DISTINGUISHED
STAFF FELLOWS
AT ORNL

GS Jung

Eugene P. Wigner Fellow

Where and when did you earn your PhD?

I received my PhD in civil and environmental engineering from Massachusetts Institute of Technology in 2019.

What was the subject of your dissertation?

My dissertation focused on developing multiscale models to understand fracture and synthesis processes of 2D materials such as graphene, tungsten disulfide, and molybdenum disulfide. Using computational methods, I examined how these materials behave when such 2D crystals structurally fail or form grain boundaries at the atomic level, to understand fundamental mechanisms at the atomic scale and how it can change the macroscale properties.

What was your dissertation's major contribution to your field?

The tools and parameters I developed help scientists understand how 2D materials deform and fail under various conditions and how 3D structural design of 2D graphene can tune materials' thermal and mechanical properties, to contribute to the design of 2D materials. My tools recently were utilized to reveal the mechanisms of 2D molybdenum disulfide crystal growth in collaboration with the Center for Nanophase Materials Sciences at ORNL.

Who is your ORNL mentor and where are you working on campus?

My mentor is Stephan Irle, Computational Chemistry and Nanomaterial group leader in the Computational Sciences and Engineering Division. I work in the Computational Chemistry and Nanomaterial Group.

What will your fellowship research focus on?

My fellowship research focuses on developing integrated multiscale models that enable predictive design and simulation of materials of interest at ORNL. For this purpose, I am developing computational tools including sampling methods, parameters, and machine-learned atomic potentials, which eventually will provide an essential modeling frame for materials design and synthesis in both continuum-level simulation and experiments.

What is your project's expected contribution to your field?

My project aims to develop essential tools of multiscale models for universal materials. The main contribution will be understanding mechanical and thermodynamical behaviors of materials. In the longer term, I hope my project will be the cornerstone of a virtual lab where novel materials can be designed, synthesized, and characterized. I am working on ORNL's C4WRD project, which aims to develop the underlying and translational science supporting development of coal-derived carbon fibers. I am working to understand how the molecular precursors from coal can form carbon fiber and how their mechanical properties can be designed.

What are your research interests?

After I earned my master's degree, I worked 3 years at LG making LCDs to satisfy my requirement for military duty as a Korean citizen. I found a need for appropriate models that could significantly reduce the time and cost for research and development. After that, I joined a Korean computing institute to learn about high-performance computing (HPC) before coming to the United States to study. Both experiences have guided my current research interests to build a virtual lab where materials can be designed, synthesized, and characterized by combining and bridging advanced computational methods at different scales. I'm excited to be able to use ORNL's world-leading high-performance computing resources and opportunities to collaborate with world-leading experts.

What led you to science and your specific discipline?

When I was a teenager, I saw the movie "The Invisible Man." The story involves a scientist trying to develop a medicine to make human tissue, and therefore human beings, invisible using computers. He tries to make a molecule and check its performance and stability with computer simulations. The scientist's process of experimentation looked very interesting and made me want to develop such tools using computers. Later on, I learned that quantum mechanics can predict the properties of materials. However, I realized quantum mechanics' focus on the atomic scale was only part of the full story and started to learn various theoretical approaches that consider different length and time scales.

What did you do before coming to ORNL?

I earned graduate and undergraduate degrees in physics at universities in Japan and then worked at LG in Korea, using experimental analysis and simulations to advance the technology behind touch panels embedded in LCDs. I also did HPC at the Korean Institute of Science and Technology Information, developing classical molecular dynamics with MPI/OpenMPI. At MIT, I worked more on the application side of modeling using molecular dynamics simulations to understand the atomic-scale behaviors of materials (e.g., 2D crystals, biominerals, and collagen). I developed my own tools and parameters for those applications.

Could you share an interesting fact or two about yourself?

I did vocals for 3 years in a pop band during my undergrad years in Japan. About 3 years ago, before COVID-19 drove everyone to video meetings, I started getting together with friends in Asia via Skype on Saturday mornings to discuss and study a particular interest of mine—machine learning. The things I've learned is very helpful for my research.