Hao Dong

List of Publications by Year
in descending order

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	An electrostatic-variable coarse-grained model for predicting enthalpy of vaporization, surface tension, diffusivity, conductivity, and dielectric constant of aqueous ionic liquid. Journal of Molecular Liquids, 2022, 346, 118230.	4.9	6
2	Surface Stability and Morphology of Calcium Phosphate Tuned by pH Values and Lactic Acid Additives: Theoretical and Experimental Study. ACS Applied Materials & Interfaces, 2022, 14, 4836-4851.	8.0	16
3	A bottom-up design strategy for controllable self-assembly based on the isotropic double-well potential. Physical Chemistry Chemical Physics, 2022, , .	2.8	0
4	Global Fold Switching of the RafH Protein: Diverse Structures with a Conserved Pathway. Journal of Physical Chemistry B, 2022, 126, 2979-2989.	2.6	2
5	Research on Impact Resistance of Reinforced Concrete Beams Strengthened with Carbon Fiber Reinforced Polymer Grid and Engineered Cementitious Composites. Polymers, 2022, 14, 1951.	4.5	6
6	Structures and Spectroscopic Properties of Large Molecules and Condensed-Phase Systems Predicted by Generalized Energy-Based Fragmentation Approach. Accounts of Chemical Research, 2021, 54, 169-181.	15.6	36
7	Computationâ€driven synthesis of pentothal sodium. International Journal of Quantum Chemistry, 2021, 121, e26624.	2.0	0
8	The Morphology of Hydroxyapatite Nanoparticles Regulates Cargo Recognition in Clathrin-Mediated Endocytosis. Frontiers in Molecular Biosciences, 2021, 8, 627015.	3.5	13
9	Strengthening of Precast RC Frame to Mitigate Progressive Collapse by Externally Anchored Carbon Fiber Ropes. Polymers, 2021, 13, 1306.	4.5	5
10	Effects of Cholesterol on the Partitioning of a Drug Molecule in Lipid Bilayers. Journal of Physical Chemistry B, 2021, 125, 5338-5345.	2.6	4
11	Selfâ€Assembled Peptide Nanoâ€Superstructure towards Enzyme Mimicking Hydrolysis. Angewandte Chemie, 2021, 133, 17301-17307.	2.0	12
12	Structures of wild-type and H451N mutant human lymphocyte potassium channel KV1.3. Cell Discovery, 2021, 7, 39.	6.7	14
13	Selfâ€Assembled Peptide Nanoâ€Superstructure towards Enzyme Mimicking Hydrolysis. Angewandte Chemie - International Edition, 2021, 60, 17164-17170.	13.8	69
14	Stable, active CO2 reduction to formate via redox-modulated stabilization of active sites. Nature Communications, 2021, 12, 5223.	12.8	145
15	Machine learning on properties of multiscale multisource hydroxyapatite nanoparticles datasets with different morphologies and sizes. Npj Computational Materials, 2021, 7, .	8.7	19
16	Two-dimensional Mo-based compounds for the Li-O2 batteries: Catalytic performance and electronic structure studies. Energy Storage Materials, 2021, 41, 650-655.	18.0	35
17	Mutants only partially represent characteristics of calcium-release-activated calcium channel gating. Chinese Journal of Chemical Physics, 2021, 34, 915-924.	1.3	0
18	Gating and regulation of the calcium releaseâ€activated calcium channel: Recent progress from experiments and molecular modeling. Biopolymers, 2020, 111, e23392.	2.4	1

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19	After-Pulse Characterizations of Geiger-Mode 4H-SiC Avalanche Photodiodes. IEEE Photonics Technology Letters, 2020, 32, 706-709.	2.5	5
20	Evaluation of thermoplastic polyolefin materials for the hard shed of composite insulators. Journal of Applied Polymer Science, 2020, 137, 49080.	2.6	6
21	Scorpion toxin inhibits the voltageâ€gated proton channel using a Zn²⁺â€like longâ€range conformational coupling mechanism. British Journal of Pharmacology, 2020, 177, 2351-2364.	5.4	14
22	Accurate and Efficient Prediction of NMR Parameters of Condensed-Phase Systems with the Generalized Energy-Based Fragmentation Method. Journal of Chemical Theory and Computation, 2020, 16, 2995-3005.	5.3	19
23	A Two-Ended Data-Driven Accelerated Sampling Method for Exploring the Transition Pathways between Two Known States of Protein. Journal of Chemical Theory and Computation, 2020, 16, 4631-4640.	5.3	9
24	Toward a Model for Activation of Orai Channel. IScience, 2019, 16, 356-367.	4.1	24
25	Achieving Rich Mixed-Valence Polysulfide/Carbon Nanotube Films toward Ultrahigh Volume Energy Density and Largely Deformable Pseudocapacitors. ACS Applied Materials & Interfaces, 2019, 11, 25271-25282.	8.0	7
26	Aromatic amineâ€terminated polysulfide oligomer: Synthesis and application in selfâ€healable polyurea. Journal of Polymer Science Part A, 2019, 57, 1460-1466.	2.3	11
27	In Situ Imaging Facet-Induced Spatial Heterogeneity of Electrocatalytic Reaction Activity at the Subparticle Level via Electrochemiluminescence Microscopy. Analytical Chemistry, 2019, 91, 6829-6835.	6.5	35
28	Equilibria between the K+ binding and cation vacancy conformations of potassium channels. Protein and Cell, 2019, 10, 533-537.	11.0	1
29	A Dataâ€Driven Accelerated Sampling Method for Searching Functional States of Proteins. Advanced Theory and Simulations, 2019, 2, 1800171.	2.8	6
30	Principles Governing Catalytic Activity of Self-Assembled Short Peptides. Journal of the American Chemical Society, 2019, 141, 223-231.	13.7	47
31	Identification of molecular determinants that govern distinct STIM2 activation dynamics. PLoS Biology, 2018, 16, e2006898.	5.6	29
32	Terahertz spectra of DNA nucleobase crystals: A joint experimental and computational study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 179, 255-260.	3.9	31
33	Molecular Mechanism of Self-Assembly of Aromatic Oligoamides into Interlocked Double-Helix Foldamers. Journal of Physical Chemistry B, 2017, 121, 10064-10072.	2.6	11
34	Entropy and Polarity Control the Partition and Transportation of Drug-like Molecules in Biological Membrane. Scientific Reports, 2017, 7, 17749.	3.3	21
35	Accurate Prediction of NMR Chemical Shifts in Macromolecular and Condensed-Phase Systems with the Generalized Energy-Based Fragmentation Method. Journal of Chemical Theory and Computation, 2017, 13, 5231-5239.	5.3	28
36	Understanding the Boronâ€“Nitrogen Interaction and Its Possible Implications in Drug Design. Journal of Physical Chemistry B, 2015, 119, 14393-14401.	2.6	5

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37	Counterion-Assisted Cation Transport in a Biological Calcium Channel. Journal of Physical Chemistry B, 2014, 118, 9668-9676.	2.6	15
38	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. Chemical Science, 2013, 4, 2776.	7.4	21
39	Pore waters regulate ion permeation in a calcium release-activated calcium channel. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 17332-17337.	7.1	65
40	Gating mechanism of a P2X4 receptor developed from normal mode analysis and molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 4140-4145.	7.1	51
41	Glycines: Role in Î±-Helical Membrane Protein Structures and a Potential Indicator of Native Conformation. Biochemistry, 2012, 51, 4779-4789.	2.5	71
42	Atomistic mechanism for the activation and desensitization of an AMPA-subtype glutamate receptor. Nature Communications, 2011, 2, 354.	12.8	50
43	Effects of Macromolecular Crowding on Protein Conformational Changes. PLoS Computational Biology, 2010, 6, e1000833.	3.2	82
44	Insight into the Mechanism of the Influenza A Proton Channel from a Structure in a Lipid Bilayer. Science, 2010, 330, 509-512.	12.6	422
45	A computational study towards understanding the mechanism of phosphodiester cleavage by two mononuclear Zn(ii) complexes. Physical Chemistry Chemical Physics, 2010, 12, 10434.	2.8	5
46	Understanding the Role of Intra- and Intermolecular Interactions in the Formation of Single- and Double-Helical Structures of Aromatic Oligoamides: A Computational Study. Journal of Physical Chemistry A, 2009, 113, 1335-1342.	2.5	24
47	Estimation on the Individual Hydrogen-Bond Strength in Molecules with Multiple Hydrogen Bonds. Journal of Physical Chemistry A, 2007, 111, 2941-2945.	2.5	52