Hujun Shen

List of Publications by Year
in descending order

51 papers	**1,017** citations	471509 **17** h-index	454955 **30** g-index
51 all docs	**51** docs citations	**51** times ranked	**1056** citing authors

#	ARTICLE	IF	CITATIONS
1	Second-Order Nonlinear Optics Response of the Boron-Dipyrromethenes-Based Mislinked Expanded Porphyrins: Revealing the Role of the −BF$_2$ Group. Journal of Physical Chemistry Letters, 2022, 13, 412-418.	4.6	7
2	Toward Rational Design of Dual-Metal-Site Catalysts: Catalytic Descriptor Exploration. ACS Catalysis, 2022, 12, 3420-3429.	11.2	40
3	Regulating the structure and morphology of nickel sulfides for electrochemical energy storage: The role of solvent pH. Chemical Engineering Journal, 2022, 441, 136130.	12.7	7
4	Different Binding Modes of SARS-CoV-1 and SARS-CoV-2 Fusion Peptides to Cell Membranes: The Influence of Peptide Helix Length. Journal of Physical Chemistry B, 2022, 126, 4261-4271.	2.6	6
5	Adsorption of Organic Molecules and Surfactants on Graphene: A Coarse-Grained Study. Journal of Physical Chemistry A, 2021, 125, 700-711.	2.5	2
6	Electronic Spin Moment As a Catalytic Descriptor for Fe Single-Atom Catalysts Supported on C$_2$N. Journal of the American Chemical Society, 2021, 143, 4405-4413.	13.7	138
7	Structural, transport, thermal, and electrochemical properties of (La1−xSrx)2CoO4±δ cathode in solid-oxide fuel cells. Journal of Applied Electrochemistry, 2021, 51, 411-423.	2.9	3
8	Extension of the CAVS model to the simulation of helical peptides in a membrane environment. Physical Chemistry Chemical Physics, 2021, 23, 12850-12863.	2.8	1
9	Effects of native defects and cerium impurity on the monoclinic BiVO$_4$ photocatalyst obtained *via* PBE+*U* calculations. Physical Chemistry Chemical Physics, 2020, 22, 25297-25305.	2.8	17
10	Atom-Pair Catalysts Supported by N-Doped Graphene for the Nitrogen Reduction Reaction: *d*-Band Center-Based Descriptor. Journal of Physical Chemistry Letters, 2020, 11, 6320-6329.	4.6	82
11	Hybrid Density Functional Theory Study of Native Defects and Nonmetal (C, N, S, and P) Doping in a Bi$_2$WO$_6$ Photocatalyst. ACS Omega, 2020, 5, 29081-29091.	3.5	33
12	Interfacial Water Structure at Zwitterionic Membrane/Water Interface: The Importance of Interactions between Water and Lipid Carbonyl Groups. ACS Omega, 2020, 5, 18080-18090.	3.5	7
13	An ultra-effective pathway for fully removing the oxygen components of graphene oxide by a flame-assisted microwave process. Dalton Transactions, 2020, 49, 6964-6968.	3.3	4
14	An intermittent microwave-exfoliated non-expansive graphite oxide process for highly-efficient production of high-quality graphene. Journal of Colloid and Interface Science, 2020, 565, 288-294.	9.4	9
15	Effect of Cholesterol and 6-Ketocholestanol on Membrane Dipole Potential and Sterol Flip-Flop Motion in Bilayer Membranes. Langmuir, 2019, 35, 11232-11241.	3.5	5
16	Effects of Ether Linkage on Membrane Dipole Potential and Cholesterol Flip-Flop Motion in Lipid Bilayer Membranes. Journal of Physical Chemistry B, 2019, 123, 7818-7828.	2.6	7
17	Comparative study of the binding mode between cytochrome P450 17A1 and prostate cancer drugs in the absence of haem iron. Journal of Biomolecular Structure and Dynamics, 2019, 37, 4161-4170.	3.5	7
18	Molecular Dynamics Simulations of Ether- and Ester-Linked Phospholipid Bilayers: A Comparative Study of Water Models. Journal of Physical Chemistry B, 2018, 122, 9399-9408.	2.6	6

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19	Effect of Cholesterol on Membrane Dipole Potential: Atomistic and Coarse-Grained Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2018, 14, 3780-3795.	5.3	14
20	Molecular Dynamics Simulations of Iron/Graphite Interfacial Behaviors: Influence of Oxygen. ISIJ International, 2018, 58, 1022-1027.	1.4	9
21	Effects of electrostatic interaction on the properties of ionic liquids correlated with the change of free volume. Physical Chemistry Chemical Physics, 2017, 19, 5389-5395.	2.8	10
22	Extension of CAVS coarse-grained model to phospholipid membranes: The importance of electrostatics. Journal of Computational Chemistry, 2017, 38, 971-980.	3.3	8
23	Effects of mutations on active site conformation and dynamics of RNA-dependent RNA polymerase from Coxsackievirus B3. Journal of Molecular Graphics and Modelling, 2017, 77, 330-337.	2.4	1
24	Exploring the Relation among Free Volume, Electrostatic Interaction, and Side Chain Flexibility of Ether-Functionalized Ionic Liquids by Molecular Dynamics Simulations. ChemistrySelect, 2017, 2, 5545-5551.	1.5	5
25	Coarse-Grained Modeling of Nucleic Acids Using Anisotropic Gay–Berne and Electric Multipole Potentials. Journal of Chemical Theory and Computation, 2016, 12, 676-693.	5.3	47
26	Coarse-Grained Model for Water Involving a Virtual Site. Journal of Physical Chemistry B, 2016, 120, 733-739.	2.6	19
27	Mechanistic insight into the functional transition of the enzyme guanylate kinase induced by a single mutation. Scientific Reports, 2015, 5, 8405.	3.3	4
28	An anisotropic coarse-grained model based on Gay-Berne and electric multipole potentials and its application to simulate a DMPC bilayer in an implicit solvent model. Journal of Computational Chemistry, 2015, 36, 1103-1113.	3.3	16
29	Liposomal nanohybrid cerasomes for mitochondria-targeted drug delivery. Journal of Materials Chemistry B, 2015, 3, 7291-7299.	5.8	26
30	A bimodal MRI and NIR liposome nanoprobe for tumor targeted molecular imaging. Journal of Materials Chemistry B, 2015, 3, 8832-8841.	5.8	9
31	Bridging the Missing Link between Structure and Fidelity of the RNA-Dependent RNA Polymerase from Poliovirus through Free Energy Simulations. Journal of Chemical Theory and Computation, 2014, 10, 5195-5205.	5.3	5
32	Anisotropic Coarse-Grained Model for Proteins Based On Gay–Berne and Electric Multipole Potentials. Journal of Chemical Theory and Computation, 2014, 10, 731-750.	5.3	44
33	Exploring the Proton Conductance and Drug Resistance of BM2 Channel through Molecular Dynamics Simulations and Free Energy Calculations at Different pH Conditions. Journal of Physical Chemistry B, 2013, 117, 982-988.	2.6	20
34	Coarse-grained simulations for organic molecular liquids based on Gay-Berne and electric multipole potentials. Journal of Molecular Modeling, 2013, 19, 551-558.	1.8	10
35	Theoretical Elucidation of the Origin for Assembly of the DAP12 Dimer with Only One NKG2C in the Lipid Membrane. Journal of Physical Chemistry B, 2013, 117, 4789-4797.	2.6	6
36	Molecular Recognition of Human Angiotensin-Coverting Enzyme I (hACE I) and Different Inhibitors. Current Topics in Medicinal Chemistry, 2013, 13, 1211-1221.	2.1	0

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37	Investigation Binding Patterns of Human Carboxylesterase I (hCES I) with Broad Substrates by MD Simulations. Current Topics in Medicinal Chemistry, 2013, 13, 1222-1233.	2.1	1
38	What Is the Role of Motif D in the Nucleotide Incorporation Catalyzed by the RNA-dependent RNA Polymerase from Poliovirus?. PLoS Computational Biology, 2012, 8, e1002851.	3.2	46
39	Specific and Sensitive Fluorescence Anisotropy Sensing of Guanine-Quadruplex Structures via a Photoinduced Electron Transfer Mechanism. Analytical Chemistry, 2012, 84, 8088-8094.	6.5	32
40	Chiral elasticity of DNA. Soft Matter, 2012, 8, 10090.	2.7	1
41	Exploring the Dynamics of Four RNA-Dependent RNA Polymerases by a Coarse-Grained Model. Journal of Physical Chemistry B, 2012, 116, 14515-14524.	2.6	18
42	A Review of Physics-Based Coarse-Grained Potentials for theÂSimulations of Protein Structure and Dynamics. Annual Reports in Computational Chemistry, 2012, 8, 129-148.	1.7	19
43	Investigation of Family 18 Chitinases and Inhibitors by Computer-Aided Approaches. Current Drug Targets, 2012, 13, 502-511.	2.1	5
44	Molecular Dynamics Simulations of Viral RNA Polymerases Link Conserved and Correlated Motions of Functional Elements to Fidelity. Journal of Molecular Biology, 2011, 410, 159-181.	4.2	79
45	Fast and accurate computation schemes for evaluating vibrational entropy of proteins. Journal of Computational Chemistry, 2011, 32, 3188-3193.	3.3	79
46	Gay-Berne and electrostatic multipole based coarse-grain potential in implicit solvent. Journal of Chemical Physics, 2011, 135, 155104.	3.0	36
47	An Improved Functional Form for the Temperature Scaling Factors of the Components of the Mesoscopic UNRES Force Field for Simulations of Protein Structure and Dynamics. Journal of Physical Chemistry B, 2009, 113, 8738-8744.	2.6	42
48	Implementation of a Serial Replica Exchange Method in a Physics-Based United-Residue (UNRES) Force Field. Journal of Chemical Theory and Computation, 2008, 4, 1386-1400.	5.3	7
49	On the Bidirectionality of the JWKB Connection Formula at a Linear Turning Point. Collection of Czechoslovak Chemical Communications, 2005, 70, 740-754.	1.0	3
50	JWKB method as an exact technique. International Journal of Quantum Chemistry, 2004, 99, 336-352.	2.0	13
51	Effects of Fluorination and Molybdenum Codoping on Monoclinic $BiVO_4$ Photocatalyst by HSE Calculations. ACS Omega, 0, , .	3.5	2