STEVENS INSTITUTE of TECHNOLOGY
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# *In silico* Design of Nano-Bio Interaction: Theoretical Approach for Nanomedicine and Nanostructuring

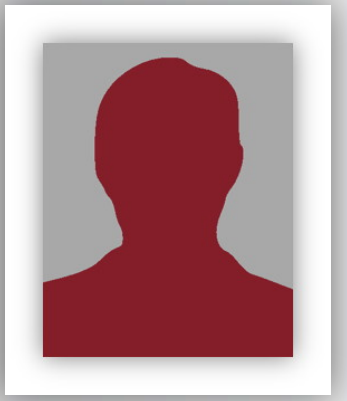

## Dr. Seung-gu Kang

Computational Biology Center, IBM T.J. Watson Research Center



**ABSTRACT:** Interfacial dynamics between nano-bio systems determines structure and function of nanomaterials with versatile applications in biological and medical sciences. Molecular level understanding of nano-bio interactions is thus essential in designing *de novo* nanomaterials with desired function and structure, which would be even more critical in evaluating potential adverse effects related to nanotoxicity. However, the intermolecular interactions are often not well understood due to intricate interplays between various weak forces. In this talk, I introduce large scale molecular dynamics (MD) simulations with two recent studies in nanomedicine and peptide self-assembly. First, I'll show how metallofullerenol $Gd@C_{82}(OH)_{22}$, originally developed as a high-contrasting imaging agent, can inhibit matrix metalloproteinase-9 (MMP-9), a key enzyme required for cancer proliferation and migration. $Gd@C_{82}(OH)_{22}$ showed specific antitumoral efficacies in vivo experiment with human pancreatic cancer. Using MD simulations, we revealed binding dynamics of the nanoparticle on MMP-9, and specified driving forces along the proposed inhibitory pathway. Our finding provides theoretical basis for atomistic details of inhibitory mechanism of $Gd@C_{82}(OH)_{22}$ as a potential nanodrug, as well as important insight in designing *de novo* nano-therapeutics. Then, I will discuss surface-assisted peptide self-assembly. Recently, we found that 9-residue amyloid-like peptides called GAV-9 can form highly-organized epitaxial assembly with different morphologies depending on substrate surfaces and salt condition: "flat" on hydrophobic graphite surface, while "upright" on hydrophilic mica and even multilayered in high salt condition. We found that, in addition to polarity, the lattice structure of basal surface closely incorporates with peptide structure, determining molecular packing and thus overall morphology. Energetic investigation revealed that the longitudinal and transversal growths are each differently driven by hydrophobic and hydrophilic interactions. Furthermore, we showed that the high salt condition drive not only multiple-layered conformation, but also different packing mode. Our findings show complexities in soft matter interactions, but also imply that adjusting weak forces plays an important role in nanostructure designs.


**BIOGRAPHY:** Dr. Seung-gu Kang received his B.S. in Chemistry, and M.S. with ultrafast laser spectroscopy from Yonsei University in 1996 and 1998, respectively. For 40 months of military service, he worked as a full-time lecturer in Chemistry Dept. of Korea Air-Force Academy. Then, he received his Ph.D. in Chemistry from Penn in 2009, where he studied in theoretical biophysics. Currently, he is working as a post-doc in Computational Biology Center of IBM T.J. Watson Research Center, focusing on protein-protein and protein-nano interactions using large scale molecular dynamics simulations.



## EVENT DETAILS

**DATE:**
Wednesday Sept. 25, 2013

**TIME:**
1:00 PM

**LOCATION:**
Carnegie, Room 315
Stevens Institute of Technology

**ATTENDANCE:**
This event is open to Stevens' Faculty, Students, Staff, and Invited Guests