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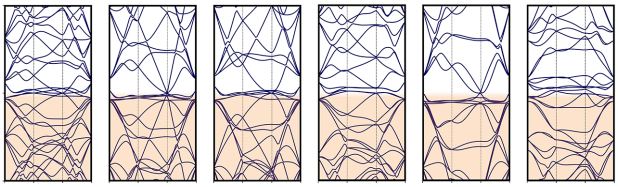
A simulation driven by artificial intelligence demonstrates researchers can pick desired properties of materials by controlling layer composition and geometry, with wide-ranging opportunities for applications.



Two-dimensional layered materials, such as graphene, have many potential applications, including information processing, communication, and energy. Tailored design of these materials could enable the development of devices with functionalities not possible through conventional materials.

Tritsaris et al. show it is possible to design materials with finely tuned electronic properties through control of the composition, stacking, and twisting of their vertically stacked graphene-like layers.

They calculated properties, including an important semiconductor property known as energy band gap, of thousands of combinations of single-layer structures and found there is always a combination that exhibits a target property. Measuring such a large number of materials in the lab would be too resource intensive.

“The simulation acted like an autonomous virtual lab driven by calculators and predictive algorithms that replaced experts in designing and conducting experiments,” said author Georgios Tritsaris.

The authors used a simple 1D model, which captured the physics of 2D materials at much lower computational cost. They combined this model with a simulation driven by intelligent computational agents, a key concept in artificial intelligence, to interactively explore the materials space. By using realistic 2D models of layered molybdenum disulfide and graphene, the authors subsequently determined the 1D results carried over to 2D materials.

This work builds on the team’s previous research in twisted 2D layered materials and machine learning. In addition, the artificial intelligence-aided simulation could be useful for the accelerated design and discovery of other types of materials or molecules.

“Based on these developments, researchers in the field can confidently continue to invest effort into developing models and methods towards the tailored design of 2D layered materials,” Tritsaris said.

Source: “Computational design of moiré assemblies aided by artificial intelligence,” by Georgios A. Tritsaris, Stephen Carr, and Gabriel R. Schleder, *Applied Physics Reviews* (2021). The article can be accessed at https://aip.scitation.org/doi/full/10.1063/5.0044511.

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