Accelerating materials design with AI emulators and generators

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Materials design is a challenging and time-consuming process that requires exploring a vast and complex chemical space. To accelerate this process, we present MatterSim and MatterGen, two novel models that can emulate and propose novel materials with desired properties.
MatterSim is a machine learning model actively trained from large-scale first-principles computations for efficient atomistic simulations at first-principles level and accurate prediction of materials' properties across the periodic table and across a wide range of temperatures and pressures.
MatterGen is an atomistic generative model that can propose novel and stable materials across the periodic table. Furthermore, the model can be fine-tuned to conditionally generate stable, novel materials with desired chemistry, symmetry, as well as mechanical, electronic, and magnetic properties.
These models unlock the large-scale discovery, exploration, and simulation of novel crystalline materials under a wide range of thermodynamic conditions, and open new possibilities for computational materials design.