Hello this is Don and I’m a Ph.D. researcher from the University of Minnesota and my research was sponsored by the University of Minnesota MRSEC program. Today I’m going to tell a little story about “Can AI Help Materials Design and Discovery?”

The founder of Google Brain, Andrew Ng, has said that Artificial Intelligence is the new electricity... and it is going to start an equally large transformation in many industries. And this statement, made about five years ago is absolutely true because in today’s world we are seeing AI interacting with us, helping us understand the world and make decisions.

For example, conventional computer visual models have achieved great performance in detecting human features such as face, gender, and ages. For example, this is a photo of one of my research groups and as you can see the computer vision model already does excellent jobs at detecting human faces and predicting their ages and genders. And it is also able to generate natural language to describe the image. This is achieved by using deep-learning models including convolutional neural networks and transformers which were trained to learn specific features and fingerprints from these images to fulfill these tasks.

A.I. is also challenging the way we do scientific research. Here is an example that A.I. was used to accelerate the discovery and design of network-forming materials from simulations. So, the functional materials with network structures have many exciting applications such as: drug delivery; water purification; lithium ion batteries; and photonics.

Starting from a molecular structure, which is usually a good educated guess, we can perform molecular simulation to generate the trajectories of the self-assembly behavior, which helps storing the molecular structure and their corresponding properties into a database. Here it is desirable to have an automated structure detection tool, or functionality, that helps us accelerate the whole process. And this is where the A.I. machine learning techniques come into play.
However, even though the models already did great, model generalization is still not very straightforward. The facial recognition model has been trained with millions of human faces. But it does not do so good in these examples of course for these apes and aliens because the models were not simply trained for these. So the takeaway from this analogy is that machine learning is also data-centric, that we need enough good data to train a model toward specific tasks. Luckily, we have access to an extensive amount of high-quality data from our previous simulations.

So, for example, here is a simulation box containing three hundred molecules. And, if we look at this simulation trajectory of a self-assembly process from a disordered structure to an ordered structure, our naked eye cannot tell any difference or any major difference between these frames.

However, when we feed this trajectory into our pre-trained neural networks or A.I. models, using these models that were trained using previous simulation data, and we are able to get classification results or as inference results.

So, as we can see from here, the snapshot we can get the probabilistic scores for each different structure. And as the trajectory evolves, we can see that the probability of this, each frame to become a network or double gyroid is approaching one, and this is because the model learns to select these specific features that helps making the decisions. So the takeaway here is that A.I. learns distinguishing features such as the viewing angles, the points used for classification and even this surface.

Finally, when we put all these pieces together, the screening process is accelerated by A.I. therefore it can guide the chemical synthesis and characterization. This helps us to achieve the ultimate goal of inverse designing a collection of molecules targeting specific applications. Thank you for listening.