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New Materials Simulation Lab will advance materials by harnessing the power of computer simulations

The College of Engineering celebrated the opening of a new lab space for the Materials Simulation Laboratory in the Department of Chemical Engineering and Materials Science (CHEMS) on Monday, Aug. 7. The lab has an open floor plan and is located in Room 1105 on the first floor of the College of Engineering Building.

Yue Qi and Philip Eisenlohr, both associate professors in CHEMS, established the lab in the fall of 2013. It has been building multi-scale modeling tools to simulate and design materials for Li-ion batteries, fuel cells and lightweight materials for desired functionality and mechanical properties.

In the past four years, Qi and Eisenlohr have brought more than $3 million in grants to fund the lab. The lab has graduated two master’s degree students and will see two PhD defenses early this autumn. The new lab space currently hosts about 15 researchers, mostly PhD students.

Qi said the Materials Simulations Lab advances the understanding and prediction of material behavior at scales from atomistic to macroscopic through modeling and simulation.

“We have been really fortunate to attract talented MSU students to the lab,” she said. “They are friendly and productive. The members in the Materials Simulation Lab have authored 55 papers in the past four years.

“The diverse material problems we can simulate in the lab allowed us to collaborate with faculty members not only in CHEMS, but also in the Departments of Mechanical Engineering, Computer Science and Engineering, Computational Mathematics, Science and Engineering, and Chemistry. We are very excited about the new lab space and looking forward to its growth,” Qi added.
Eisenlohr, who works in computational materials mechanics, said students are able to harness the power of computer simulations in the new lab.

“Our students approach a wide variety of materials science questions by combining numerical simulation techniques and experimentation,” Eisenlohr explained. “They range from electronic structure and atomistic transport phenomena up to the functional and structural properties of energy materials, advanced engineering alloys, and fundamental aspects of material deformation and deformability.

“We are truly delighted to have the College of Engineering dedicate this open and collaborative space to host our graduate students, post-docs, and visiting scientists for them to interact across physical scales and research topics,” he added.

Donald Morelli, chair of the Department of Chemical Engineering and Materials Science, said theory, computation, and numerical simulation are playing more important roles in the design and functioning of advanced materials.

“This new computational laboratory will allow our faculty to continue to pursue ground-breaking research at the frontiers of their fields, and will be an important tool in the preparation of our students for careers in materials science and engineering in academia, government laboratories, and industry,” Morelli said.