Neural Networks Predict Crystal Stability

SAN DIEGO, Sept. 21, 2018 – Researchers at the University of California, San Diego (UCSD) are using neural networks to predict the stability of materials in two classes of crystals: garnets and perovskites.

They trained artificial neural networks to predict a crystal's formation energy using just two inputs: electronegativity and ionic radius of the constituent atoms. Based on this work, they developed models that can identify stable materials in two classes of crystals. According to the team, its models are up to 10× more accurate than previous machine learning models and are fast enough to efficiently screen thousands of materials in a matter of hours on a laptop.

"Garnets and perovskites are used in LED lights, rechargeable lithium-ion batteries, and solar cells. These neural networks have the potential to greatly accelerate the discovery of new materials for these and other important applications," said researcher Weike Ye.

The team has made their models publicly accessible via a web application at http://crystals.ai so that others can use the neural networks to compute the formation energy of any garnet or perovskite composition on the fly.

"Predicting the stability of materials is a central problem in materials science, physics and chemistry," said professor Shyue Ping Ong. "On one hand, you have traditional chemical intuition such as Linus Pauling's five rules . . . On the

other, you have expensive quantum mechanical computations to calculate the energy gained from forming a crystal . . . What we have done is to use artificial neural networks to bridge these two worlds."

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