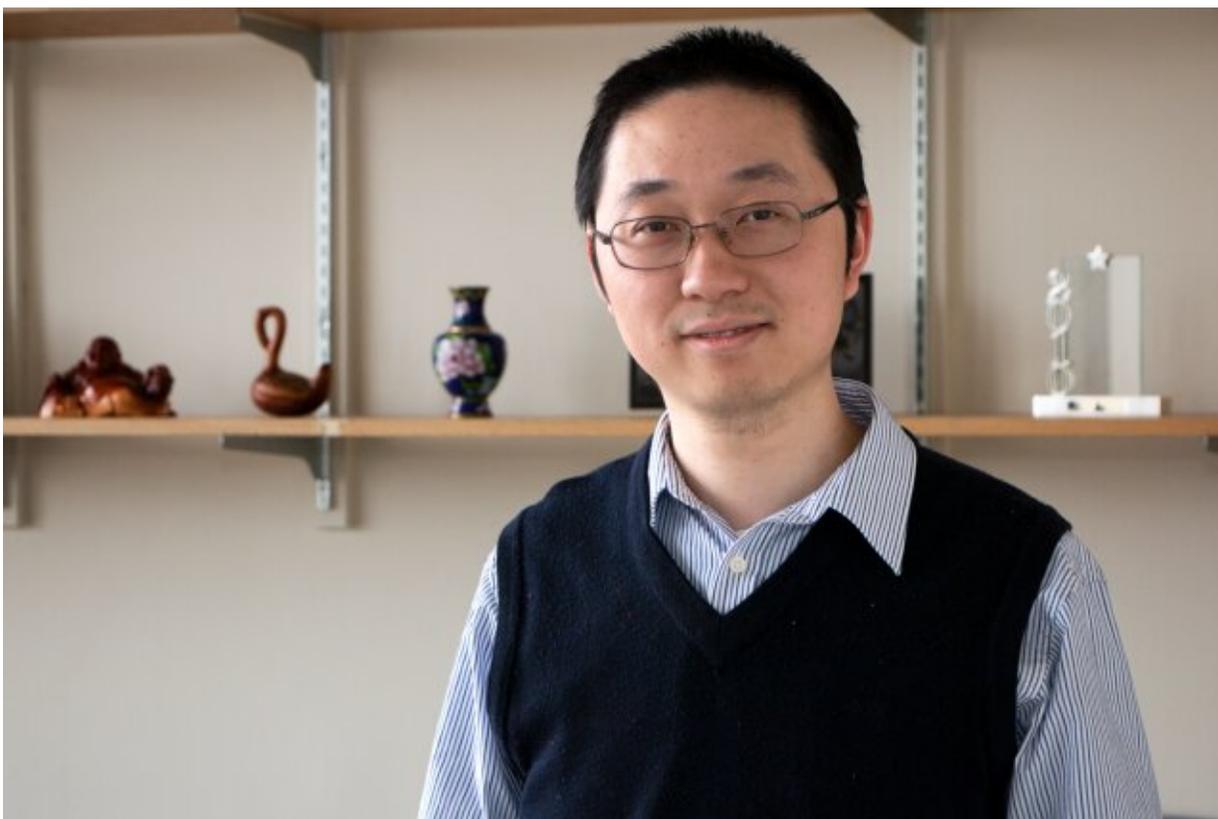


How artificial intelligence is supercharging materials science

October 4 2019, by Denis Paiste



MIT Associate Professor Juejun "JJ" Hu. Credit: Denis Paiste/Materials Research Laboratory

Machine learning and artificial intelligence are increasingly being used in materials science research. For example, MIT associate professor of

materials science and engineering Juejun "JJ" Hu developed an algorithm that enhances the performance of a chip-based spectrometer, and Atlantic Richfield Associate Professor of Energy Studies Elsa A. Olivetti built an artificial-intelligence system that scours through scientific papers to deduce materials science "recipes."

These and other MIT professors, as well as keynote speaker Brian Storey, Toyota Research Institute's director of accelerated materials design and discovery, will discuss insights and breakthroughs in their research using machine learning at the MIT Materials Research Laboratory's annual Materials Day Symposium on Wednesday, Oct. 9 in Kresge Auditorium.

Associate Professor Hu recently explained what led to his breakthrough spectrometer, and why he is optimistic that [machine learning](#) and [artificial intelligence](#) are becoming an everyday tool in materials research.

Q: Your spectrometer work in particular made use of machine learning techniques. How is the new approach changing the process of discovery in materials science?

A: Basically, we developed a new spectrometer technology that allows us to shrink big components onto a small silicon chip and still maintain high performance. We developed an [algorithm](#) that allows us to extract the information with much better signal-to-noise ratio. We have validated the algorithm for many different kinds of spectrum. The algorithm identifies separate colors of light by comparing two repeated measurements to mitigate the impact of measurement noises. The algorithm improves resolution by 100 percent compared to the textbook limits, called the Rayleigh limits.

Q: How are you using machine learning to identify new optical materials and designs for your work on mid-infrared lenses composed of optical antenna arrays?

A: We are collaborating with a group at UMass [the University of Massachusetts] to develop a deep learning algorithm for designing "metasurfaces," which are a kind of optical device where instead of using conventional geometric curvature to construct, say, a lens, you use an array of specially designed optical antennas to impart phase delay on the incoming light, and therefore we can achieve all kind of functionalities. One big problem with metasurfaces is that conventionally, when people would design these metasurfaces, they would do it essentially by trial and error.

We have set up a deep learning algorithm. The algorithm allows us to train it with existing data. So as we train it, eventually the algorithm becomes "smart." The algorithm can evaluate the workability of irregular shapes that go beyond conventional shapes like circles and rectangles. It can recognize hidden connections between complex geometries and the electromagnetic response, which is usually not trivial, and it can find these hidden relations faster than conventional full-scale simulations. The algorithm can also screen out potential combinations of materials and functions that just won't work. If you use conventional methods, you have to waste lots of time to exhaust all the possible design space and then come to this conclusion, but now our algorithm can tell you really quickly.

Q: What other advances are facilitating use of machine learning in materials science?

A: The other thing we are seeing is now we also have much easier access to very powerful, cloud-based computational facilities that are commercially available. So that combination of hardware, easy access, very powerful computing resources, and the new algorithms, that's what enables us to make new innovations. Again, for example, with metasurfaces, if you look at old designs, people were pretty much using regular geometries like circles, squares, rectangles, but we, as well as many others in the community, are all now moving on to topologically optimized optical devices. And to design those structures, the combination of new algorithms and powerful computational resources is the key to design huge devices like macroscopic, topologically optimized optics in three-dimensional space.

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