Seonghan Kim

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Summary

Conducting research across a broad range of chemistry, biophysics, and nanomaterials using computational tools including physics-based molecular modeling, molecular dynamics (MD) simulations, enhanced sampling methods, free energy calculations, quantum chemistry, and scientific software development (CHARMM-GUI).

Education

Ph.D., Bioengineering, Lehigh University, PA Advisor: Wonpil Im, Ph.D. (homepage)	2019-2023
Graduate student, Chemistry, NC State University, NC	2017-2018
M.S., Chemistry, Kwangwoon University, Seoul, South Korea Advisor: Rakwoo Chang, Ph.D. (homepage)	2014-2016
B.S., Chemistry (Intensive Education Program), Kwangwoon University, Seoul, South Korea	2008-2014

Research Experience

Postdoctoral Research Associate, Oak Ridge National Laboratory   2024-
- Molecular modeling and simulation of bio/polymer systems for Biopreparedness Research Virtual Environment (BRaVE) project
  - Modeling and simulation of polyelectrolyte and polyzwitterion brushes on nanosurfaces, using multiscale simulation (quantum calculation and all-atom) methods to study dynamics of the polymers and their interactions with proteins.
  - Comparing results with sum frequency generation (SFG), surface plasmon resonance (SPR), neutron reflectometry (NR), and atomic force microscopy (AFM) experiments to provide a molecular-level of understanding in a fast-paced research environment.

Ph.D. Student, Department of Bioengineering, Lehigh University   2019-2023
- Comparison of cross-docking performance of docking programs
  - Studying effects of input ligand pre-processing and parameters by utilizing AutoDock Vina, RxDock, Smina, DiffDock, and FABind.
- Molecular basis of human olfactory receptor activation (collaboration with experiments)
  - Modeling and running MD simulation of an olfactory GPCR, examining the binding/unbinding behaviors of ligand to the binding pocket. Applied post translational modification (PTM), lipidation.
- CHARMM-GUI Bicelle Builder development
  - Developed a user-friendly web-based platform for modeling and simulation of bicelle systems.
- Interactions between peptides and 2D nanosheets (collaboration with experiments)
  - Investigation of nano-bio interface system to gain insights into the dynamical behavior of peptides at different concentrations on each using MD simulation. Collaboration with experimental groups.
- Nanomaterial Modeler development
  - Contributed to its capability to generate 400+ nanomaterials such as metals, silica, battery oxides, etc., for modeling and simulations of nanomaterial systems. Wrote MD simulation input files for major MD packages including CHARMM, NAMD, OpenMM, GROMACS, and LAMMPS.
- SARS-CoV-2 RBD variants and human receptors interaction (collaboration with experiments)
  - Conducted MD simulations to evaluate stability of RBD of SARS-CoV-2 and Neuropilin-1 receptor generated by AlphaFold2 to investigate protein-protein interactions.

- Built systems and conducted enhanced sampling simulations, steered molecular dynamics (SMD), to characterize the binding interactions between ACE2 and the RBD of SARS-CoV-2 variants, including the wild type, Alpha, Beta, Gamma, Delta, Epsilon, Kappa, and Omicron variants. Identified key interacting residues and effects of each mutation between RBD and ACE2.
- Compared SARS-CoV-2 and SARS-CoV-1 in terms of their interactions with human ACE2 receptor, identified key interacting residues and effects of glycans by inducing PTM, glycosylation, and suggested their dissociation mechanism by utilizing SMD simulation.

Graduate Student, Department of Chemistry, NC State University 2017-2018
- Characterization of perinone series using the ultrafast transient absorption spectroscopy
- DFT calculations of perinone series

Graduate Research Assistant, Chemistry, Kwangwoon University (collaboration with experiments) 2014-2016
- Effects of oxidized lipid bilayer membranes by plasma treatment
- Computational study of DOPC/DSPC mixture membrane systems

Undergraduate Research Fellow, Chemistry, Kwangwoon University 2012-2014
- Mechanism study of reaction of MIO enzyme using DFT and QM/MM
- The EDISON project - development of computer programs for physical chemistry education

Selected Publications (*equal contribution) | [Google Scholar](#) Citations: 508 | h-index: 8 | i10-index: 7 (as of 01-21-2025)

1. Choi, C.*; Bae, J.*; **Kim, S.**; Lee, S.; Kang, H.; Kim, J.; Bang, I.; Kim, K.; Huh, W.; Seok, C.; Park, H.; Im. W.; Choi, H.
   Understanding the molecular mechanisms of odorant binding and activation of the human OR52 family.
   Nat. Commun. **2023**, 14, 8105 ([doi:10.1038/s41467-023-43983-9](#)) | Citations: 13

2. **Kim, S.**; Liu, Y.; Ziarnik, M.; Cao, Y.; Zhang, X. F.; Im, W.
   Binding of Human ACE2 and RBD of Omicron Enhanced by Unique Interaction Patterns among SARS-CoV-2 Variants of Concern.
   J. Comput. Chem. **2023***, 44, 594-601* ([doi:10.1002/jcc.27025](#)) | Citations: 75

3. Choi, Y. K.*; Kern, N. R.*; **Kim, S.***; Jo, S.; Brooks, B. R.; Tadmor, E.; Heinz, H.; Lee, J.; Im. W.
   CHARMM-GUI Nanomaterial Modeler for Modeling and Simulations of Nanomaterials.
   J. Chem. Theory Comput. **2022**, *18*, 479-493 ([doi:10.1021/acs.jctc.1c00996](#)) | Citations: 115

4. Kanhaiya, K.; **Kim, S**.; Im, W.; Heinz, H.
   Accurate Simulation of Surfaces and Interfaces of Ten FCC Metals and Steel using Lennard-Jones Potentials.
   NPJ. Comput. Mater. **2021**, 7 (1), 17 ([doi:10.1038/s41524-020-00478-1](#)) | Citations: 70

5. **Kim, S.**; Liu, Y.; Lei, Z.; Dicker, J.; Cao, Y.; Zhang, X. F.; Im, W.
   Differential Interactions between Human ACE2 and Spike RBD of SARS-CoV-2 Variants of Concern.
   J. Chem. Theory Comput. **2021**, *17*, 7972-7979 ([doi:10.1021/acs.jctc.1c00965](#)) | Citations: 98

6. Cao, W.*; Dong, C.*; **Kim, S.***; Hou, D.; Tai, W.; Du, L.; Im, W.; Zhang, X. F.
   Biomechanical characterization of SARS-CoV-2 spike RBD and human ACE2 protein-protein interaction.
   [[News Article](#)]
   Biophys. J. **2021**, *120* (6), 1011-1019 ([doi:10.1016/j.bpj.2021.02.007](#)) | Citations: 107

Invited Talks

1. The 68th Biophysical Society Annual Meeting, Los Angeles, CA. January 2025.
2. Department of Chemistry, Chungbuk National University, South Korea. December 2024.

Conference & Symposium Presentations

1. **Kim, S.**; Yang, Z.; Carrillo, J-M.; Ganesh, P.; Retterer, S. The 68th Biophysical Society Annual Meeting, Los Angeles, CA. January 2025.
2. **Kim, S.**; Yang, Z.; Carrillo, J-M.; Ganesh, P.; Retterer, S. Computational Medicinal Chemistry School, Novartis Institutes for Biomedical Research, Cambridge, MA. October 2024.
3. **Kim, S.**; Yang, Z.; Carrillo, J-M.; Ganesh, P.; Retterer, S. ORNL OLCF User Meeting, Oak Ridge, TN. September 2024.
4. **Kim, S.**; Walker, C.; Carrillo, J-M.; Ganesh, P. Retterer, S. ORNL CNMS User Meeting, Knoxville, TN. August 2024.
5. **Kim, S.**; Im, W. 2023 Biophysics Summer School: Soft Living Matter, Rethymno, Crete, Greece. August 2023.
6. **Kim, S.**; Im. W. Korean American Society in Biotech and Pharmaceuticals Spring Symposium, Waltham, MA. June 2023.
7. **Kim, S.**; Kern, N.; Baryiames, C.; Tieleman, P.; Columbus, L.; Im, W. The 67th Biophysical Society Annual Meeting, San Diego, CA. February 2023.
8. **Kim, S.**; Liu, Y.; Lei, Z.; Dicker, J.; Cao, Y.; Zhang, X. F.; Im, W. The 66th Biophysical Society Annual Meeting, San Francisco, CA. February 2022.
9. **Kim, S.**; R. Chang. The 250th American Chemical Society & Exhibition, Boston, MA. August 2015.

Scientific Service

Peer Review
- Biochemistry   2024
- Langmuir   2024
- Virus Research   2023
- [Annual Reviews in Biophysics](#) (contribution to the scientific discussion in the manuscript)   2023
- Informatics in Medicine Unlocked   2022

Awards

- Elizabeth V. Stout Dissertation Award, Lehigh University   2024
- Best Student Poster Award, Bioengineering Graduate Research Day, Lehigh University   2023
- Teaching Certificate Award, NC State University   2018
- International Travel Award, The 250th American Chemical Society National Meetings   2015
- Physical Chemistry Best Student Poster Award, Korean Chemical Society Meetings   2014

Teaching and Mentoring Experience

Lehigh University   2021-2023
- Mentoring undergraduate and high school students
- Methods and Logics in Biological Research (a special lecture to first year PhD students)
- VMD Tutorial (to junior group members)
- Chemistry Lab

NC State University   2017-2018
- General Chemistry Lab
- Quantitative Chemistry and Lab

Kwangwoon University   2013-2015
- General Chemistry Lab
- Chemistry Colloquium