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	Electronic Spin Moment As a Catalytic Descriptor for Fe Single-Atom Catalysts Supported on C₂N. Journal of the American Chemical Society, 2021, 143, 4405-4413.	13.7	138
2	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
3	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
4	Fast and accurate computation schemes for evaluating vibrational entropy of proteins. Journal of Computational Chemistry, 2011, 32, 3188-3193.	3.3	79
5	Coarse-Grained Modeling of Nucleic Acids Using Anisotropic Gayâ€“Berne and Electric Multipole Potentials. Journal of Chemical Theory and Computation, 2016, 12, 676-693.	5.3	47
6	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
7	Anisotropic Coarse-Grained Model for Proteins Based On Gayâ€“Berne and Electric Multipole Potentials. Journal of Chemical Theory and Computation, 2014, 10, 731-750.	5.3	44
8	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
9	Toward Rational Design of Dual-Metal-Site Catalysts: Catalytic Descriptor Exploration. ACS Catalysis, 2022, 12, 3420-3429.	11.2	40
10	Gay-Berne and electrostatic multipole based coarse-grain potential in implicit solvent. Journal of Chemical Physics, 2011, 135, 155104.	3.0	36
11	Hybrid Density Functional Theory Study of Native Defects and Nonmetal (C, N, S, and P) Doping in a Bi₂WO₆Photocatalyst. ACS Omega, 2020, 5, 29081-29091.	3.5	33
12	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
13	Liposomal nanohybrid cerasomes for mitochondria-targeted drug delivery. Journal of Materials Chemistry B, 2015, 3, 7291-7299.	5.8	26
14	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
15	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
16	Coarse-Grained Model for Water Involving a Virtual Site. Journal of Physical Chemistry B, 2016, 120, 733-739.	2.6	19
17	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
18	Effects of native defects and cerium impurity on the monoclinic BiVO₄ photocatalyst obtained via PBE+U calculations. Physical Chemistry Chemical Physics, 2020, 22, 25297-25305.	2.8	17

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19	An anisotropic coarseâ€grained model based on <scp>G</scp>ayâ€“<scp>B</scp>erne 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
20	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
21	JWKB method as an exact technique. International Journal of Quantum Chemistry, 2004, 99, 336-352.	2.0	13
22	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
23	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
24	A bimodal MRI and NIR liposome nanoprobe for tumor targeted molecular imaging. Journal of Materials Chemistry B, 2015, 3, 8832-8841.	5.8	9
25	Molecular Dynamics Simulations of Iron/Graphite Interfacial Behaviors: Influence of Oxygen. ISIJ International, 2018, 58, 1022-1027.	1.4	9
26	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
27	Extension of CAVS coarseâ€grained model to phospholipid membranes: The importance of electrostatics. Journal of Computational Chemistry, 2017, 38, 971-980.	3.3	8
28	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
29	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
30	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
31	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
32	Second-Order Nonlinear Optics Response of the Boron-Dipyrromethenes-Based Mislinked Expanded Porphyrins: Revealing the Role of the â^'BF₂ Group. Journal of Physical Chemistry Letters, 2022, 13, 412-418.	4.6	7
33	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
34	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
35	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
36	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

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37	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
38	Exploring the Relation among Free Volume, Electrostatic Interaction, and Side Chain Flexibility of Etherâ€Functionalized Ionic Liquids by Molecular Dynamics Simulations. ChemistrySelect, 2017, 2, 5545-5551.	1.5	5
39	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
40	Investigation of Family 18 Chitinases and Inhibitors by Computer-Aided Approaches. Current Drug Targets, 2012, 13, 502-511.	2.1	5
41	Mechanistic insight into the functional transition of the enzyme guanylate kinase induced by a single mutation. Scientific Reports, 2015, 5, 8405.	3.3	4
42	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
43	Structural, transport, thermal, and electrochemical properties of (La1â^'xSrx)2CoO4Â±Î´ cathode in solid-oxide fuel cells. Journal of Applied Electrochemistry, 2021, 51, 411-423.	2.9	3
44	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
45	Adsorption of Organic Molecules and Surfactants on Graphene: A Coarse-Grained Study. Journal of Physical Chemistry A, 2021, 125, 700-711.	2.5	2
46	Effects of Fluorination and Molybdenum Codoping on Monoclinic BiVO₄ Photocatalyst by HSE Calculations. ACS Omega, 0, , .	3.5	2
47	Chiral elasticity of DNA. Soft Matter, 2012, 8, 10090.	2.7	1
48	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
49	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
50	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
51	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