

# 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	Protein corona mitigates the cytotoxicity of graphene oxide by reducing its physical interaction with cell membrane. <i>Nanoscale</i> , 2015, 7, 15214-15224.	5.6	204
2	Molecular mechanism of pancreatic tumor metastasis inhibition by Gd@C <sub>82</sub> (OH) <sub>22</sub> and its implication for de novo design of nanomedicine. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 15431-15436.	7.1	200
3	Computational design of a protein crystal. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 7304-7309.	7.1	157
4	Interactions Between Proteins and Carbon-Based Nanoparticles: Exploring the Origin of Nanotoxicity at the Molecular Level. <i>Small</i> , 2013, 9, 1546-1556.	10.0	132
5	Highly Tunable Photoluminescent Properties of Amphiphilic Conjugated Block Copolymers. <i>Journal of the American Chemical Society</i> , 2010, 132, 9931-9933.	13.7	131
6	Directing Noble Metal Ion Chemistry within a Designed Ferritin Protein. <i>Biochemistry</i> , 2008, 47, 12729-12739.	2.5	84
7	How force unfolding differs from chemical denaturation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 3413-3418.	7.1	83
8	Hydrated Excess Protons Can Create Their Own Water Wires. <i>Journal of Physical Chemistry B</i> , 2015, 119, 9212-9218.	2.6	83
9	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. <i>PLoS Medicine</i> , 2015, 12, e1001900.	8.4	66
10	Gd-Metallofullerenol Nanomaterial Suppresses Pancreatic Cancer Metastasis by Inhibiting the Interaction of Histone Deacetylase 1 and Metastasis-Associated Protein 1. <i>ACS Nano</i> , 2015, 9, 6826-6836.	14.6	64
11	Hydrophobic Interaction Drives Surface-Assisted Epitaxial Assembly of Amyloid-like Peptides. <i>Journal of the American Chemical Society</i> , 2013, 135, 3150-3157.	13.7	56
12	Nanomedicine: de novo design of nanodrugs. <i>Nanoscale</i> , 2014, 6, 663-677.	5.6	56
13	Salts drive controllable multilayered upright assembly of amyloid-like peptides at mica/water interface. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 8543-8548.	7.1	46
14	Computational protein design: structure, function and combinatorial diversity. <i>Current Opinion in Chemical Biology</i> , 2007, 11, 329-334.	6.1	42
15	Non-destructive Inhibition of Metallofullerenol Gd@C <sub>82</sub> (OH) <sub>22</sub> on WW domain: Implication on Signal Transduction Pathway. <i>Scientific Reports</i> , 2012, 2, 957.	3.3	41
16	Interaction of Amyloid Inhibitor Proteins with Amyloid Beta Peptides: Insight from Molecular Dynamics Simulations. <i>PLoS ONE</i> , 2014, 9, e113041.	2.5	40
17	Structural Damage of a $\beta$ -Sheet Protein upon Adsorption onto Molybdenum Disulfide Nanotubes. <i>Journal of Physical Chemistry C</i> , 2016, 120, 6796-6803.	3.1	39
18	Characterization of a Novel Water Pocket Inside the Human Cx26 Hemichannel Structure. <i>Biophysical Journal</i> , 2014, 107, 599-612.	0.5	34

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19	Large scale molecular simulations of nanotoxicity. Wiley Interdisciplinary Reviews: Systems Biology and Medicine, 2014, 6, 329-343.	6.6	34
20	Robust Denaturation of Villin Headpiece by MoS2 Nanosheet: Potential Molecular Origin of the Nanotoxicity. Scientific Reports, 2016, 6, 28252.	3.3	33
21	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
22	Molecular Mechanism of Surface-Assisted Epitaxial Self-Assembly of Amyloid-like Peptides. ACS Nano, 2012, 6, 9276-9282.	14.6	29
23	Structural and electronic properties of uranium-encapsulated Au <sub>14</sub> cage. Scientific Reports, 2015, 4, 5862.	3.3	29
24	Molecular mechanism of Gd@C <sub>82</sub> (OH) <sub>22</sub> increasing collagen expression: Implication for encaging tumor. Biomaterials, 2018, 152, 24-36.	11.4	26
25	Dual Inhibitory Pathways of Metallofullerenol Gd@C <sub>82</sub> (OH) <sub>22</sub> on Matrix Metalloproteinase-2: Molecular insight into drug-like nanomedicine. Scientific Reports, 2014, 4, 4775.	3.3	25
26	Charging nanoparticles: increased binding of Gd@C <sub>82</sub> (OH) <sub>22</sub> derivatives to human MMP-9. Nanoscale, 2018, 10, 5667-5677.	5.6	25
27	Impacts of fullerene derivatives on regulating the structure and assembly of collagen molecules. Nanoscale, 2013, 5, 7341.	5.6	24
28	Effect of ligands on the characteristics of (CdSe) <sub>13</sub> quantum dots. RSC Advances, 2014, 4, 27146-27151.	3.6	23
29	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
30	Metallofullerenol Gd@C <sub>82</sub> (OH) <sub>22</sub> distracts the proline-rich-motif from putative binding on the SH3 domain. Nanoscale, 2013, 5, 2703.	5.6	22
31	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
32	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
33	Size-dependent impact of CNTs on dynamic properties of calmodulin. Nanoscale, 2014, 6, 12828-12837.	5.6	18
34	Modeling and Structural Characterization of the Sweet Taste Receptor Heterodimer. ACS Chemical Neuroscience, 2019, 10, 4579-4592.	3.5	18
35	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
36	Toward high permeability, selectivity and controllability of water desalination with FePc nanopores. Physical Chemistry Chemical Physics, 2016, 18, 8140-8147.	2.8	11

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37	Concentration-dependent binding of CdSe quantum dots on the SH3 domain. <i>Nanoscale</i> , 2018, 10, 351-358.	5.6	8
38	Analysis of Training and Seed Bias in Small Molecules Generated with a Conditional Graph-Based Variational Autoencoder—Insights for Practical AI-Driven Molecule Generation. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 801-816.	5.4	5
39	CASTELO: clustered atom subtypes aided lead optimization—a combined machine learning and molecular modeling method. <i>BMC Bioinformatics</i> , 2021, 22, 338.	2.6	4
40	Molecular Recognition of Metabotropic Glutamate Receptor Type 1 (mGluR1): Synergistic Understanding with Free Energy Perturbation and Linear Response Modeling. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6393-6404.	2.6	2
41	Molecular mechanism of phosphoinositides' specificity for the inwardly rectifying potassium channel Kir2.2. <i>Chemical Science</i> , 2018, 9, 8352-8362.	7.4	2
42	Rare Dissipative Transitions Punctuate the Initiation of Chemical Denaturation in Proteins. <i>Biophysical Journal</i> , 2018, 114, 812-821.	0.5	0
43	Molecular Insight of Metallofullerenol GD@C82(OH)22 in Cancer Anti-Metastasis: In Silico Modeling of Nanodrug. <i>Biophysical Journal</i> , 2018, 114, 690a.	0.5	0
44	Functional modification of phosphatidylinositol-specific phospholipase C from <i>Bacillus cereus</i> by computer modeling and site-directed mutagenesis. <i>FASEB Journal</i> , 2006, 20, A900.	0.5	0
45	Chapter 9. Protein Design: Tailoring Sequence, Structure, and Folding Properties. <i>RSC Biomolecular Sciences</i> , 2008, , 188-213.	0.4	0