

# Seung-gu Kang, Ph.D.

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## Education and training

- 2002 – 2009 Ph.D. Chemistry, University of Pennsylvania, Philadelphia, PA, USA  
“Probabilistic computational protein design: Advances in methodology and the incorporation of non-biological molecular components”, Prof. Jeffery G. Saven
- 1996 – 1998 M.S. Chemistry, Yonsei University, Seoul, Korea
- 1992 – 1996 B.S. Chemistry, Yonsei University, Seoul, Korea

## Professional experiences

- 2011 – Postdoctoral research fellow, IBM T.J. Watson Research Center, Yorktown Height, NY, USA
- 2010 – 2010 Postdoctoral fellow in Chemistry, University of Pennsylvania, Philadelphia, PA, USA
- 1998 – 2002 Korea Air Force Academy, Lecturer in Chemistry, Chungju, Korea

## Publications

1. Yang X<sup>†</sup>, **Kang SG**<sup>†</sup>, Zhou R, “Nanomedicine: de novo design of nanodrugs”, *Nanoscale*, **2014**, 6:663-77. (<sup>†</sup> Equal contribution)
2. Das P, **Kang SG**, Temple S, Belfort GE, Chaperone binding to amyloid beta oligomers inhibits aggregation: insight from molecular dynamics simulations”, *Plos. Comp. Biol.*, **2013**, in review.
3. **Kang SG**, Das P, McGrane SJ, Martin AJ, Huynh T, Royyuru AK, Taylor AJ, Jones PG, Zhou R, “Molecular recognition of metabotropic glutamate receptor type 1 (mGluR1): Synergistic understanding with free energy perturbation and linear response modeling”, *J. Phys. Chem. B*, **2013**, in review.
4. Jimenez-Cruz C, **Kang SG**, Zhou R, “Large-scale molecular simulations for nanotoxicity”, *WIREs Systems Biology and Medicine*, **2013**, in review.
5. Araya-Secchi R, **Kang SG**, Huynh T, Bernardin A, Martinez AD, Saez JC, Perez-Acle T, Zhou R, “Characterization of a novel water pocket inside the human Cx26 hemi-channel structure”, *Biophysical J.*, **2013**, in review.
6. Stirnemann G, **Kang SG**, Zhou R, Berne BJ, “How force unfolding differs from thermal or chemical denaturation”, *Proc. Natl. Acad. Sci. USA*, **2013**, in review.
7. Xia Z<sup>†</sup>, Chen H<sup>†</sup>, **Kang SG**, Huynh T, Fang J, Lamothe P, Walker B, Zhou R, “The complex and specific pMHC interactions with diverse HIV-1 TCR clonotypes reveal a structural basis for alterations in CTL function”, *(Nature) Scientific Reports*, **2013**, in review.
8. Yin X<sup>†</sup>, Zhao L<sup>†</sup>, **Kang SG**, Pan J, Song Y, Zhang M, Xing G, Wang F, Li J, Zhou R, Zhao Y, “Impact of fullerene derivatives on regulating the structure and assembly of collagen molecules”, *Nanoscale*, **2013**, 5:7341-8. (<sup>†</sup> Equal contribution)
9. Dai B<sup>†</sup>, **Kang SG**<sup>†</sup>, Huynh T, Lei H, Castelli M, Hu J, Zhang Y, Zhou R, “Salts drive controllable multi-layered upright assembly of amyloid-like peptides at mica/water interface”, *Proc. Natl. Acad. Sci. USA*, **2013**, 110:8543-8. (<sup>†</sup> Equal contribution)
10. **Kang SG**, Huynh T, Zhou R, “Metallofullerenol Gd@C<sub>82</sub>(OH)<sub>22</sub> distracts the proline-rich motif from putative binding on the SH3 domain”, *Nanoscale*, **2013**, 5:2703-12.
11. **Kang SG**, Huynh T, Xia Z, Zhang Y, Fang H, Wei G, Zhou R, “Hydrophobic interaction drives surface-assisted epitaxial assembly of amyloid-like peptides”, *Journal of American Chemical Society*, **2013**, 135:3150-7.
12. **Kang SG**, Huynh T, Zhou R, “Non-destructive inhibition of metallofullerenol Gd@C<sub>82</sub>(OH)<sub>22</sub> on WW domain: Implication on signal transduction pathway”, *(Nature) Scientific Reports*, **2012**, 2:957 (DOI:10.1038/srep.00957).

13. **Kang SG**, Li H, Huynh T, Zhang F, Xia Z, Zhang Y, Zhou R, "Molecular mechanism of surface-assisted epitaxial self-assembly of amyloid-like peptides", *ACS Nano*, **2012**, 6:9276-82.
14. Zuo G, **Kang SG**, Xiu P, Zhao Y, Zhou R, "Interaction between proteins and carbon-based nanoparticles: Exploring the origin of nanotoxicity at the molecular level", *Small*, **2012**, DOI:10.1002/smll.201201381.
15. **Kang SG**, Zhou G, Yang P, Liu Y, Sun B, Huynh T, Meng H, Zhao L, Xing G, Chen C, Zhao Y, Zhou R, "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", *Proc. Natl. Acad. Sci. USA*, **2012**, 109:15431-6. (featured in *PNAS Highlight*, *MIT-Technology Review*, *Nature-SciBX*, *PNNL News* and *IBM Research*)
16. Lanci CJ<sup>†</sup>, MacDermaid CM<sup>†</sup>, **Kang SG**, Acharya R, North B, Yang X, Qiu XJ, DeGrado WF, Saven JG, "Computation design of a protein crystal", *Proc. Natl. Acad. Sci. USA*, **2012**, 109:7304-9. (<sup>†</sup> Equal contribution)
17. Xia Z, Huynh T, **Kang SG**, Zhou R, "Free energy simulation reveal that both hydrophobic and polar interactions are important for influenza hemagglutinin antibody binding", *Biophysical Journal*, **2012**, 102:1453-61.
18. Park SJ, **Kang SG**, Saven JG, Park SJ, "Highly tunable photoluminescent properties of amphiphilic conjugated block copolymers", *Journal of American Chemical Society*, **2010**, 132:9331-33.
19. Tang J<sup>†</sup>, **Kang SG**<sup>†</sup>, Saven JG, Gai F, "Characterization of the cofactor-induced folding mechanism of a zinc-binding peptide using computationally designed mutants", *Journal of Molecular Biology*, **2009**, 389:90-102. (<sup>†</sup> Equal contribution)
20. Butts CA, Swift J, **Kang SG**, Constanzo LD, Christianson DW, Saven JG, Dmochowski IJ, "Directing noble metal ion chemistry within a designed ferritin protein", *Biochemistry*, **2008**, 47:12729-39.
21. **Kang SG**, Saven JG, "Computational protein design: structure, function and combinatorial diversity", *Current Opinion in Chemical Biology*, **2007**, 11:329-34.
22. **Kang SG**, Chae WS, Kim YR, Jung JS, Lee SH, "Electronic energy dynamics of photoexcited ternary Zintl phase LiSbTe<sub>2</sub> and the distance estimation between trap sites", *Chemical Physics*, **2000**, 256:295-305.

#### Manuscripts in preparation

1. Kang SG, et al, "How to deactivate cancer-related gene expression: Molecular mechanism of carbon-based nanodrug on histone deacetylase", aiming for *Nature Biotech*.
2. Kang SG, et al, "Between cell death and survival: Combined effect of carbon-based nanodrug on cell survival pathway of TNF- $\alpha$  response", aiming for *Proc. Natl. Acad. Sci. USA*.
3. Kang SG, et al, "Molecular mechanism of carbon-based nanodrug on immune regulation through Toll-like receptor, aiming for *Proc. Natl. Acad. Sci. USA*.
4. Kang SG, et al, "Dual inhibitory pathways of metallofullerenol Gd@C<sub>82</sub>(OH)<sub>22</sub> on matrix metalloproteinase-2: Insight into anti-metastatic nanomedicines".
5. Kang SG, et al, "Molecular mechanism of membrane translocation of inorganic quantum dots".

#### Book Chapters

1. **Kang SG**, Zhou R, "Protein and Nanoparticle Interactions: Perspectives of Nanomedicine and Nanotoxicity", *Molecular Modeling at the Atomic Scale: Methods and Applications in Quantitative Biology*, Ed. by Zhou R, Taylor & Francis Books, Inc., **2013**, in press.
2. Lehmann A, Lanci CJ, Petty II TJ, **Kang SG**, Saven JG, "Protein Design: Tailoring Sequence, Structure and Folding Properties", *Protein Folding, Misfolding and Aggregation*, Ed. by Muñoz V, The Royal Society of Chemistry: Cambridge, **2008**, 188-213
3. **Kang SG**, Kim YR, "Solid-state Electronic Energy Dynamics using Power Saturation Spectroscopy", *Solid State Chemistry*, Ed. by Yo CH, Freedom Academy Pub. Co., **2003**

## **Patents**

1. **Kang SG**, Luan B, Zhou R, "A new chemical compound targeting receptor SecA for Citrus Greening disease", **2013**, DISCLOSURE NO. YOR820131858.
2. Luan B, **Kang SG**, Zhou R, "A new chemical compound targeting receptor transcription factor for Citrus Greening disease", **2013**, DISCLOSURE NO. YOR820131859.

## **Honors and Awards**

1. Eminence and Excellence Award, IBM for "Systematic ligand designs for sensory membrane protein", **2011**.
2. IBM Accomplishment Award, IBM for "*De novo* design of nanomedicine: implications from nanotoxicity", **2013**.
3. Eminence and Excellence Award, IBM for "drug design for Citrus Greening disease", **2013**.
4. Outstanding Technical Achievement Award (OTAA, the highest technical award of IBM), IBM, in review.