Generative adversarial networks for inverse design of two-dimensional topological insulators

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Despite rapid growth in use cases for generative artificial intelligence, its ability to design purpose built materials remains in a nascent phase. Materials generation is dominated by stable diffusion networks, however alternative architectures can offer distinct advantages[1,2]. We explore the use of an adversarial network for the design of stable, two-dimensional topological insulators.

While a handful of two-dimensional topological insulators have been predicted, the size of the band-gap, a measure of topological protection, remains a concern in most candidate compounds. Adversarial networks offer a route to overcome this challenge by incorporating multiple discriminators capable of biasing the network towards stable, large band gap topological materials[3].

The implementation strategy is further unique by taking a multi-stage approach. In the first stage the adversarial network is trained and 2000 generated materials are relaxed within density functional theory and examined for evidence of non-trivial topology. The resulting data is then used to fine tune a new discriminator layer in stage II. In the second stage a universal force field fine-tuned using the data from stage I which is able to accurately predict the phonon modes and band-gap of generated materials providing important real-time feedback on the dynamic stability of generated crystal structures[4].

The hit-rate for stable topological insulators is thus dramatically increased in stage II by leveraging the power of universal force fields in the inverse design process. Resulting materials and their potential synthesis are discussed.

References

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[3] Long, Teng, et al. "Constrained crystals deep convolutional generative adversarial network for the inverse design of crystal structures." *npj Computational Materials* 7.1 (2021): 66.

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Figures

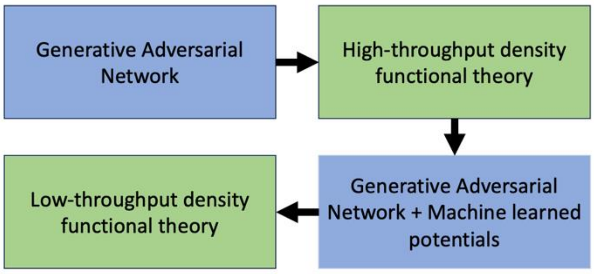

Figure 1. Workflow staggering machine-learning and density functional theory for inverse design of stable topological insulators including universal machine learned potential as a discriminator.

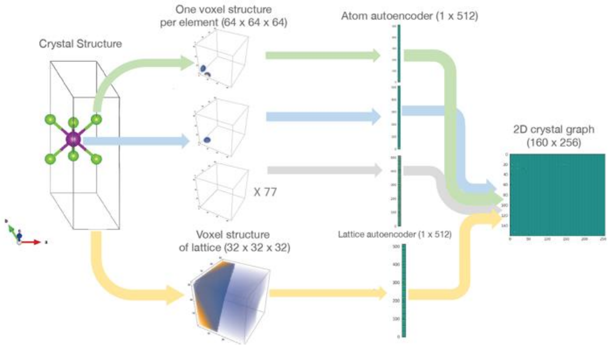

Figure 2. Creation of voxel images for two-dimensional crystals which are then encoded as vectors to form two-dimensional crystal graphs suitable for training a convolutional neural network.