Seung-gu Kang

List of Publications by Year
in descending order

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45 papers	2,006 citations	257450 24 h-index	265206 42 g-index
46 all docs	46 docs citations	46 times ranked	3466 citing authors

#	Article	IF	Citations
1	Analysis of Training and Seed Bias in Small Molecules Generated with a Conditional Graph-Based Variational Autoencoderâ”€Insights for Practical AI-Driven Molecule Generation. Journal of Chemical Information and Modeling, 2022, 62, 801-816.	5.4	5
2	CASTELO: clustered atom subtypes aided lead optimizationâ€”a combined machine learning and molecular modeling method. BMC Bioinformatics, 2021, 22, 338.	2.6	4
3	Structural cavities are critical to balancing stability and activity of a membrane-integral enzyme. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 22146-22156.	7.1	23
4	Modeling and Structural Characterization of the Sweet Taste Receptor Heterodimer. ACS Chemical Neuroscience, 2019, 10, 4579-4592.	3.5	18
5	Charging nanoparticles: increased binding of Gd@C₈₂(OH)₂₂ derivatives to human MMP-9. Nanoscale, 2018, 10, 5667-5677.	5.6	25
6	Rare Dissipative Transitions Punctuate the Initiation of Chemical Denaturation in Proteins. Biophysical Journal, 2018, 114, 812-821.	0.5	0
7	T cell receptors for the HIV KK10 epitope from patients with differential immunologic control are functionally indistinguishable. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 1877-1882.	7.1	15
8	Molecular Insight of Metallofullerenol GD@C82(OH)22 in Cancer Anti-Metastasis: In Silico Modeling of Nanodrug. Biophysical Journal, 2018, 114, 690a.	0.5	0
9	Molecular mechanism of Gd@C 82 (OH) 22 increasing collagen expression: Implication for encaging tumor. Biomaterials, 2018, 152, 24-36.	11.4	26
10	Concentration-dependent binding of CdSe quantum dots on the SH3 domain. Nanoscale, 2018, 10, 351-358.	5.6	8
11	Molecular mechanism of phosphoinositides' specificity for the inwardly rectifying potassium channel Kir2.2. Chemical Science, 2018, 9, 8352-8362.	7.4	2
12	Structural Damage of a Î²-Sheet Protein upon Adsorption onto Molybdenum Disulfide Nanotubes. Journal of Physical Chemistry C, 2016, 120, 6796-6803.	3.1	39
13	Robust Denaturation of Villin Headpiece by MoS2 Nanosheet: Potential Molecular Origin of the Nanotoxicity. Scientific Reports, 2016, 6, 28252.	3.3	33
14	Toward high permeability, selectivity and controllability of water desalination with FePc nanopores. Physical Chemistry Chemical Physics, 2016, 18, 8140-8147.	2.8	11
15	Selection of an HLA-C*03:04-Restricted HIV-1 p24 Gag Sequence Variant Is Associated with Viral Escape from KIR2DL3+ Natural Killer Cells: Data from an Observational Cohort in South Africa. PLoS Medicine, 2015, 12, e1001900.	8.4	66
16	Hydrated Excess Protons Can Create Their Own Water Wires. Journal of Physical Chemistry B, 2015, 119, 9212-9218.	2.6	83
17	Gdâ€“Metallofullerenol Nanomaterial Suppresses Pancreatic Cancer Metastasis by Inhibiting the Interaction of Histone Deacetylase 1 and Metastasis-Associated Protein 1. ACS Nano, 2015, 9, 6826-6836.	14.6	64
18	Protein corona mitigates the cytotoxicity of graphene oxide by reducing its physical interaction with cell membrane. Nanoscale, 2015, 7, 15214-15224.	5.6	204

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19	Structural and electronic properties of uranium-encapsulated Au14 cage. Scientific Reports, 2015, 4, 5862.	3.3	29
20	Interaction of Amyloid Inhibitor Proteins with Amyloid Beta Peptides: Insight from Molecular Dynamics Simulations. PLoS ONE, 2014, 9, e113041.	2.5	40
21	How force unfolding differs from chemical denaturation. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 3413-3418.	7.1	83
22	Molecular Recognition of Metabotropic Glutamate Receptor Type 1 (mGluR1): Synergistic Understanding with Free Energy Perturbation and Linear Response Modeling. Journal of Physical Chemistry B, 2014, 118, 6393-6404.	2.6	2
23	Nanomedicine: de novo design of nanodrugs. Nanoscale, 2014, 6, 663-677.	5.6	56
24	Effect of ligands on the characteristics of (CdSe)₁₃quantum dots. RSC Advances, 2014, 4, 27146-27151.	3.6	23
25	Characterization of a Novel Water Pocket Inside the Human Cx26 Hemichannel Structure. Biophysical Journal, 2014, 107, 599-612.	0.5	34
26	Size-dependent impact of CNTs on dynamic properties of calmodulin. Nanoscale, 2014, 6, 12828-12837.	5.6	18
27	Large scale molecular simulations of nanotoxicity. Wiley Interdisciplinary Reviews: Systems Biology and Medicine, 2014, 6, 329-343.	6.6	34
28	The complex and specific pMHC interactions with diverse HIV-1 TCR clonotypes reveal a structural basis for alterations in CTL function. Scientific Reports, 2014, 4, 4087.	3.3	22
29	Dual Inhibitory Pathways of Metallofullerenol Gd@C82(OH)22 on Matrix Metalloproteinase-2: Molecular insight into drug-like nanomedicine. Scientific Reports, 2014, 4, 4775.	3.3	25
30	Interactions Between Proteins and Carbonâ€Based Nanoparticles: Exploring the Origin of Nanotoxicity at the Molecular Level. Small, 2013, 9, 1546-1556.	10.0	132
31	Metallofullerenol Gd@C82(OH)22 distracts the proline-rich-motif from putative binding on the SH3 domain. Nanoscale, 2013, 5, 2703.	5.6	22
32	Hydrophobic Interaction Drives Surface-Assisted Epitaxial Assembly of Amyloid-like Peptides. Journal of the American Chemical Society, 2013, 135, 3150-3157.	13.7	56
33	Impacts of fullerene derivatives on regulating the structure and assembly of collagen molecules. Nanoscale, 2013, 5, 7341.	5.6	24
34	Salts drive controllable multilayered upright assembly of amyloid-like peptides at mica/water interface. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 8543-8548.	7.1	46
35	Non-destructive Inhibition of Metallofullerenol Gd@C82(OH)22 on WW domain: Implication on Signal Transduction Pathway. Scientific Reports, 2012, 2, 957.	3.3	41
36	Molecular mechanism of pancreatic tumor metastasis inhibition by Gd@C ₈₂ (OH) ₂₂ and its implication for de novo design of nanomedicine. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 15431-15436.	7.1	200

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37	Molecular Mechanism of Surface-Assisted Epitaxial Self-Assembly of Amyloid-like Peptides. ACS Nano, 2012, 6, 9276-9282.	14.6	29
38	Free-Energy Simulations Reveal that Both Hydrophobic and Polar Interactions Are Important for Influenza Hemagglutinin Antibody Binding. Biophysical Journal, 2012, 102, 1453-1461.	0.5	30
39	Computational design of a protein crystal. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 7304-7309.	7.1	157
40	Highly Tunable Photoluminescent Properties of Amphiphilic Conjugated Block Copolymers. Journal of the American Chemical Society, 2010, 132, 9931-9933.	13.7	131
41	Characterization of the Cofactor-Induced Folding Mechanism of a Zinc-Binding Peptide Using Computationally Designed Mutants. Journal of Molecular Biology, 2009, 389, 90-102.	4.2	19
42	Directing Noble Metal Ion Chemistry within a Designed Ferritin Protein[,]. Biochemistry, 2008, 47, 12729-12739.	2.5	84
43	Chapter 9. Protein Design: Tailoring Sequence, Structure, and Folding Properties. RSC Biomolecular Sciences, 2008, , 188-213.	0.4	0
44	Computational protein design: structure, function and combinatorial diversity. Current Opinion in Chemical Biology, 2007, 11, 329-334.	6.1	42
45	Functional modification of phosphatidylinositolâ€specific phospholipase C from Bacillus cereus by computer modeling and siteâ€directed mutagenesis. FASEB Journal, 2006, 20, A900.	0.5	0