Chemical engineers outline new approach to materials design

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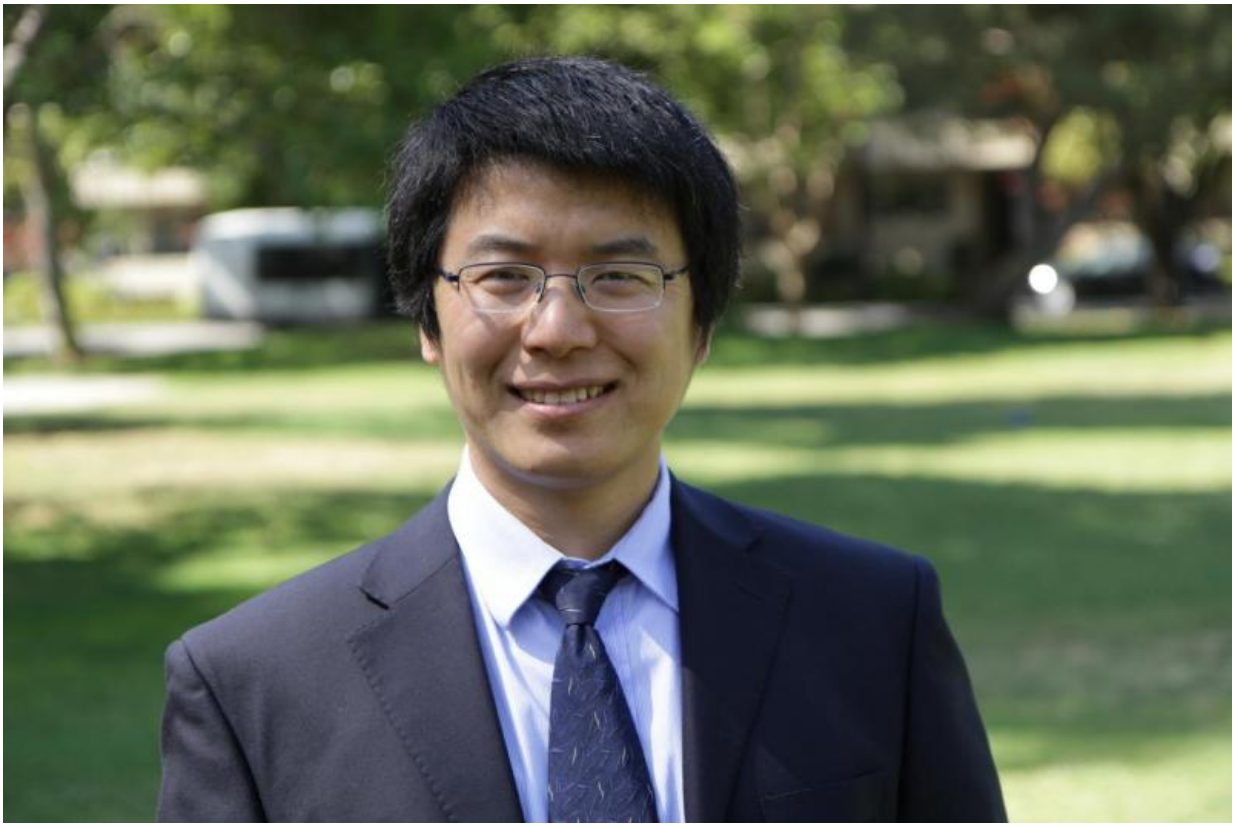

Hongliang Xin and members of his Virginia Tech chemical engineering research group, and fellow faculty member Luke Achenie developed a novel approach that should significantly accelerate materials discovery. Credit: Virginia Tech

A novel approach that should "significantly accelerate materials

discovery" is the subject of a new article in the *Journal of Physical Chemistry Letters* .

The findings reveal a unique model that enables fast and accurate prediction of novel alloy materials for efficient chemical conversions.

Two Virginia Tech chemical engineering faculty members, Luke Achenie and Hongliang Xin, along with Xianfeng Ma and Zheng Li from Xin's research group, authored the article in the peer-reviewed journal.

"This is the first example of learning from data in catalysis. We anticipate that this new approach will have a huge impact in future materials design," Xin said.

Catalysis is the increase in the rate of a chemical reaction due to the addition of a substance called a catalyst. Catalysts come in multiple forms including: acids, solid metal, nanoparticles, and large protein molecules or enzymes in human bodies.

Ninety percent of industrially important chemicals are made using catalysts. It is a major field in applied science; hence the importance of the new approach by the Virginia Tech chemical engineering members.

The mixture of two or more metals with very precise atomic structures and compositions "has shown great promise for catalyzing many chemical and electrochemical reactions," Xin said.

In the past, testing of mixed blends of metals has produced novel physical and chemical properties. "However the process is very time-consuming and costly to search for highly optimized alloys" using the conventional approaches, Achenie added.

So that is why Achenie and Xin decided to use existing data to train

computer algorithms to make predictions of new materials, a field called machine learning. This approach captures complex, nonlinear interactions of molecules on metal surfaces through artificial neural networks, thus allowing "large scale exploration alloy materials space," according to their article.

They specifically concentrated on the electrochemical reduction of carbon dioxide on metal electrodes "because of the current interest in this process for sustainable production of fuels and value added chemicals," Xin explained.

Carbon dioxide (CO2) is a versatile industrial material, used in everything from fire extinguishers to oil recovery to carbonated beverages, but it is also a major greenhouse gas. Conversion of CO2 to something useful could dramatically reduce its emission into the atmosphere and help alleviate the global warming problem.

With their model and their design approach, they have identified a few promising copper multi-metallics with a higher energy conversion efficiency and possibly higher selectivity in carbon dioxide electro-reduction to ethylene, an extremely useful chemical in industry for making plastics.

"This study opens a new way for designing metal-based catalysts with complexities, for example, geometry and composition, promoters and poisons, defects, and nano-effects," Xin said.

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