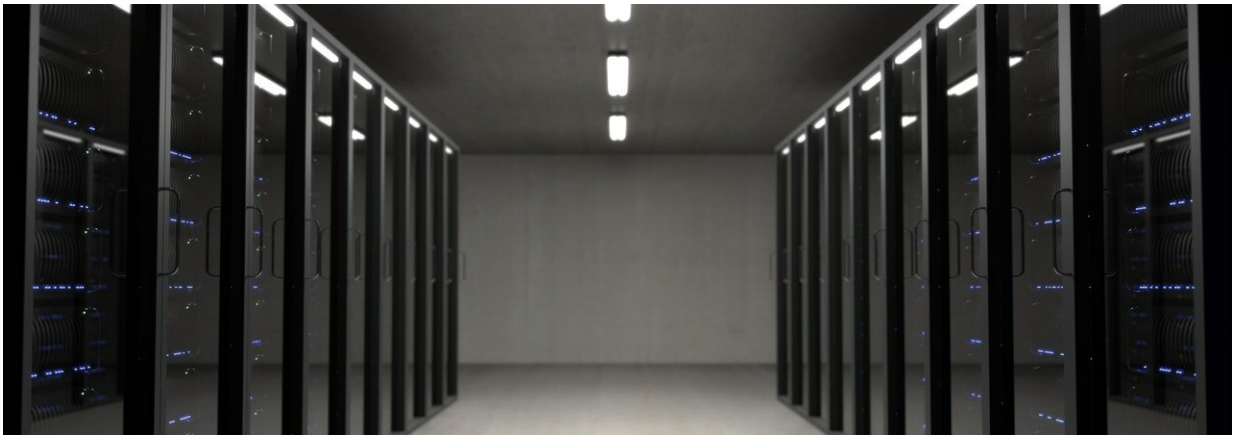
Teaching computers to intelligently design 'billions' of possible materials

April 2 2019, by Eric Stann



At the University of Missouri, researchers in the College of Engineering are applying one of the first uses of deep learning — the technology computers use to intelligently perform tasks such as recognizing language and driving autonomous vehicles — to the field of materials science. Credit: University of Missouri-Columbia

Discovering how atoms—such as a single layer of carbon atoms found in graphene, one of the world's strongest materials—work to create a solid material is currently a major research topic in the field of materials science, or the design and discovery of new materials. At the University of Missouri, researchers in the College of Engineering are applying one of the first uses of deep learning—the technology computers use to intelligently perform tasks such as recognizing language and driving

autonomous vehicles—to the field of materials science.

"You can train a computer to do what it would take many years for people to otherwise do," said Yuan Dong, a research assistant professor of mechanical and aerospace engineering and lead researcher on the study. "This is a good starting point."

Dong worked with Jian Lin, an assistant professor of mechanical and aerospace engineering, to determine if there was a way to predict the billions of possibilities of material structures created when certain carbon atoms in graphene are replaced with non-carbon atoms.

"If you put atoms in certain configurations, the material will behave differently," Lin said. "Structures determine the properties. How can you predict these properties without doing experiments? That's where computational principles come in."

Lin and Dong partnered with Jianlin Cheng, a William and Nancy Thompson Professor of Electrical Engineering and Computer Science at MU, to input a few thousand known combinations of graphene structures and their properties into deep learning models. From there, it took about two days for the high-performance computer to learn and predict the properties of the billions of other possible structures of graphene without having to test each one separately.

Researchers envision future uses of this artificial intelligence assistive technology in designing many different graphene related or other two-dimensional materials. These materials could be applied to the construction of LED televisions, touch screens, smartphones, solar cells, missiles and explosive devices.

"Give an intelligent computer system any design, and it can predict the properties," Cheng said. "This trend is emerging in the material science

field. It's a great example of applying artificial intelligence to change the standard process of material design in this field."

The study, "Bandgap prediction by deep learning in configurationally hybridized graphene and boron nitride," was published in *npj Computational Materials*.

More information: Yuan Dong et al. Bandgap prediction by deep learning in configurationally hybridized graphene and boron nitride, *npj Computational Materials* (2019). DOI: 10.1038/s41524-019-0165-4

Provided by University of Missouri-Columbia