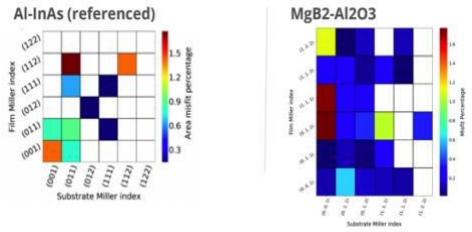
Materials by the Numbers

Andrea Hwang is headed to UC Berkeley to study computational materials science as a Ph.D. student

Growing up in the Bay Area of California, **Andrea Hwang** *(B.S. 2021)* was interested in physics and chemistry, but had no awareness of materials science. In fact, she arrived at Carnegie Mellon in fall 2017 as a chemistry major. That changed quickly, however, when she enrolled in "Engineering the Materials of the Future," taught by **Professor Noa Marom.**

"I realized that materials science actually brings together the best aspects of both physics and chemistry," Hwang explains. "I was fascinated not by looking at materials at the atomic scale, but by looking at their larger structures and their patterns of behavior. It was interesting to see the various ways you could customize materials for a specific application. I quickly changed my major to MSE."

Hwang spent three years in Marom's research group as an undergraduate assistant, using computer simulation tools to better understand materials bonds, structures, and properties. Specifically, she investigated materials improvements that would support advances in quantum computing. "Quantum computing has the capability to enhance supercomputing, but it requires new processes and new materials," says Hwang. "It's been exciting to work with Professor Marom on these kinds of innovations." Along the way, Hwang added a minor in Electronic Materials to reflect her growing interest in developing materials for quantum computing applications.



Results of lattice matching for interfaces with different substrate and film orientations: on the left, a cubic interface between Al and InAs and on the right, a hexagonal interface between MgB_2 and Al_2O_3.

Hwang also worked as a research intern at IBM, developing new materials for magnetoelectronics and spintronics applications. An internship at Northwestern in summer 2020 allowed her to focus on computational modeling of soft matter. Her computational models of phase transitions required her to write her own scripts to calculate and plot desired materials properties.

Structure Prediction of Epitaxial Inorganic Interfaces

Hwang's honors research project at CMU focused on predicting the structure and electronic properties of interfaces between inorganic materials, which are at the core of semiconductor, spintronic, and quantum devices.

To this end, she collaborated with Ph.D. students **Shuyang Yang, Saeed Moayedpour**, and **Derek Dardzinski.** The team implemented in the Ogre code new functionalities of lattice and surface matching [see: arXiv:2103.13947 (2021)]. Hwang's contribution was writing functions to convert between cubic and hexagonal Miller indices, a notation system in crystallography for defining planes in crystal lattices, which is used in Ogre to construct interface structures.

She presented the preliminary results of her research at CMU's Meeting of the Minds event in May. At MSE's Commencement ceremony, Hwang received the Hubert I. Aaronson Undergraduate Award.

A Pioneer in the Lab — and Eventually the Classroom

"Computational modeling is an incredible way to analyze and predict materials behavior for complex applications like electronics," Hwang notes. "But computational materials scientists are breaking new ground, and that means creating entirely new techniques."

Hwang will continue pioneering new computational modeling techniques this fall as a doctoral student at the University of California, Berkeley.

Eventually, Hwang hopes to work as a faculty member, leading a research team and educating the next generation of materials scientists. "From introducing me to the field of materials science to serving as my research advisor, Professor Marom has been an inspiration to me. And I've been positively impacted by every one of my professors at Carnegie Mellon," says Hwang. "I hope to one day influence future materials scientists and support continuing innovation in our field."