

# Ali A Hassanali

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/3931679/publications.pdf>

Version: 2024-02-01

67  
papers

3,767  
citations

185998

28  
h-index

128067

60  
g-index

69  
all docs

69  
docs citations

69  
times ranked

4572  
citing authors

#	ARTICLE	IF	CITATIONS
1	Water Determines the Structure and Dynamics of Proteins. <i>Chemical Reviews</i> , 2016, 116, 7673-7697.	23.0	645
2	Protons and Hydroxide Ions in Aqueous Systems. <i>Chemical Reviews</i> , 2016, 116, 7642-7672.	23.0	358
3	Proton transfer through the water gossamer. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 13723-13728.	3.3	320
4	Hydration Dynamics and Time Scales of Coupled Water-Protein Fluctuations. <i>Journal of the American Chemical Society</i> , 2007, 129, 3376-3382.	6.6	232
5	Proton Transfer and Structure-Specific Fluorescence in Hydrogen Bond-Rich Protein Structures. <i>Journal of the American Chemical Society</i> , 2016, 138, 3046-3057.	6.6	182
6	On the recombination of hydronium and hydroxide ions in water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 20410-20415.	3.3	154
7	Model for the Water-Amorphous Silica Interface: The Undissociated Surface. <i>Journal of Physical Chemistry B</i> , 2007, 111, 11181-11193.	1.2	125
8	Anomalous water diffusion in salt solutions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 3310-3315.	3.3	124
9	Aqueous solutions: state of the art in <i>ab initio</i> molecular dynamics. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2014, 372, 20120482.	1.6	121
10	Charge transfer across H <sub>2</sub> O hydrogen bonds stabilizes oil droplets in water. <i>Science</i> , 2021, 374, 1366-1370.	6.0	88
11	DNA Binding to the Silica Surface. <i>Journal of Physical Chemistry B</i> , 2015, 119, 11030-11040.	1.2	82
12	Decomposition of the Experimental Raman and Infrared Spectra of Acidic Water into Proton, Special Pair, and Counterion Contributions. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5246-5252.	2.1	74
13	Charge transfer as a ubiquitous mechanism in determining the negative charge at hydrophobic interfaces. <i>Nature Communications</i> , 2020, 11, 901.	5.8	68
14	Structure and Dynamics of the Instantaneous Water/Vapor Interface Revisited by Path-Integral and Ab Initio Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2015, 119, 10079-10086.	1.2	61
15	Thermal transport at a nanoparticle-water interface: A molecular dynamics and continuum modeling study. <i>Journal of Chemical Physics</i> , 2019, 150, 114701.	1.2	57
16	Origin of Slow Relaxation Following Photoexcitation of W7 in Myoglobin and the Dynamics of Its Hydration Layer. <i>Journal of Physical Chemistry B</i> , 2008, 112, 16121-16134.	1.2	54
17	<i>Ab Initio</i> Quality NMR Parameters in Solid-State Materials Using a High-Dimensional Neural-Network Representation. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 765-773.	2.3	51
18	Probing Defects and Correlations in the Hydrogen-Bond Network of ab Initio Water. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1953-1964.	2.3	51

#	ARTICLE	IF	CITATIONS
19	The Role of Quantum Effects on Structural and Electronic Fluctuations in Neat and Charged Water. Journal of Physical Chemistry B, 2014, 118, 13226-13235.	1.2	48
20	A Molecular Dynamics Study of Lys-Trp-Lys:Å Structure and Dynamics in Solution Following Photoexcitation. Journal of Physical Chemistry B, 2006, 110, 10497-10508.	1.2	46
21	The Dissociated Amorphous Silica Surface: Model Development and Evaluation. Journal of Chemical Theory and Computation, 2010, 6, 3456-3471.	2.3	45
22	The Fuzzy Quantum Proton in the Hydrogen Chloride Hydrates. Journal of the American Chemical Society, 2012, 134, 8557-8569.	6.6	45
23	Hydrogen Bonds and Life in the Universe. Life, 2018, 8, 1.	1.1	43
24	The excess proton at the air-water interface: The role of instantaneous liquid interfaces. Journal of Chemical Physics, 2017, 146, 244703.	1.2	42
25	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.	1.3	41
26	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.	1.2	32
27	Ultrafast Dynamics of Nonequilibrium Electron Transfer in Photoinduced Redox Cycle: Solvent Mediation and Conformation Flexibility. Journal of Physical Chemistry B, 2012, 116, 9130-9140.	1.2	31
28	The role of the umbrella inversion mode in proton diffusion. Chemical Physics Letters, 2014, 599, 133-138.	1.2	31
29	An AIMD Study of CPD Repair Mechanism in Water: Role of Solvent in Ring Splitting. Journal of Physical Chemistry B, 2011, 115, 3860-3871.	1.2	30
30	Role of Quantum Vibrations on the Structural, Electronic, and Optical Properties of 9-Methylguanine. Journal of Physical Chemistry A, 2015, 119, 10816-10827.	1.1	28
31	Toward Understanding Optical Properties of Amyloids: A Reaction Path and Nonadiabatic Dynamics Study. Journal of the American Chemical Society, 2020, 142, 18042-18049.	6.6	28
32	Nuclear quantum effects in a HIV/cancer inhibitor: The case of ellipticine. Journal of Chemical Physics, 2016, 145, 205102.	1.2	24
33	Hydrogen Bond Networks and Hydrophobic Effects in the Amyloid Î²<sub>30</sub>â€“35</sub> Chain in Water: A Molecular Dynamics Study. Journal of Chemical Information and Modeling, 2017, 57, 1548-1562.	2.5	24
34	On the Role of Nonspherical Cavities in Short Length-Scale Density Fluctuations in Water. Journal of Physical Chemistry A, 2017, 121, 370-380.	1.1	24
35	Short hydrogen bonds enhance nonaromatic protein-related fluorescence. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	24
36	One-Dimensional Confinement Inhibits Water Dissociation in Carbon Nanotubes. Journal of Physical Chemistry Letters, 2018, 9, 5029-5033.	2.1	23

#	ARTICLE	IF	CITATIONS
37	Spontaneously Forming Dendritic Voids in Liquid Water Can Host Small Polymers. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 5585-5591.	2.1	21
38	Static and dynamic properties of the water/amorphous silica interface: a model for the undissociated surface. <i>Journal of Computer-Aided Materials Design</i> , 2007, 14, 53-63.	0.7	18
39	On-off transition and ultrafast decay of amino acid luminescence driven by modulation of supramolecular packing. <i>IScience</i> , 2021, 24, 102695.	1.9	18
40	Unveiling the Janus-Like Properties of OH <sup>+</sup> . <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 272-278.	2.1	17
41	Low energy optical excitations as an indicator of structural changes initiated at the termini of amyloid proteins. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 23931-23942.	1.3	17
42	Ab Initio Molecular Dynamics Study of the Mechanism of Proton Recombination with a Weak Base. <i>Journal of Physical Chemistry B</i> , 2014, 118, 13903-13912.	1.2	16
43	Emergence of Electric Fields at the Water-C12E6 Surfactant Interface. <i>Journal of the American Chemical Society</i> , 2021, 143, 15103-15112.	6.6	16
44	Intracellular A $\beta$ 242 Aggregation Leads to Cellular Thermogenesis. <i>Journal of the American Chemical Society</i> , 2022, 144, 10034-10041.	6.6	16
45	Insights into the Emerging Networks of Voids in Simulated Supercooled Water. <i>Journal of Physical Chemistry B</i> , 2020, 124, 2180-2190.	1.2	14
46	High-Dimensional Fluctuations in Liquid Water: Combining Chemical Intuition with Unsupervised Learning. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3136-3150.	2.3	14
47	A Data Science Approach to Understanding Water Networks Around Biomolecules: The Case of Tri-Alanine in Liquid Water. <i>Journal of Physical Chemistry B</i> , 2018, 122, 7895-7906.	1.2	13
48	A multi-scale perspective of gas transport through soap-film membranes. <i>Molecular Systems Design and Engineering</i> , 2020, 5, 911-921.	1.7	13
49	A computational study on the role of water and conformational fluctuations in Hsp90 in response to inhibitors. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 96, 107510.	1.3	12
50	Structural and dynamical fingerprints of the anomalous dielectric properties of water under confinement. <i>Physical Review Materials</i> , 2021, 5, .	0.9	10
51	Quantum mechanical effects in zwitterionic amino acids: The case of proline, hydroxyproline, and alanine in water. <i>Journal of Chemical Physics</i> , 2018, 148, 222826.	1.2	9
52	Understanding the quantum mechanical properties of hydrogen bonds in solvated biomolecules from cluster calculations. <i>Journal of Molecular Liquids</i> , 2018, 263, 501-509.	2.3	8
53	First-passage fingerprints of water diffusion near glutamine surfaces. <i>Soft Matter</i> , 2020, 16, 9202-9216.	1.2	8
54	Squeezing Oil into Water under Pressure: Inverting the Hydrophobic Effect. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 4826-4833.	2.1	7

#	ARTICLE	IF	CITATIONS
55	The behavior of methane-water mixtures under elevated pressures from simulations using many-body potentials. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	7
56	Hierarchical lattice models of hydrogen-bond networks in water. <i>Physical Review E</i> , 2018, 97, 062113.	0.8	6
57	Understanding Förster Energy Transfer through the Lens of Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7281-7288.	2.3	6
58	Statistical physics of inhomogeneous transport: Unification of diffusion laws and inference from first-passage statistics. <i>Physical Review E</i> , 2022, 106, .	0.8	6
59	Biomolecules at the amorphous silica/water interface: Binding and fluorescence anisotropy of peptides. <i>Colloids and Surfaces B: Biointerfaces</i> , 2017, 157, 83-92.	2.5	5
60	A study of polybromide chain formation using carbon nanomaterials via density functional theory approach. <i>Cogent Engineering</i> , 2016, 3, 1261509.	1.1	5
61	Model Folded Hydrophobic Polymers Reside in Highly Branched Voids. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 183-189.	2.1	5
62	Structural and dynamical heterogeneities at glutamine-water interfaces. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16083-16094.	1.3	4
63	Simulation of Liquids with the Tight-Binding Density-Functional Approach and Improved Atomic Charges. <i>Journal of Physical Chemistry B</i> , 2020, 124, 7421-7432.	1.2	4
64	Coupled Local-Mode Approach for the Calculation of Vibrational Spectra: Application to Protonated Water Clusters. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 9226-9232.	2.1	4
65	Learning the Hydrophobic, Hydrophilic, and Aromatic Character of Amino Acids from Thermal Relaxation and Interfacial Thermal Conductance. <i>Journal of Physical Chemistry B</i> , 2022, 126, 670-678.	1.2	4
66	How to determine solubility in binary mixtures from neutron scattering data: The case of methane and water. <i>Journal of Chemical Physics</i> , 2022, 156, 054502.	1.2	3
67	Growing Materials Science in Africa – The Case of the African School for Electronic Structure Methods and Applications (ASESMA). <i>MRS Advances</i> , 2018, 3, 2183-2201.	0.5	1