

# Hao Dong

## List of Publications by Year in descending order

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47  
papers

1,585  
citations

361413

20  
h-index

302126

39  
g-index

48  
all docs

48  
docs citations

48  
times ranked

1862  
citing authors

#	ARTICLE	IF	CITATIONS
1	Insight into the Mechanism of the Influenza A Proton Channel from a Structure in a Lipid Bilayer. <i>Science</i> , 2010, 330, 509-512.	12.6	422
2	Stable, active CO <sub>2</sub> reduction to formate via redox-modulated stabilization of active sites. <i>Nature Communications</i> , 2021, 12, 5223.	12.8	145
3	Effects of Macromolecular Crowding on Protein Conformational Changes. <i>PLoS Computational Biology</i> , 2010, 6, e1000833.	3.2	82
4	Glycines: Role in $\alpha$ -Helical Membrane Protein Structures and a Potential Indicator of Native Conformation. <i>Biochemistry</i> , 2012, 51, 4779-4789.	2.5	71
5	Self-Assembled Peptide Nano-Superstructure towards Enzyme Mimicking Hydrolysis. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 17164-17170.	13.8	69
6	Pore waters regulate ion permeation in a calcium release-activated calcium channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 17332-17337.	7.1	65
7	Estimation on the Individual Hydrogen-Bond Strength in Molecules with Multiple Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2941-2945.	2.5	52
8	Gating mechanism of a P2X <sub>4</sub> receptor developed from normal mode analysis and molecular dynamics simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 4140-4145.	7.1	51
9	Atomistic mechanism for the activation and desensitization of an AMPA-subtype glutamate receptor. <i>Nature Communications</i> , 2011, 2, 354.	12.8	50
10	Principles Governing Catalytic Activity of Self-Assembled Short Peptides. <i>Journal of the American Chemical Society</i> , 2019, 141, 223-231.	13.7	47
11	Structures and Spectroscopic Properties of Large Molecules and Condensed-Phase Systems Predicted by Generalized Energy-Based Fragmentation Approach. <i>Accounts of Chemical Research</i> , 2021, 54, 169-181.	15.6	36
12	<i>In Situ</i> Imaging Facet-Induced Spatial Heterogeneity of Electrocatalytic Reaction Activity at the Subparticle Level via Electrochemiluminescence Microscopy. <i>Analytical Chemistry</i> , 2019, 91, 6829-6835.	6.5	35
13	Two-dimensional Mo-based compounds for the Li-O <sub>2</sub> batteries: Catalytic performance and electronic structure studies. <i>Energy Storage Materials</i> , 2021, 41, 650-655.	18.0	35
14	Terahertz spectra of DNA nucleobase crystals: A joint experimental and computational study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 179, 255-260.	3.9	31
15	Identification of molecular determinants that govern distinct STIM2 activation dynamics. <i>PLoS Biology</i> , 2018, 16, e2006898.	5.6	29
16	Accurate Prediction of NMR Chemical Shifts in Macromolecular and Condensed-Phase Systems with the Generalized Energy-Based Fragmentation Method. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5231-5239.	5.3	28
17	Understanding the Role of Intra- and Intermolecular Interactions in the Formation of Single- and Double-Helical Structures of Aromatic Oligoamides: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1335-1342.	2.5	24
18	Toward a Model for Activation of Orai Channel. <i>IScience</i> , 2019, 16, 356-367.	4.1	24

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19	Ab initio calculations and validation of the pH-dependent structures of the His37-Trp41 quartet, the heart of acid activation and proton conductance in the M2 protein of Influenza A virus. <i>Chemical Science</i> , 2013, 4, 2776.	7.4	21
20	Entropy and Polarity Control the Partition and Transportation of Drug-like Molecules in Biological Membrane. <i>Scientific Reports</i> , 2017, 7, 17749.	3.3	21
21	Accurate and Efficient Prediction of NMR Parameters of Condensed-Phase Systems with the Generalized Energy-Based Fragmentation Method. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2995-3005.	5.3	19
22	Machine learning on properties of multiscale multisource hydroxyapatite nanoparticles datasets with different morphologies and sizes. <i>Npj Computational Materials</i> , 2021, 7, .	8.7	19
23	Surface Stability and Morphology of Calcium Phosphate Tuned by pH Values and Lactic Acid Additives: Theoretical and Experimental Study. <i>ACS Applied Materials &amp; Interfaces</i> , 2022, 14, 4836-4851.	8.0	16
24	Counterion-Assisted Cation Transport in a Biological Calcium Channel. <i>Journal of Physical Chemistry B</i> , 2014, 118, 9668-9676.	2.6	15
25	Scorpion toxin inhibits the voltage-gated proton channel using a Zn <sup>2+</sup> -like long-range conformational coupling mechanism. <i>British Journal of Pharmacology</i> , 2020, 177, 2351-2364.	5.4	14
26	Structures of wild-type and H451N mutant human lymphocyte potassium channel KV1.3. <i>Cell Discovery</i> , 2021, 7, 39.	6.7	14
27	The Morphology of Hydroxyapatite Nanoparticles Regulates Cargo Recognition in Clathrin-Mediated Endocytosis. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 627015.	3.5	13
28	Self-Assembled Peptide Nano-Superstructure towards Enzyme Mimicking Hydrolysis. <i>Angewandte Chemie</i> , 2021, 133, 17301-17307.	2.0	12
29	Molecular Mechanism of Self-Assembly of Aromatic Oligoamides into Interlocked Double-Helix Foldamers. <i>Journal of Physical Chemistry B</i> , 2017, 121, 10064-10072.	2.6	11
30	Aromatic amine-terminated polysulfide oligomer: Synthesis and application in self-healable polyurea. <i>Journal of Polymer Science Part A</i> , 2019, 57, 1460-1466.	2.3	11
31	A Two-Ended Data-Driven Accelerated Sampling Method for Exploring the Transition Pathways between Two Known States of Protein. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4631-4640.	5.3	9
32	Achieving Rich Mixed-Valence Polysulfide/Carbon Nanotube Films toward Ultrahigh Volume Energy Density and Largely Deformable Pseudocapacitors. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 25271-25282.	8.0	7
33	A Data-Driven Accelerated Sampling Method for Searching Functional States of Proteins. <i>Advanced Theory and Simulations</i> , 2019, 2, 1800171.	2.8	6
34	Evaluation of thermoplastic polyolefin materials for the hard shed of composite insulators. <i>Journal of Applied Polymer Science</i> , 2020, 137, 49080.	2.6	6
35	An electrostatic-variable coarse-grained model for predicting enthalpy of vaporization, surface tension, diffusivity, conductivity, and dielectric constant of aqueous ionic liquid. <i>Journal of Molecular Liquids</i> , 2022, 346, 118230.	4.9	6
36	Research on Impact Resistance of Reinforced Concrete Beams Strengthened with Carbon Fiber Reinforced Polymer Grid and Engineered Cementitious Composites. <i>Polymers</i> , 2022, 14, 1951.	4.5	6

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37	A computational study towards understanding the mechanism of phosphodiester cleavage by two mononuclear Zn(ii) complexes. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 10434.	2.8	5
38	Understanding the Boron–Nitrogen Interaction and Its Possible Implications in Drug Design. <i>Journal of Physical Chemistry B</i> , 2015, 119, 14393-14401.	2.6	5
39	After-Pulse Characterizations of Geiger-Mode 4H-SiC Avalanche Photodiodes. <i>IEEE Photonics Technology Letters</i> , 2020, 32, 706-709.	2.5	5
40	Strengthening of Precast RC Frame to Mitigate Progressive Collapse by Externally Anchored Carbon Fiber Ropes. <i>Polymers</i> , 2021, 13, 1306.	4.5	5
41	Effects of Cholesterol on the Partitioning of a Drug Molecule in Lipid Bilayers. <i>Journal of Physical Chemistry B</i> , 2021, 125, 5338-5345.	2.6	4
42	Global Fold Switching of the RafH Protein: Diverse Structures with a Conserved Pathway. <i>Journal of Physical Chemistry B</i> , 2022, 126, 2979-2989.	2.6	2
43	Equilibria between the K <sup>+</sup> binding and cation vacancy conformations of potassium channels. <i>Protein and Cell</i> , 2019, 10, 533-537.	11.0	1
44	Gating and regulation of the calcium release-activated calcium channel: Recent progress from experiments and molecular modeling. <i>Biopolymers</i> , 2020, 111, e23392.	2.4	1
45	Computation-driven synthesis of pentothal sodium. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26624.	2.0	0
46	A bottom-up design strategy for controllable self-assembly based on the isotropic double-well potential. <i>Physical Chemistry Chemical Physics</i> , 2022, , .	2.8	0
47	Mutants only partially represent characteristics of calcium-release-activated calcium channel gating. <i>Chinese Journal of Chemical Physics</i> , 2021, 34, 915-924.	1.3	0