conjecture on distance dependent polarization relaxation in solvation dynamics. Journal of Chemical Physics, 1989, 91, 2594-2598.	1.2	30
52	Molecular Origin of the Debyeâ€'Huckelâ€'Onsager Limiting Law of Ion Conductance and Its Extension to High Concentrations:Â Mode Coupling Theory Approach to Electrolyte Friction. Journal of the American Chemical Society, 1999, 121, 4082-4083.	6.6	29
53	Effects of hydrogen-bond environment on single particle and pair dynamics in liquid water. Journal of Chemical Sciences, 2001, 113, 591-601.	0.7	28
54	Dynamics of ionic and hydrophobic solutes in water-methanol mixtures of varying composition. Journal of Chemical Physics, 2005, 123, 234501.	1.2	28

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55	Hydration structure and dynamics of a hydroxide ion in water clusters of varying size and temperature: Quantum chemical and ab initio molecular dynamics studies. Chemical Physics, 2012, 400, 154-164.	0.9	27
56	Microscopic study of inertial and viscoelastic effects in dipolar solvation dynamics. Journal of Chemical Physics, 1993, 99, 553-562.	1.2	26
57	Solute size effects on the solvation structure and diffusion of ions in liquid methanol under normal and cold conditions. Journal of Chemical Physics, 2006, 124, 084507.	1.2	26
58	A first-principles theoretical study of hydrogen-bond dynamics and vibrational spectral diffusion in aqueous ionic solution: Water in the hydration shell of a fluoride ion. Pure and Applied Chemistry, 2012, 85, 27-40.	0.9	26
59	Pressure effects on the tracer diffusion and orientational relaxation of hydrogen bonding solutes in ambient and supercooled water. Chemical Physics Letters, 2003, 373, 79-86.	1.2	25
60	Dynamics of polar solvation: Route to single exponential relaxation via translational diffusion. Proceedings of the Indian Academy of Sciences - Section A, 1988, 100, 353-357.	0.2	25
61	An analysis of voids and necks in supercritical water. Journal of Molecular Liquids, 2011, 163, 1-6.	2.3	24
62	A Hybrid QM/MM Simulation Study of Intramolecular Proton Transfer in the Pyridoxal 5â€²-Phosphate in the Active Site of Transaminase: Influence of Active Site Interaction on Proton Transfer. Journal of Physical Chemistry B, 2014, 118, 11077-11089.	1.2	24
63	Ultrafast Vibrational Echo Spectroscopy of Liquid Water from First-Principles Simulations. Journal of Physical Chemistry B, 2015, 119, 11215-11228.	1.2	24
64	Dynamics of ion solvation in electrolyte solutions: dependence on salt concentration. Chemical Physics Letters, 1995, 244, 314-320.	1.2	22
65	Preferential solvation, ion pairing, and dynamics of concentrated aqueous solutions of divalent metal nitrate salts. Journal of Chemical Physics, 2017, 147, 244503.	1.2	22
66	Nonideality in diffusion of ionic and hydrophobic solutes and pair dynamics in water-acetone mixtures of varying composition. Journal of Chemical Physics, 2007, 127, 024503.	1.2	21
67	Transimination Reaction at the Active Site of Aspartate Aminotransferase: A Proton Hopping Mechanism through Pyridoxal 5â€²-Phosphate. ACS Catalysis, 2019, 9, 6276-6283.	5.5	21
68	Molecular relaxation in simple dipolar liquids confined between two solid surfaces. Chemical Physics, 1998, 231, 65-80.	0.9	20
69	Creating Interfaces by Stretching the Solvent Is Key to Metallic Ammonia Solutions. Angewandte Chemie - International Edition, 2007, 46, 3676-3679.	7.2	20
70	An ab initio molecular dynamics study of the frequency dependence of rotational motion in liquid water. Journal of Molecular Liquids, 2008, 143, 31-34.	2.3	20
71	Hydrogen bond dynamics and vibrational spectral diffusion in aqueous solution of acetone: A first principles molecular dynamics study#. Journal of Chemical Sciences, 2012, 124, 215-221.	0.7	20
72	Wetting and dewetting of narrow hydrophobic channels by orthogonal electric fields: Structure, free energy, and dynamics for different water models. Journal of Chemical Physics, 2015, 143, 224708.	1.2	20

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73	Proton transfer through hydrogen bonds in two-dimensional water layers: A theoretical study based on ab initio and quantum-classical simulations. Journal of Chemical Physics, 2015, 142, 044701.	1.2	20
74	Anisotropic structure and dynamics of the solvation shell of a benzene solute in liquid water from ab initio molecular dynamics simulations. Physical Chemistry Chemical Physics, 2016, 18, 6132-6145.	1.3	20
75	An interpretation of the bifurcation of orientational relaxation processes in a supercooled liquid. Journal of Chemical Physics, 1990, 93, 8991-9001.	1.2	19
76	Binding of hydrogen bonding solutes at liquidâ€“vapour interfaces of molecular fluids. Chemical Physics Letters, 2004, 400, 515-519.	1.2	19
77	A first principles theoretical study of the hydration structure and dynamics of an excess proton in water clusters of varying size and temperature. Chemical Physics, 2011, 387, 92-102.	0.9	19
78	Diffusion of ions in supercritical water: Dependence on ion size and solvent density and roles of voids and necks. Journal of Molecular Liquids, 2011, 162, 12-19.	2.3	19
79	A first principles simulation study of vibrational spectral diffusion in aqueous NaBr solutions: Dynamics of water in ion hydration shells. Chemical Physics, 2013, 412, 13-21.	0.9	18
80	Exploring the structure and dynamics of nano-confined water molecules using molecular dynamics simulations. Molecular Simulation, 2015, 41, 463-470.	0.9	18
81	Microscopic free energy functional for polarization fluctuations: Generalization of Marcusâ€“Felderhof expression. Journal of Chemical Physics, 1991, 94, 2258-2261.	1.2	17
82	A first principles molecular dynamics study of lithium atom solvation in binary liquid mixture of water and ammonia: Structural, electronic, and dynamical properties. Journal of Chemical Physics, 2011, 134, 024519.	1.2	17
83	Dynamics of electrolyte solutions at finite wave vectors: Theoretical results for ions in a molecular solvent. Journal of Chemical Physics, 1997, 106, 2360-2371.	1.2	16
84	An ab initio molecular dynamics study of supercritical aqueous ionic solutions: Hydrogen bonding, rotational dynamics and vibrational spectral diffusion. Chemical Physics, 2011, 387, 48-55.	0.9	16
85	A first principles molecular dynamics study of vibrational spectral diffusion and hydrogen bond dynamics in liquid methanol. Chemical Physics, 2012, 408, 36-42.	0.9	16
86	Spatial and Orientational Structure of the Hydration Shell of Benzene in Sub- and Supercritical Water. Journal of Physical Chemistry B, 2015, 119, 8600-8612.	1.2	16
87	Ab Initio Molecular Dynamics Simulation of the Phosphate Ion in Water: Insights into Solvation Shell Structure, Dynamics, and Kosmotropic Activity. Journal of Physical Chemistry B, 2017, 121, 10519-10529.	1.2	16
88	Effects of tert-Butyl Alcohol on Water at the Liquidâ€“Vapor Interface: Structurally Bulk-like but Dynamically Slow Interfacial Water. Journal of Physical Chemistry C, 2018, 122, 9374-9388.	1.5	16
89	Effects of Boron Nitride Nanotube on the Secondary Structure of AÎ²(1â€“42) Trimer: Possible Inhibitory Effect on Amyloid Formation. Journal of Physical Chemistry B, 2020, 124, 1928-1940.	1.2	16
90	An ab initio molecular dynamics study of diffusion, orientational relaxation and hydrogen bond dynamics in acetoneâ€“water mixtures. Journal of Molecular Liquids, 2012, 165, 1-6.	2.3	15

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91	Dynamics of hydrogen bonds and vibrational spectral diffusion in liquid methanol from first principles simulations with dispersion corrected density functional. Chemical Physics, 2013, 415, 1-7.	0.9	15
92	Urea in Water: Structure, Dynamics, and Vibrational Echo Spectroscopy from First-Principles Simulations. Journal of Physical Chemistry B, 2019, 123, 3325-3336.	1.2	15
93	Water in Confinement between Nanowalls: Results for Hexagonal Boron Nitride versus Graphene Sheets from Ab Initio Molecular Dynamics. Journal of Physical Chemistry C, 2019, 123, 6130-6140.	1.5	15
94	Collective orientational relaxation in a dense liquid of ellipsoidal molecules. Physica A: Statistical Mechanics and Its Applications, 1990, 169, 246-262.	1.2	14
95	A molecular theory of frequency and waveâ€vectorâ€dependent dynamic response functions of electrolyte solutions. Journal of Chemical Physics, 1996, 104, 8662-8670.	1.2	14
96	Excess Electron and Lithium Atom Solvation in Water Clusters at Finite Temperature: An ab Initio Molecular Dynamics Study of the Structural, Spectral, and Dynamical Behavior of (H2O)6â^'and Li(H2O)6. Journal of Physical Chemistry A, 2010, 114, 11869-11878.	1.1	14
97	All-Atom Simulations of Human ACE2-Spike Protein RBD Complexes for SARS-CoV-2 and Some of its Variants: Nature of Interactions and Free Energy Diagrams for Dissociation of the Protein Complexes. Journal of Physical Chemistry B, 2022, 126, 5375-5389.	1.2	14
98	Force constants of solvent polarization fluctuations: Softening at intermediate wave vectors. Journal of Chemical Physics, 1989, 91, 7181-7186.	1.2	13
99	Molecular Dynamics Study of the Liquidâ^'Vapor Interface of Acetonitrile:Â Equilibrium and Dynamical Properties. Journal of Physical Chemistry B, 2005, 109, 20558-20564.	1.2	13
100	Electron solvation in water-ammonia mixed clusters: Structure, energetics, and the nature of localization states of the excess electron. Journal of Chemical Physics, 2007, 126, 234510.	1.2	13
101	Dynamics of supercritical methanol of varying density from first principles simulations: Hydrogen bond fluctuations, vibrational spectral diffusion, and orientational relaxation. Journal of Chemical Physics, 2013, 138, 224501.	1.2	13
102	Orientational order and dynamics of interfacial water near a hexagonal boron-nitride sheet: An ab initio molecular dynamics study. Journal of Chemical Physics, 2017, 147, 164704.	1.2	13
103	Relationship between energy gap time correlation and fluorescence stokes shift correlation functions in solvation dynamics. Chemical Physics Letters, 1990, 165, 93-99.	1.2	12
104	Liquidâ^'Vapor Interfaces of Simple Electrolyte Solutions:Â Molecular Dynamics Results for Ions in Stockmayer Fluids. Journal of Physical Chemistry B, 2003, 107, 12705-12712.	1.2	12
105	Vibrational echo spectral observables and frequency fluctuations of hydration shell water around a fluoride ion from first principles simulations. Journal of Chemical Sciences, 2017, 129, 1069-1080.	0.7	12
106	Free energy landscapes of prototropic tautomerism in pyridoxal 5â€²â€phosphate schiff bases at the active site of an enzyme in aqueous medium. Journal of Computational Chemistry, 2018, 39, 1629-1638.	1.5	12
107	Computer simulations of dipolar liquids near charged solid surfaces: electric-field-induced modifications of structure and dynamics of interfacial solvent. Computational and Theoretical Chemistry, 1998, 455, 1-8.	1.5	11
108	A theoretical study of outersphere electron transfer reactions in electrolyte solutions. Journal of Chemical Physics, 1999, 110, 1569-1580.	1.2	11

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109	Pressure effects on diffusion in liquid ammonia : A simulation study using a combination of isobaric-isothermal and microcanonical molecular dynamics. Indian Journal of Physics, 2009, 83, 91-100.	0.9	11
110	Solvation structure of nanoscopic hydrophobic solutes in supercritical water: Results for varying thickness of hydrophobic walls, soluteâ€“solvent interaction and solvent density. Chemical Physics, 2012, 408, 28-35.	0.9	11
111	Bornâ€“Oppenheimer Molecular Dynamics Simulations of a Bromate Ion in Water Reveal Its Dual Kosmotropic and Chaotropic Behavior. Journal of Physical Chemistry B, 2018, 122, 2090-2101.	1.2	11
112	Solvation Shell of the Nitrite Ion in Water: An Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry B, 2020, 124, 7194-7204.	1.2	11
113	Dielectric relaxation of binary dipolar liquids. Chemical Physics, 1995, 195, 93-105.	0.9	10
114	Single particle and pair dynamics in waterâ€“formic acid mixtures containing ionic and neutral solutes: Nonideality in dynamical properties. Journal of Chemical Physics, 2008, 128, 184506.	1.2	10
115	Hydrogen bonded structure, polarity, molecular motion and frequency fluctuations at liquid-vapor interface of a water-methanol mixture: An ab initio molecular dynamics study. Journal of Chemical Physics, 2014, 141, 134703.	1.2	10
116	An ab initio molecular dynamics study of the liquid-vapor interface of an aqueous NaCl solution: Inhomogeneous density, polarity, hydrogen bonds, and frequency fluctuations of interfacial molecules. Journal of Chemical Physics, 2014, 141, 194705.	1.2	10
117	Nature of hydration shells of a polyoxyâ€anion with a large cationic centre: The case of iodate ion in water. Journal of Computational Chemistry, 2018, 39, 1226-1235.	1.5	10
118	Temperature dependence of the ultrafast vibrational echo spectroscopy of OD modes in liquid water from first principles simulations. Physical Chemistry Chemical Physics, 2019, 21, 6485-6498.	1.3	10
119	Structure, Dynamics, and the Free Energy of Solute Adsorption at Liquidâ^'Vapor Interfaces of Simple Dipolar Systems:â€‰ Molecular Dynamics Results for Pure and Mixed Stockmayer Fluids. Journal of Physical Chemistry B, 2007, 111, 12500-12507.	1.2	9
120	Microscopic solvation of a lithium atom in water-ammonia mixed clusters: Solvent coordination and electron localization in presence of a counterion. Journal of Chemical Physics, 2008, 129, 024511.	1.2	9
121	SINGLE-PARTICLE AND PAIR DYNAMICAL PROPERTIES OF ACETONEâ€“METHANOL MIXTURES CONTAINING CHARGED AND NEUTRAL SOLUTES: A MOLECULAR DYNAMICS STUDY. Journal of Theoretical and Computational Chemistry, 2011, 10, 261-278.	1.8	9
122	Water under Supercritical Conditions: Hydrogen Bonds, Polarity, and Vibrational Frequency Fluctuations from Ab Initio Simulations with a Dispersion Corrected Density Functional. ACS Omega, 2018, 3, 3453-3462.	1.6	9
123	Structure and dynamics of mixed dipolar liquids near solid surfaces: a molecular dynamics simulation study. Chemical Physics, 1999, 242, 353-366.	0.9	8
124	A first principles molecular dynamics study of the solvation structure and migration kinetics of an excess proton and a hydroxide ion in binary water-ammonia mixtures. Journal of Chemical Physics, 2012, 136, 114509.	1.2	8
125	Voids and necks in liquid ammonia and their roles in diffusion of ions of varying size. Journal of Computational Chemistry, 2012, 33, 843-852.	1.5	8
126	Effects of dispersion interaction on vibrational spectral diffusion in aqueous NaBr solutions: An ab initio molecular dynamics study. Chemical Physics, 2015, 448, 1-8.	0.9	8

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127	Infrared Spectral and Dynamical Properties of Water Confined in Nanobubbles at Hybrid Interfaces of Diamond and Graphene: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2017, 121, 23455-23462.	1.5	8
128	Interactions of the AÎ²(1â€“42) Peptide with Boron Nitride Nanoparticles of Varying Curvature in an Aqueous Medium: Different Pathways to Inhibit Î²-Sheet Formation. Journal of Physical Chemistry B, 2021, 125, 11159-11178.	1.2	8
129	Electron transfer reactions in electrolyte solutions: effects of ion atmosphere and solvent relaxation. Chemical Physics Letters, 1996, 253, 456-462.	1.2	7
130	Solvation of fullerene and fulleride ion in liquid ammonia: Structure and dynamics of the solvation shells. Journal of Chemical Physics, 2012, 137, 134501.	1.2	7
131	Two-Dimensional Infrared Spectroscopy of Aqueous Solutions of Metal Nitrates: Slowdown of Spectral Diffusion in the Presence of Divalent Cations. Journal of Physical Chemistry B, 2020, 124, 7391-7404.	1.2	7
132	Electrolyte dynamics effect on adiabatic outersphere electron transfer reactions. Computational and Theoretical Chemistry, 1996, 361, 123-134.	1.5	6
133	Rotational dielectric friction and molecular relaxation at metal-solvent interfaces. Journal of Molecular Liquids, 1998, 77, 77-93.	2.3	6
134	An ab initio molecular dynamics study of benzene in water at supercritical conditions: Structure, dynamics, and polarity of hydration shell water and the solute. Journal of Chemical Physics, 2019, 151, 044508.	1.2	6
135	A <scp>QM</scp>/<scp>MM</scp> simulation study of transamination reaction at the active site of aspartate aminotransferase: Free energy landscape and proton transfer pathways. Journal of Computational Chemistry, 2020, 41, 2684-2694.	1.5	6
136	Transport of hydrated nitrate and nitrite ions through graphene nanopores in aqueous medium. Journal of Computational Chemistry, 2020, 41, 1850-1858.	1.5	6
137	Effects of stearyl alcohol monolayer on the structure, dynamics and vibrational sum frequency generation spectroscopy of interfacial water. Physical Chemistry Chemical Physics, 2022, 24, 7374-7386.	1.3	6
138	Surface charge induced modifications of the structure and dynamics of mixed dipolar liquids at solidâ€“liquid interfaces: A molecular dynamics simulation study. Journal of Chemical Physics, 2000, 113, 8817-8826.	1.2	5
139	Structure of a mixed dipolar liquid near a metal surface: A combined approach of weighted density and perturbative approximations. Physical Review E, 2000, 62, 1017-1024.	0.8	5
140	Hydration and translocation of an excess proton in water clusters: Anab initio molecular dynamics study. Pramana - Journal of Physics, 2005, 65, 763-768.	0.9	5
141	Water structure near single and multi-layer nanoscopic hydrophobic plates of varying separation and interaction potentials. Bulletin of Materials Science, 2008, 31, 525-532.	0.8	5
142	Structural, single-particle and pair dynamical properties of acetoneâ€“chloroform mixtures with dissolved solutes. Chemical Physics, 2011, 383, 41-49.	0.9	5
143	Ab initio molecular dynamics studies of hydrogen bonded structure, molecular motion, and frequency fluctuations of water in the vicinity of azide ions. Journal of Chemical Physics, 2015, 142, 164505.	1.2	5
144	Wetting behavior of nonpolar nanotubes in simple dipolar liquids for varying nanotube diameter and solute-solvent interactions. Journal of Chemical Physics, 2015, 142, 034704.	1.2	5

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145	Dynamics of water in conical solvation shells around a benzene solute under different thermodynamic conditions. Physical Chemistry Chemical Physics, 2018, 20, 18328-18339.	1.3	5
146	Ab Initio Molecular Dynamics Study of Aqueous Solutions of Magnesium and Calcium Nitrates: Hydration Shell Structure, Dynamics and Vibrational Echo Spectroscopy. Journal of Physical Chemistry B, 2022, 126, 528-544.	1.2	5
147	Microscopic expression for time-dependent solvation energy of ions and dipoles in dense polar liquids. Proceedings of the Indian Academy of Sciences - Section A, 1989, 101, 83-88.	0.2	5
148	Solvent effects on outersphere electron transfer reactions in mixed dipolar liquids. Chemical Physics, 1998, 238, 285-300.	0.9	4
149	Nonlinear theory of metal-solvent interface using the density functional approach. Physical Review E, 1999, 59, 3140-3146.	0.8	4
150	Dynamics of polarization relaxation in a dipolar mixture at a solidâ€“liquid interface. Journal of Chemical Physics, 2000, 113, 377-384.	1.2	4
151	Interfacial structure of a mixed dipolar liquid in contact with a charged solid surface. Journal of Chemical Physics, 2000, 112, 10467-10475.	1.2	4
152	Nonideality in diffusion of ionic and neutral solutes and hydrogen bond dynamics in dimethyl sulfoxideâ€“chloroform mixtures of varying composition. Journal of Computational Chemistry, 2011, 32, 2679-2689.	1.5	4
153	Structure and Dynamics of the Liquidâ€“Liquid Interface of an Aqueous NaCl Solution with Liquid Carbon Tetrachloride from First-Principles Simulations. Journal of Physical Chemistry C, 2014, 118, 23083-23091.	1.5	4
154	Effects of dispersion interactions on the structure, polarity, and dynamics of liquid-vapor interface of an aqueous NaCl solution: Results of first principles simulations at room temperature. Journal of Chemical Physics, 2018, 148, 024702.	1.2	4
155	Dynamics of vibrational spectral diffusion in water: Effects of dispersion interactions, temperature, density, system size and fictitious orbital mass. Journal of Molecular Liquids, 2018, 249, 169-178.	2.3	4
156	On the issue of closed versus open forms of gamma-aminobutyric acid (GABA) in water: Ab initio molecular dynamics and metadynamics studies. Journal of Chemical Physics, 2018, 148, 194503.	1.2	4
157	Dynamics of ion atmosphere relaxation around a newly created dipolar solute. Chemical Physics, 1996, 208, 1-7.	0.9	3
158	Effects of ion atmosphere relaxation on dipole isomerization reactions in electrolyte solutions. Computational and Theoretical Chemistry, 1998, 422, 49-55.	1.5	3
159	Structure and dynamics of water at liquidâ€“vapour interfaces covered by surfactant monolayers of neutral stearic acid and charged stearate ions. Journal of Molecular Liquids, 2008, 140, 33-38.	2.3	3
160	A first principles molecular dynamics study of excess electron and lithium atom solvation in waterâ€“ammonia mixed clusters: Structural, spectral, and dynamical behaviors of [(H $_2$2O) $_5$5NH $_3]^-$3]â^' and Li(H $_2$2O) $_5$5NH $_3$3 at finite temperature. Journal of Chemical Physics, 2011, 134, 034302.	1.2	3
161	Frequency dependence of the reorientational motion of OD bonds of deuterated methanol in liquid phase: A first principles molecular dynamics study. Journal of Molecular Liquids, 2013, 182, 43-47.	2.3	3
162	Solvation of narrow pores of graphene-like plates in simple dipolar liquids: Wetting and dewetting behavior and solvent dynamics for varying pore width and soluteâ€“solvent interaction. Chemical Physics, 2015, 457, 78-86.	0.9	3

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