Ali A Hassanali

List of Publications by Year
in descending order

67	3,767	186265 28	128289 60
papers	citations	h-index	g-index

69	69	69	4572
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Learning the Hydrophobic, Hydrophilic, and Aromatic Character of Amino Acids from Thermal Relaxation and Interfacial Thermal Conductance. Journal of Physical Chemistry B, 2022, 126, 670-678.	2.6	4
2	How to determine solubility in binary mixtures from neutron scattering data: The case of methane and water. Journal of Chemical Physics, 2022, 156, 054502.	3.0	3
3	Model Folded Hydrophobic Polymers Reside in Highly Branched Voids. Journal of Physical Chemistry Letters, 2022, 13, 183-189.	4.6	5
4	High-Dimensional Fluctuations in Liquid Water: Combining Chemical Intuition with Unsupervised Learning. Journal of Chemical Theory and Computation, 2022, 18, 3136-3150.	5.3	14
5	The behavior of methaneâ€“water mixtures under elevated pressures from simulations using many-body potentials. Journal of Chemical Physics, 2022, 156, .	3.0	7
6	Intracellular Aî²42 Aggregation Leads to Cellular Thermogenesis. Journal of the American Chemical Society, 2022, 144, 10034-10041.	13.7	16
7	Statistical physics of inhomogeneous transport: Unification of diffusion laws and inference from first-passage statistics. Physical Review E, 2022, 106, .	2.1	6
8	Structural and dynamical fingerprints of the anomalous dielectric properties of water under confinement. Physical Review Materials, 2021, 5, .	2.4	10
9	Short hydrogen bonds enhance nonaromatic protein-related fluorescence. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	24
10	On-off transition and ultrafast decay of amino acid luminescence driven by modulation of supramolecular packing. IScience, 2021, 24, 102695.	4.1	18
11	Coupled Local-Mode Approach for the Calculation of Vibrational Spectra: Application to Protonated Water Clusters. Journal of Physical Chemistry Letters, 2021, 12, 9226-9232.	4.6	4
12	Emergence of Electric Fields at the Waterâ€“C12E6 Surfactant Interface. Journal of the American Chemical Society, 2021, 143, 15103-15112.	13.7	16
13	Charge transfer across Câ€“Hâ‹…â‹…â‹…O hydrogen bonds stabilizes oil droplets in water. Science, 2021, 374, 1366-1370.	12.6	88
14	A computational study on the role of water and conformational fluctuations in Hsp90 in response to inhibitors. Journal of Molecular Graphics and Modelling, 2020, 96, 107510.	2.4	12
15	Simulation of Liquids with the Tight-Binding Density-Functional Approach and Improved Atomic Charges. Journal of Physical Chemistry B, 2020, 124, 7421-7432.	2.6	4
16	Understanding FÃ¶rster Energy Transfer through the Lens of Molecular Dynamics. Journal of Chemical Theory and Computation, 2020, 16, 7281-7288.	5.3	6
17	Toward Understanding Optical Properties of Amyloids: A Reaction Path and Nonadiabatic Dynamics Study. Journal of the American Chemical Society, 2020, 142, 18042-18049.	13.7	28
18	First-passage fingerprints of water diffusion near glutamine surfaces. Soft Matter, 2020, 16, 9202-9216.	2.7	8

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19	Squeezing Oil into Water under Pressure: Inverting the Hydrophobic Effect. Journal of Physical Chemistry Letters, 2020, 11, 4826-4833.	4.6	7
20	A multi-scale perspective of gas transport through soap-film membranes. Molecular Systems Design and Engineering, 2020, 5, 911-921.	3.4	13
21	Insights into the Emerging Networks of Voids in Simulated Supercooled Water. Journal of Physical Chemistry B, 2020, 124, 2180-2190.	2.6	14
22	Charge transfer as a ubiquitous mechanism in determining the negative charge at hydrophobic interfaces. Nature Communications, 2020, 11, 901.	12.8	68
23	Structural and dynamical heterogeneities at glutamineâ€“water interfaces. Physical Chemistry Chemical Physics, 2019, 21, 16083-16094.	2.8	4
24	Spontaneously Forming Dendritic Voids in Liquid Water Can Host Small Polymers. Journal of Physical Chemistry Letters, 2019, 10, 5585-5591.	4.6	21
25	Thermal transport at a nanoparticle-water interface: A molecular dynamics and continuum modeling study. Journal of Chemical Physics, 2019, 150, 114701.	3.0	57
26	Low energy optical excitations as an indicator of structural changes initiated at the termini of amyloid proteins. Physical Chemistry Chemical Physics, 2019, 21, 23931-23942.	2.8	17
27	Growing Materials Science in Africa â€“ The Case of the African School for Electronic Structure Methods and Applications (ASESMA). MRS Advances, 2018, 3, 2183-2201.	0.9	1
28	Hierarchical lattice models of hydrogen-bond networks in water. Physical Review E, 2018, 97, 062113.	2.1	6
29	A Data Science Approach to Understanding Water Networks Around Biomolecules: The Case of Tri-Alanine in Liquid Water. Journal of Physical Chemistry B, 2018, 122, 7895-7906.	2.6	13
30	Hydrogen Bonds and Life in the Universe. Life, 2018, 8, 1.	2.4	43
31	Understanding the quantum mechanical properties of hydrogen bonds in solvated biomolecules from cluster calculations. Journal of Molecular Liquids, 2018, 263, 501-509.	4.9	8
32	Quantum mechanical effects in zwitterionic amino acids: The case of proline, hydroxyproline, and alanine in water. Journal of Chemical Physics, 2018, 148, 222826.	3.0	9
33	One-Dimensional Confinement Inhibits Water Dissociation in Carbon Nanotubes. Journal of Physical Chemistry Letters, 2018, 9, 5029-5033.	4.6	23
34	A computational study on how structure influences the optical properties in model crystal structures of amyloid fibrils. Physical Chemistry Chemical Physics, 2017, 19, 4030-4040.	2.8	41
35	Hydrogen Bond Networks and Hydrophobic Effects in the Amyloid Î²_{30â€“35} Chain in Water: A Molecular Dynamics Study. Journal of Chemical Information and Modeling, 2017, 57, 1548-1562.	5.4	24
36	On the Role of Nonspherical Cavities in Short Length-Scale Density Fluctuations in Water. Journal of Physical Chemistry A, 2017, 121, 370-380.	2.5	24

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37	Decomposition of the Experimental Raman and Infrared Spectra of Acidic Water into Proton, Special Pair, and Counterion Contributions. Journal of Physical Chemistry Letters, 2017, 8, 5246-5252.	4.6	74
38	The excess proton at the air-water interface: The role of instantaneous liquid interfaces. Journal of Chemical Physics, 2017, 146, 244703.	3.0	42
39	Biomolecules at the amorphous silica/water interface: Binding and fluorescence anisotropy of peptides. Colloids and Surfaces B: Biointerfaces, 2017, 157, 83-92.	5.0	5
40	Nuclear quantum effects in a HIV/cancer inhibitor: The case of ellipticine. Journal of Chemical Physics, 2016, 145, 205102.	3.0	24
41	Water Determines the Structure and Dynamics of Proteins. Chemical Reviews, 2016, 116, 7673-7697.	47.7	645
42	Protons and Hydroxide Ions in Aqueous Systems. Chemical Reviews, 2016, 116, 7642-7672.	47.7	358
43	Proton Transfer and Structure-Specific Fluorescence in Hydrogen Bond-Rich Protein Structures. Journal of the American Chemical Society, 2016, 138, 3046-3057.	13.7	182
44	Ab Initio Quality NMR Parameters in Solid-State Materials Using a High-Dimensional Neural-Network Representation. Journal of Chemical Theory and Computation, 2016, 12, 765-773.	5.3	51
45	Probing Defects and Correlations in the Hydrogen-Bond Network of ab Initio Water. Journal of Chemical Theory and Computation, 2016, 12, 1953-1964.	5.3	51
46	A study of polybromide chain formation using carbon nanomaterials via density functional theory approach. Cogent Engineering, 2016, 3, 1261509.	2.2	5
47	Role of Quantum Vibrations on the Structural, Electronic, and Optical Properties of 9-Methylguanine. Journal of Physical Chemistry A, 2015, 119, 10816-10827.	2.5	28
48	Unveiling the Janus-Like Properties of OH^{â€“}. Journal of Physical Chemistry Letters, 2015, 6, 272-278.	4.6	17
49	Structure and Dynamics of the Instantaneous Water/Vapor Interface Revisited by Path-Integral and Ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2015, 119, 10079-10086.	2.6	61
50	DNA Binding to the Silica Surface. Journal of Physical Chemistry B, 2015, 119, 11030-11040.	2.6	82
51	The Role of Quantum Effects on Structural and Electronic Fluctuations in Neat and Charged Water. Journal of Physical Chemistry B, 2014, 118, 13226-13235.	2.6	48
52	Ab Initio Molecular Dynamics Study of the Mechanism of Proton Recombination with a Weak Base. Journal of Physical Chemistry B, 2014, 118, 13903-13912.	2.6	16
53	Aqueous solutions: state of the art in ab initio molecular dynamics. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20120482.	3.4	121
54	Anomalous water diffusion in salt solutions. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 3310-3315.	7.1	124

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55	The role of the umbrella inversion mode in proton diffusion. Chemical Physics Letters, 2014, 599, 133-138.	2.6	31
56	Proton transfer through the water gossamer. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 13723-13728.	7.1	320
57	Ultrafast Dynamics of Nonequilibrium Electron Transfer in Photoinduced Redox Cycle: Solvent Mediation and Conformation Flexibility. Journal of Physical Chemistry B, 2012, 116, 9130-9140.	2.6	31
58	The Fuzzy Quantum Proton in the Hydrogen Chloride Hydrates. Journal of the American Chemical Society, 2012, 134, 8557-8569.	13.7	45
59	An AIMD Study of the CPD Repair Mechanism in Water: Reaction Free Energy Surface and Mechanistic Implications. Journal of Physical Chemistry B, 2011, 115, 3848-3859.	2.6	32
60	An AIMD Study of CPD Repair Mechanism in Water: Role of Solvent in Ring Splitting. Journal of Physical Chemistry B, 2011, 115, 3860-3871.	2.6	30
61	On the recombination of hydronium and hydroxide ions in water. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 20410-20415.	7.1	154
62	The Dissociated Amorphous Silica Surface: Model Development and Evaluation. Journal of Chemical Theory and Computation, 2010, 6, 3456-3471.	5.3	45
63	Origin of Slow Relaxation Following Photoexcitation of W7 in Myoglobin and the Dynamics of Its Hydration Layer. Journal of Physical Chemistry B, 2008, 112, 16121-16134.	2.6	54
64	Model for the Waterâ^'Amorphous Silica Interface:â€‰ The Undissociated Surface. Journal of Physical Chemistry B, 2007, 111, 11181-11193.	2.6	125
65	Hydration Dynamics and Time Scales of Coupled Waterâ^'Protein Fluctuations. Journal of the American Chemical Society, 2007, 129, 3376-3382.	13.7	232
66	Static and dynamic properties of the water/amorphous silica interface: a model for the undissociated surface. Journal of Computer-Aided Materials Design, 2007, 14, 53-63.	0.7	18
67	A Molecular Dynamics Study of Lys-Trp-Lys:Â Structure and Dynamics in Solution Following Photoexcitation. Journal of Physical Chemistry B, 2006, 110, 10497-10508.	2.6	46