

Rational Design of Pure Silica Zeolites Using a Generative Adversarial Network

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Rational design of nanomaterials using artificial neural networks can be a great innovation for future materials design. Though recent progress has been made in generating small organic molecules, there have been some difficulties for complicated materials like porous materials. In this work, we introduce a generative adversarial network (GAN) model that generate crystalline pure-silica zeolites. Topological analysis using coordination sequences confirmed that our model generated zeolites outside the training set of over 30,000 known zeolite structures. More importantly, our model creates materials with user-desired properties because its learning inputs deal with the property dimension of materials.