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Inverse design of multicomponent crystalline materials

Wednesday, 13 April 2022 11:00 (30 minutes)

Autonomous materials discovery with desired properties is one of the ultimate goals of materials science. We implemented and applied constrained crystal deep convolutional generative adversarial networks to design unreported (meta-)stable crystal structures. Using an image-based continuous latent space, the physical properties can be optimized while exploring a big chemical space. Our approach has been successfully applied to predict stable binary and multicomponent systems. This paves the way to achieve the inverse design of crystalline materials with optimal properties.

Poster title

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