Title: "Can A.I. Help Materials Design and Discovery?"
Speaker: Don Zhengyuan Shen, Ph.D. researcher, College of Science and Engineering, Siepmann/Lodge groups

submission for: Materials Research Science and Enginering Center (MRSEC) Science Slam, 2022, Jan 28, 2022

Format:
      [ ] indicates description of slide shown by speaker for that portion of presentation
      paragraph below indicates the words spoken over that slide

Transcript:

      [slide shows title, some atoms, the UMN MRSEC logo and speaker information]
      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?"

      [shows quote from Google Brain founder: "By replacing steam powered machines with those using electricity we transformed transportation, manufacturing, agriculture, healthcare and so on. Now, A.I. is poised to start an equally large transformation in many industries..." - Andrew Ng]
      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.

      [research group photograph with icons over each person representing data about the person such as age and gender]
      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.

      [image of research journal cover showing close up of material with regular structure]
      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.

      [diagram shows a cycle going from a molecular structure, to molecular simulations, to simulation trajectory, to a database, and back to molecular structure]
      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.

[image of monkeys and commonly held concept of space aliens showing where recognition software mistakenly considers them humans with incorrect human traits]

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.

[image showing a box-shaped section of self assembling material. As speaker continues, the atoms repeatedly arrange themselves in apparently random fashion]

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.

[graphic showing section from previous slide being fed into a pre-trained A.I.]

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.

[diagram including an example of targeting selected features and embedded video shows probablities approaching one]

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.

[diagram shows the design cycle from before and the output is novel materials]

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.