Bhabani S Mallik

List of Publications by Year
in descending order

99	1,410	448610 19	466096 32
papers	citations	h-index	g-index

100	100	100	974
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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.	0.9	7
2	Structure and rotational dynamics of water around hydrogen peroxide. Journal of Molecular Liquids, 2022, 348, 118054.	2.3	3
3	Site dependent catalytic water dissociation on anisotropic buckled black phosphorous surface. Physical Chemistry Chemical Physics, 2022, 24, 2582-2591.	1.3	2
4	2D IR spectra of the intrinsic vibrational probes of ionic liquid from dispersion corrected DFT-MD simulations. Journal of Molecular Liquids, 2022, 348, 118390.	2.3	4
5	Conformational dynamics of polymers in ethylammonium nitrate from advanced sampling methods. Computational Materials Science, 2022, 203, 111072.	1.4	3
6	An oxygen-bridged bimetallic [Cuâ€"Oâ€"Se] catalyst for Sonogashira cross-coupling. New Journal of Chemistry, 2022, 46, 1650-1657.	1.4	6
7	Recyclable Aliphatic Nitrile-Template Enabled Remote meta-Câ€"H Functionalization at Room Temperature. Journal of Organic Chemistry, 2022, 87, 2204-2221.	1.7	7
8	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.	1.1	0
9	Experimental and molecular dynamic insights on the thermophysical properties for MWCNT-Phosphonium based eutectic thermal media. Journal of Molecular Liquids, 2022, 354, 118892.	2.3	4
10	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.	0.9	5
11	Mechanistic Insights into Cobalt-Based Water Oxidation Catalysis by DFT-Based Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2022, 126, 3301-3310.	1.1	5
12	Conformation-induced vibrational spectral dynamics of hydrogen peroxide and vicinal water molecules. Physical Chemistry Chemical Physics, 2021, 23, 6665-6676.	1.3	10
13	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.	2.3	12
14	Mechanism and Electronic Perspective of Oxygen Evolution Reactions Catalyzed by [Fe(OTf)2(bpbp)]. Journal of Physical Chemistry C, 2021, 125, 1313-1322.	1.5	8
15	Insights into the structure and ionic transport in â€˜water-in-bisaltâ€™ electrolytes for lithium-ion batteries. Materials Advances, 2021, 2, 7691-7700.	2.6	4
16	Effects of Doped N, B, P, and S Atoms on Graphene toward Oxygen Evolution Reactions. ACS Omega, 2021, 6, 5368-5378.	1.6	15
17	Structure and Transport of Solvent Ligated Octahedral Mg-Ion in an Aqueous Battery Electrolyte. Journal of Chemical & Engineering Data, 2021, 66, 1543-1554.	1.0	4
18	Insignificant Effect of Temperature on the Structure and Angular Jumps of Water near a Hydrophobic Cation. ACS Omega, 2021, 6, 8356-8364.	1.6	2

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19	Proton transfer from water to aromatic N-heterocyclic anions from DFT-MD simulations. Journal of Molecular Graphics and Modelling, 2021, 103, 107818.	1.3	0
20	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.	1.5	6
21	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.	1.2	7
22	Molecular Dynamics and Emerging Network Graphs of Interactions in Dinitrile-Based Li-Ion Battery Electrolytes. Journal of Physical Chemistry B, 2021, 125, 7231-7240.	1.2	3
23	Dynamics of Ionic Liquid through Intrinsic Vibrational Probes Using the Dispersion-Corrected DFT Functionals. Journal of Physical Chemistry B, 2021, 125, 6994-7008.	1.2	11
24	Mechanistic Insight into the O₂ Evolution Catalyzed by Copper Complexes with Tetra- and Pentadentate Ligands. Journal of Physical Chemistry A, 2021, 125, 6461-6473.	1.1	4
25	Aqueous Affinity and Interfacial Dynamics of Anisotropic Buckled Black Phosphorous. Journal of Physical Chemistry B, 2021, 125, 7527-7536.	1.2	6
26	Solvent-Assisted Li-Ion Transport and Structural Heterogeneity in Fluorinated Battery Electrolytes. Journal of Physical Chemistry B, 2021, 125, 10551-10561.	1.2	4
27	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.	2.5	7
28	Amphiphilicity of Intricate Layered Graphene/g-C₃N₄ Nanosheets. Journal of Physical Chemistry B, 2021, 125, 11697-11708.	1.2	5
29	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.	1.1	5
30	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.	1.7	7
31	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.	1.3	22
32	Solubility and solvation free energy of a cardiovascular drug, LASSBio-294, in ionic liquids: A computational study. Journal of Molecular Liquids, 2020, 301, 112449.	2.3	32
33	Aqueous hydroxyl group as the vibrational probe to access the hydrophobicity of amide derivatives. Journal of Molecular Liquids, 2020, 301, 112395.	2.3	6
34	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.	1.5	15
35	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.	1.1	3
36	Negligible Effect on the Structure and Vibrational Spectral Dynamics of Water Molecules Near Hydrophobic Solutes. ChemistrySelect, 2020, 5, 11549-11559.	0.7	0

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37	Ionic conductance and viscous drag in water-in-salt electrolytes for lithium and sodium ion batteries and supercapacitors. Materials Today Communications, 2020, 25, 101588.	0.9	18
38	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.	2.3	1
39	Computational mechanistic study on molecular catalysis of water oxidation by cyclam ligand-based iron complex. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	6
40	Conformational Free-Energy Landscapes of Alanine Dipeptide in Hydrated Ionic Liquids from Enhanced Sampling Methods. Journal of Physical Chemistry B, 2020, 124, 6728-6737.	1.2	5
41	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.	2.3	3
42	Cohesiveness and Nondiffusive Rotational Jump Dynamics of Protic Ionic Liquid from Dispersion-Corrected FPMD Simulations. Journal of Physical Chemistry B, 2020, 124, 10752-10765.	1.2	5
43	Conformational dynamics of aqueous hydrogen peroxide from first principles molecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 28286-28296.	1.3	9
44	Ion-induced free energy landscapes of AÎ²33â€“42 peptide dimer in wet ionic liquids. Journal of Molecular Liquids, 2020, 318, 114026.	2.3	4
45	Detailed characterization of dioxouranium(vi) complexes with a symmetrical tetradentate N2O2-benzil bis(isonicotinoyl hydrazone) ligand. Dalton Transactions, 2020, 49, 10603-10612.	1.6	9
46	Ultrafast Aqueous Dynamics in Concentrated Electrolytic Solutions of Lithium Salt and Ionic Liquid. Journal of Physical Chemistry B, 2020, 124, 9898-9912.	1.2	12
47	Conformational dynamics of amyloid-Î² (16â€“22) peptide in aqueous ionic liquids. RSC Advances, 2020, 10, 33248-33260.	1.7	5
48	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.	1.1	3
49	Ionic Dynamics of Hydroxylammonium Ionic Liquids: A Classical Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2020, 124, 4960-4974.	1.2	11
50	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.	1.1	5
51	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.	1.2	3
52	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.	1.2	9
53	Distinctive behavior and two-dimensional vibrational dynamics of water molecules inside glycine solvation shell. RSC Advances, 2020, 10, 6658-6670.	1.7	12
54	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.	2.3	10

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55	Reaction Mechanism and Free Energy Barriers for the Chemisorption of CO₂ by Ionic Entities. Journal of Physical Chemistry A, 2020, 124, 836-848.	1.1	14
56	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.	1.2	20
57	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.	2.3	4
58	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.	2.3	20
59	Rattling Transport of Lithium Ion in the Cavities of Model Solid Electrolyte Interphase. Journal of Physical Chemistry C, 2019, 123, 25015-25024.	1.5	2
60	Dynamics and Spectral Response of Water Molecules around Tetramethylammonium Cation. Journal of Physical Chemistry B, 2019, 123, 8753-8766.	1.2	24
61	Heterogeneous Occupancy and Vibrational Dynamics of Spatially Patterned Water Molecules. Journal of Physical Chemistry B, 2019, 123, 4278-4290.	1.2	2
62	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.	1.2	4
63	Solvation Structure and Dynamics of Alkali Metal Halides in an Ionic Liquid from Classical Molecular Dynamics Simulations. ACS Omega, 2019, 4, 19556-19564.	1.6	9
64	Interstitial Voids and Resultant Density of Liquid Water: A First-Principles Molecular Dynamics Study. ACS Omega, 2018, 3, 2010-2017.	1.6	23
65	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.	1.2	32
66	Association of Nucleobases in Hydrated Ionic Liquid from Biased Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2018, 122, 9635-9645.	1.2	7
67	Nondiffusive Rotational Jump Dynamics in Ethyl Ammonium Nitrate. Journal of Physical Chemistry B, 2018, 122, 9738-9746.	1.2	6
68	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.	1.5	21
69	Biosolvation Nature of Ionic Liquids: Molecular Dynamics Simulation of Methylated Nucleobases in Hydrated 1-Ethyl-3-methylimidazolium Acetate. ACS Omega, 2018, 3, 8344-8354.	1.6	14
70	Iron promoted C3â€“H nitration of 2H-indazole: direct access to 3-nitro-2H-indazoles. Organic and Biomolecular Chemistry, 2018, 16, 5113-5118.	1.5	41
71	Ultrafast Vibrational Spectroscopy of Aqueous Solution of Methylamine from First Principles MD Simulations. ChemistrySelect, 2017, 2, 74-83.	0.7	20
72	Protic ammonium carboxylate ionic liquids: insight into structure, dynamics and thermophysical properties by alkyl group functionalization. Physical Chemistry Chemical Physics, 2017, 19, 10358-10370.	1.3	31

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73	Time-dependent vibrational spectral analysis of first principles trajectory of methylamine with wavelet transform. Physical Chemistry Chemical Physics, 2017, 19, 9912-9922.	1.3	17
74	Structure and Dynamics of Hydroxyl-Functionalized Protic Ammonium Carboxylate Ionic Liquids. Journal of Physical Chemistry A, 2017, 121, 8097-8107.	1.1	28
75	Alkali Metal and Alkaline Earth Metal Complexes with the Bis(boraneâ€diphenylphosphanyl)amido Ligand â€“ Synthesis, Structures, and Catalysis for Ringâ€Opening Polymerization of Ìµâ€Caprolactone. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2016, 642, 118-127.	0.6	18
76	Proton transfer from water to anion: Free energy profile from first principles metadynamics simulations. Journal of Molecular Liquids, 2016, 219, 810-814.	2.3	10
77	A delicate case of unidirectional proton transfer from water to an aromatic heterocyclic anion. Physical Chemistry Chemical Physics, 2016, 18, 29979-29986.	1.3	8
78	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.	0.9	9
79	Formation of BH3 Adducts with Pyridine-2-Methylaminophosphine ligands: An experimental and computational study. Journal of Chemical Sciences, 2016, 128, 53-60.	0.7	2
80	Heavier group 2 metal complexes with a flexible scorpionate ligand based on 2-mercaptopyridine. RSC Advances, 2015, 5, 51413-51420.	1.7	12
81	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.	0.5	4
82	Functionalisation of Imidazolin-2-imine to Corresponding Phosphinamine, Chalcogenide (O, S, Se, Te), and Borane Compounds. Australian Journal of Chemistry, 2015, 68, 127.	0.5	8
83	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.	2.3	21
84	Effects of Temperature on the Structure and Dynamics of Aqueous Mixtures ofN,N-Dimethylformamide. Journal of Chemical & Engineering Data, 2014, 59, 3250-3257.	1.0	19
85	Unprecedented Calcium Metallaâ€macrocycle Having Phosphinoselenoic Amide and Diphenylphosphinate in the Coordination Sphere. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2014, 640, 994-999.	0.6	8
86	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
87	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.	1.8	9
88	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
89	Understanding the solubility of triamino-trinitrobenzene in hydrous tetramethylammonium fluoride: a first principles molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2012, 14, 4884.	1.3	14
90	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

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91	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
92	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.	1.2	37
93	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
94	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
95	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
96	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
97	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
98	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.	1.2	78
99	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, , .	1.2	4