HEMI Seminar

MatterGen: a generative model for inorganic materials design

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The design of functional materials with desired properties is essential in driving technological advances in areas like energy storage, catalysis, and carbon capture. Traditionally, materials design is achieved by screening a large database of known materials and filtering down candidates based on the application. Generative models provide a new paradigm for materials design by directly generating entirely novel materials given desired property constraints. In this talk, we present MatterGen, a generative model that generates stable, diverse inorganic materials across the periodic table and can further be fine-tuned to steer the generation towards a broad range of property constraints. To enable this, we introduce a new diffusion-based generative process that produces crystalline structures by gradually refining atom types, coordinates, and the periodic lattice. We further introduce adapter modules to enable fine-tuning towards any given property constraints with a labeled dataset. Compared to prior generative models, structures produced by MatterGen are more than twice as likely to be novel and stable, and more than 15 times closer to the local energy minimum. After fine-tuning, MatterGen successfully generates stable, novel materials with desired chemistry, symmetry, as well as mechanical, electronic and magnetic properties. Finally, we demonstrate multi-property materials design capabilities by proposing structures that have both high magnetic density and a chemical composition with low supply-chain risk. We believe that the quality of generated materials and the breadth of MatterGen's capabilities represent a major advancement towards creating a universal generative model for materials design.

> Tian Xie is a senior researcher and project lead at Microsoft Research AI4Science. He leads a team of researchers, engineers, and program manager to develop the next generation machine learning models for materials discovery. Before joining Microsoft, he was a postdoc in the Computer Science and Artificial Intelligence Laboratory (CSAIL) at MIT from 2020 to 2022, co-advised by Tommi Jaakkola and Regina Barzilay. He got his PhD in Materials Science and Engineering at MIT in 2020, advised by Jeffrey C. Grossman. Tian is most known for his research in graph representation learning and generative models for materials, including widely used models like CGCNN and CDVAE.

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