Bhabani S Mallik

List of Publications by Year
in descending order

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99	1,410	394421 19	414414 32
papers	citations	h-index	g-index

100	100	100	859
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Vibrational Spectral Diffusion and Hydrogen Bond Dynamics in Heavy Water from First Principles. Journal of Physical Chemistry A, 2008, 112, 5104-5112.	2.5	129
2	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.	3.0	102
3	A 118 nm vacuum ultraviolet laser/time-of-flight mass spectroscopic study of methanol and ethanol clusters in the vapor phase. Journal of Chemical Physics, 2002, 116, 6990-6999.	3.0	78
4	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.	3.0	70
5	Iron promoted C3â€“H nitration of 2H-indazole: direct access to 3-nitro-2H-indazoles. Organic and Biomolecular Chemistry, 2018, 16, 5113-5118.	2.8	41
6	Thermodynamic, Structural and Transport Properties of Tetramethyl Ammonium Fluoride: First Principles Molecular Dynamics Simulations of an Unusual Ionic Liquid. Journal of Physical Chemistry B, 2010, 114, 12577-12584.	2.6	37
7	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.	2.5	35
8	Hydroboration, Cyanosilylation, and Sequential Cyanosilylation and Hydroboration of Carbonyl Compounds in the Presence of a Ti^{IV} Amido Complex as an Efficient Catalyst. European Journal of Organic Chemistry, 2018, 2018, 3180-3192.	2.4	32
9	Solubility and solvation free energy of a cardiovascular drug, LASSBio-294, in ionic liquids: A computational study. Journal of Molecular Liquids, 2020, 301, 112449.	4.9	32
10	Protic ammonium carboxylate ionic liquids: insight into structure, dynamics and thermophysical properties by alkyl group functionalization. Physical Chemistry Chemical Physics, 2017, 19, 10358-10370.	2.8	31
11	Structure and Dynamics of Hydroxyl-Functionalized Protic Ammonium Carboxylate Ionic Liquids. Journal of Physical Chemistry A, 2017, 121, 8097-8107.	2.5	28
12	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.	1.9	26
13	Dynamics and Spectral Response of Water Molecules around Tetramethylammonium Cation. Journal of Physical Chemistry B, 2019, 123, 8753-8766.	2.6	24
14	Interstitial Voids and Resultant Density of Liquid Water: A First-Principles Molecular Dynamics Study. ACS Omega, 2018, 3, 2010-2017.	3.5	23
15	Heterogeneity in the microstructure and dynamics of tetraalkylammonium hydroxide ionic liquids: insight from classical molecular dynamics simulations and Voronoi tessellation analysis. Physical Chemistry Chemical Physics, 2020, 22, 3466-3480.	2.8	22
16	Aqueous solvation of an amide molecule from first principles molecular simulations: Structure, hydrogen bond dynamics and spectral signature. Journal of Molecular Liquids, 2015, 212, 941-946.	4.9	21
17	Novelty of Lithium Salt Solution in Sulfone and Dimethyl Carbonate-Based Electrolytes for Lithium-Ion Batteries: A Classical Molecular Dynamics Simulation Study of Optimal Ion Diffusion. Journal of Physical Chemistry C, 2018, 122, 26315-26325.	3.1	21
18	An ab initio molecular dynamics study of the frequency dependence of rotational motion in liquid water. Journal of Molecular Liquids, 2008, 143, 31-34.	4.9	20

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19	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.	1.5	20
20	Ultrafast Vibrational Spectroscopy of Aqueous Solution of Methylamine from First Principles MD Simulations. ChemistrySelect, 2017, 2, 74-83.	1.5	20
21	Structural and Thermophysical Anomalies of Liquid Water: A Tale of Molecules in the Instantaneous Low- and High-Density Regions. Journal of Physical Chemistry B, 2020, 124, 1071-1081.	2.6	20
22	Structure and stretching dynamics of water molecules around an amphiphilic amide from FPMD simulations: A case study of N,N-dimethylformamide. Journal of Molecular Liquids, 2020, 302, 112524.	4.9	20
23	Effects of Temperature on the Structure and Dynamics of Aqueous Mixtures ofN,N-Dimethylformamide. Journal of Chemical & Engineering Data, 2014, 59, 3250-3257.	1.9	19
24	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.	1.9	18
25	Alkali Metal and Alkaline Earth Metal Complexes with the Bis(boraneâ€diphenylphosphanyl)amido Ligand â€“ Synthesis, Structures, and Catalysis for Ringâ€Opening Polymerization of Ïµâ€Caprolactone. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2016, 642, 118-127.	1.2	18
26	Ionic conductance and viscous drag in water-in-salt electrolytes for lithium and sodium ion batteries and supercapacitors. Materials Today Communications, 2020, 25, 101588.	1.9	18
27	Time-dependent vibrational spectral analysis of first principles trajectory of methylamine with wavelet transform. Physical Chemistry Chemical Physics, 2017, 19, 9912-9922.	2.8	17
28	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.	1.9	16
29	Iron Complex as a Water-Oxidizing Catalyst: Free-Energy Barriers, Proton-Coupled Electron Transfer, Spin Dynamics, and Role of Water Molecules in the Reaction Mechanism. Journal of Physical Chemistry C, 2020, 124, 205-218.	3.1	15
30	Effects of Doped N, B, P, and S Atoms on Graphene toward Oxygen Evolution Reactions. ACS Omega, 2021, 6, 5368-5378.	3.5	15
31	Understanding the solubility of triamino-trinitrobenzene in hydrous tetramethylammonium fluoride: a first principles molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2012, 14, 4884.	2.8	14
32	Biosolvation Nature of Ionic Liquids: Molecular Dynamics Simulation of Methylated Nucleobases in Hydrated 1-Ethyl-3-methylimidazolium Acetate. ACS Omega, 2018, 3, 8344-8354.	3.5	14
33	Reaction Mechanism and Free Energy Barriers for the Chemisorption of CO₂ by Ionic Entities. Journal of Physical Chemistry A, 2020, 124, 836-848.	2.5	14
34	Heavier group 2 metal complexes with a flexible scorpionate ligand based on 2-mercaptopyridine. RSC Advances, 2015, 5, 51413-51420.	3.6	12
35	Ultrafast Aqueous Dynamics in Concentrated Electrolytic Solutions of Lithium Salt and Ionic Liquid. Journal of Physical Chemistry B, 2020, 124, 9898-9912.	2.6	12
36	Distinctive behavior and two-dimensional vibrational dynamics of water molecules inside glycine solvation shell. RSC Advances, 2020, 10, 6658-6670.	3.6	12

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37	A simple removable aliphatic nitrile template 2-cyano-2,2-di-isobutyl acetic acid for remote meta-selective Câ€“H functionalization. Organic Chemistry Frontiers, 2021, 8, 1959-1969.	4.5	12
38	Ionic Dynamics of Hydroxylammonium Ionic Liquids: A Classical Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2020, 124, 4960-4974.	2.6	11
39	Dynamics of Ionic Liquid through Intrinsic Vibrational Probes Using the Dispersion-Corrected DFT Functionals. Journal of Physical Chemistry B, 2021, 125, 6994-7008.	2.6	11
40	Proton transfer from water to anion: Free energy profile from first principles metadynamics simulations. Journal of Molecular Liquids, 2016, 219, 810-814.	4.9	10
41	Revisiting LiClO4 as an electrolyte for Li-ion battery: Effect of aggregation behavior on ion-pairing dynamics and conductance. Journal of Molecular Liquids, 2020, 302, 112536.	4.9	10
42	Conformation-induced vibrational spectral dynamics of hydrogen peroxide and vicinal water molecules. Physical Chemistry Chemical Physics, 2021, 23, 6665-6676.	2.8	10
43	N- versus P-co-ordination for Nâ€“B and Pâ€“B bonded BH3 adducts for various phosphinamine ligands â€“ An experimental and computational study. Journal of Molecular Structure, 2013, 1047, 302-309.	3.6	9
44	Proton transfer from water to ketyl radical anion: Assessment of critical size of hydrated cluster and free energy barrier in solution from first principles simulations. Chemical Physics, 2016, 477, 46-51.	1.9	9
45	Solvation Structure and Dynamics of Alkali Metal Halides in an Ionic Liquid from Classical Molecular Dynamics Simulations. ACS Omega, 2019, 4, 19556-19564.	3.5	9
46	Conformational dynamics of aqueous hydrogen peroxide from first principles molecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 28286-28296.	2.8	9
47	Detailed characterization of dioxouranium(vi) complexes with a symmetrical tetradentate N2O2-benzil bis(isonicotinoyl hydrazone) ligand. Dalton Transactions, 2020, 49, 10603-10612.	3.3	9
48	Connecting Correlated and Uncorrelated Transport to Dynamics of Ionic Interactions in Cyclic Ammonium-Based Ionic Liquids. Journal of Physical Chemistry B, 2020, 124, 6813-6824.	2.6	9
49	Unprecedented Calcium Metallaâ€macrocycle Having Phosphinoselenoic Amide and Diphenylphosphinate in the Coordination Sphere. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2014, 640, 994-999.	1.2	8
50	Functionalisation of Imidazolin-2-imine to Corresponding Phosphinamine, Chalcogenide (O, S, Se, Te), and Borane Compounds. Australian Journal of Chemistry, 2015, 68, 127.	0.9	8
51	A delicate case of unidirectional proton transfer from water to an aromatic heterocyclic anion. Physical Chemistry Chemical Physics, 2016, 18, 29979-29986.	2.8	8
52	Mechanism and Electronic Perspective of Oxygen Evolution Reactions Catalyzed by [Fe(OTf)2(bpbp)]. Journal of Physical Chemistry C, 2021, 125, 1313-1322.	3.1	8
53	Association of Nucleobases in Hydrated Ionic Liquid from Biased Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2018, 122, 9635-9645.	2.6	7
54	Nanostructure domains, voids, and low-frequency spectra in binary mixtures of N,N-dimethylacetamide and ionic liquids with varying cationic size. RSC Advances, 2020, 10, 1811-1827.	3.6	7

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55	Hydrogen Bond Kinetics, Ionic Dynamics, and Voids in the Binary Mixtures of Protic Ionic Liquids with Alkanolamines. Journal of Physical Chemistry B, 2021, 125, 5587-5600.	2.6	7
56	Understanding the role of fluorination in the mechanistic nature of the water splitting process catalyzed by cobalt tris-(2-pyridylmethyl)amine complexes. Sustainable Energy and Fuels, 2021, 5, 2313-2324.	4.9	7
57	Revisiting OD-stretching dynamics of methanolâ€'d4, ethanol-d6 and dilute HOD/H2O mixture with predefined potentials and wavelet transform spectra. Chemical Physics, 2022, 553, 111385.	1.9	7
58	Recyclable Aliphatic Nitrile-Template Enabled Remote meta-Câ€"H Functionalization at Room Temperature. Journal of Organic Chemistry, 2022, 87, 2204-2221.	3.2	7
59	Nondiffusive Rotational Jump Dynamics in Ethyl Ammonium Nitrate. Journal of Physical Chemistry B, 2018, 122, 9738-9746.	2.6	6
60	Aqueous hydroxyl group as the vibrational probe to access the hydrophobicity of amide derivatives. Journal of Molecular Liquids, 2020, 301, 112395.	4.9	6
61	Computational mechanistic study on molecular catalysis of water oxidation by cyclam ligand-based iron complex. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	6
62	Comparative first principlesâ€based molecular dynamics study of catalytic mechanism and reaction energetics of water oxidation reaction on 2D â€surface. Journal of Computational Chemistry, 2021, 42, 1138-1149.	3.3	6
63	Aqueous Affinity and Interfacial Dynamics of Anisotropic Buckled Black Phosphorous. Journal of Physical Chemistry B, 2021, 125, 7527-7536.	2.6	6
64	An oxygen-bridged bimetallic [Cuâ€"Oâ€"Se] catalyst for Sonogashira cross-coupling. New Journal of Chemistry, 2022, 46, 1650-1657.	2.8	6
65	Conformational Free-Energy Landscapes of Alanine Dipeptide in Hydrated Ionic Liquids from Enhanced Sampling Methods. Journal of Physical Chemistry B, 2020, 124, 6728-6737.	2.6	5
66	Cohesiveness and Nondiffusive Rotational Jump Dynamics of Protic Ionic Liquid from Dispersion-Corrected FPMD Simulations. Journal of Physical Chemistry B, 2020, 124, 10752-10765.	2.6	5
67	Conformational dynamics of amyloid-Î² (16â€"22) peptide in aqueous ionic liquids. RSC Advances, 2020, 10, 33248-33260.	3.6	5
68	Thermophysical Properties and Angular Jump Dynamics of Water: A Comparative DFT and DFT-Dispersion-Based Molecular Dynamics Study. Journal of Physical Chemistry A, 2020, 124, 6039-6049.	2.5	5
69	Amphiphilicity of Intricate Layered Graphene/g-C₃N₄ Nanosheets. Journal of Physical Chemistry B, 2021, 125, 11697-11708.	2.6	5
70	Mechanism and Dynamics of Formation of Bisoxo Intermediates and Oâ€"O Bond in the Catalytic Water Oxidation Process. Journal of Physical Chemistry A, 2021, 125, 279-290.	2.5	5
71	Vibrational spectral dynamics and ion-probe interactions of the hydrogen-bonded liquids in 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide. Chemical Physics, 2022, 559, 111519.	1.9	5
72	Mechanistic Insights into Cobalt-Based Water Oxidation Catalysis by DFT-Based Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2022, 126, 3301-3310.	2.5	5

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73	Modelling of Transition State in Grignard Reaction of Rigid N-(Aryl)imino-Acenapthenone (Ar-BIAO): A Combined Experimental and Computational Study. Australian Journal of Chemistry, 2015, 68, 931.	0.9	4
74	Vibration Spectral Dynamics of Weakly Coordinating Water Molecules near an Anion: FPMD Simulations of an Aqueous Solution of Tetrafluoroborate. Journal of Physical Chemistry B, 2019, 123, 2135-2146.	2.6	4
75	Ion-induced free energy landscapes of Aî²33â€“42 peptide dimer in wet ionic liquids. Journal of Molecular Liquids, 2020, 318, 114026.	4.9	4
76	Reciprocity between ion-dipole and hydrogen bond interactions in the binary mixtures of N,N-Dimethylformamide with ionic liquids. Journal of Molecular Liquids, 2020, 301, 112487.	4.9	4
77	Insights into the structure and ionic transport in â€˜water-in-bisaltâ€™ electrolytes for lithium-ion batteries. Materials Advances, 2021, 2, 7691-7700.	5.4	4
78	Structure and Transport of Solvent Ligated Octahedral Mg-Ion in an Aqueous Battery Electrolyte. Journal of Chemical & Engineering Data, 2021, 66, 1543-1554.	1.9	4
79	Mechanistic Insight into the O₂ Evolution Catalyzed by Copper Complexes with Tetra- and Pentadentate Ligands. Journal of Physical Chemistry A, 2021, 125, 6461-6473.	2.5	4
80	Solvent-Assisted Li-Ion Transport and Structural Heterogeneity in Fluorinated Battery Electrolytes. Journal of Physical Chemistry B, 2021, 125, 10551-10561.	2.6	4
81	2D IR spectra of the intrinsic vibrational probes of ionic liquid from dispersion corrected DFT-MD simulations. Journal of Molecular Liquids, 2022, 348, 118390.	4.9	4
82	Experimental and molecular dynamic insights on the thermophysical properties for MWCNT-Phosphonium based eutectic thermal media. Journal of Molecular Liquids, 2022, 354, 118892.	4.9	4
83	Microheterogeneity-Induced Vibrational Spectral Dynamics of Aqueous 1-Alkyl-3-methylimidazolium Tetrafluoroborate Ionic Liquids of Different Cationic Chain Lengths. Journal of Physical Chemistry B, 0, , .	2.6	4
84	Hydration behavior of protic ionic pair of methyl ammonium formate: A comparative molecular dynamics simulation study with their conjugate neutral forms. Computational and Theoretical Chemistry, 2020, 1172, 112663.	2.5	3
85	Solvent-mediated dynamics and stretching profile of amide modes: QM/MM simulations of N-methylacetamide in ionic and various molecular liquids. Journal of Molecular Liquids, 2020, 317, 114202.	4.9	3
86	Probing the vibrational dynamics of amide bands of N-methylformamide, N, N-dimethylacetamide, and N-methylacetamide in water. Computational and Theoretical Chemistry, 2020, 1190, 113001.	2.5	3
87	Structure and Conformational Response of Pure and Lithium-Doped Ionic Liquids to Pressure Alterations from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2020, 124, 2436-2449.	2.6	3
88	Molecular Dynamics and Emerging Network Graphs of Interactions in Dinitrile-Based Li-Ion Battery Electrolytes. Journal of Physical Chemistry B, 2021, 125, 7231-7240.	2.6	3
89	Structure and rotational dynamics of water around hydrogen peroxide. Journal of Molecular Liquids, 2022, 348, 118054.	4.9	3
90	Conformational dynamics of polymers in ethylammonium nitrate from advanced sampling methods. Computational Materials Science, 2022, 203, 111072.	3.0	3

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91	Formation of BH3 Adducts with Pyridine-2-Methylaminophosphine ligands: An experimental and computational study. Journal of Chemical Sciences, 2016, 128, 53-60.	1.5	2
92	Rattling Transport of Lithium Ion in the Cavities of Model Solid Electrolyte Interphase. Journal of Physical Chemistry C, 2019, 123, 25015-25024.	3.1	2
93	Heterogeneous Occupancy and Vibrational Dynamics of Spatially Patterned Water Molecules. Journal of Physical Chemistry B, 2019, 123, 4278-4290.	2.6	2
94	Insignificant Effect of Temperature on the Structure and Angular Jumps of Water near a Hydrophobic Cation. ACS Omega, 2021, 6, 8356-8364.	3.5	2
95	Site dependent catalytic water dissociation on anisotropic buckled black phosphorous surface. Physical Chemistry Chemical Physics, 2022, 24, 2582-2591.	2.8	2
96	Differing preferential ion binding to the peptide bond in ionic environment from classical and first principles molecular dynamics simulations. Journal of Molecular Liquids, 2020, 318, 114257.	4.9	1
97	Negligible Effect on the Structure and Vibrational Spectral Dynamics of Water Molecules Near Hydrophobic Solutes. ChemistrySelect, 2020, 5, 11549-11559.	1.5	0
98	Proton transfer from water to aromatic N-heterocyclic anions from DFT-MD simulations. Journal of Molecular Graphics and Modelling, 2021, 103, 107818.	2.4	0
99	Catalytic Mechanism of Competing Proton Transfer Events from Water and Acetic Acid by [Co^{II}(bpbH₂)Cl₂] for Water Splitting Processes. Journal of Physical Chemistry A, 2022, 126, 1321-1328.	2.5	0