LatMatcher - AI-Powered Tool for 2D Material Stacking and Property prediction.

Andrei Voicu Tomut [1]
Stephan Roche [12]
Jose Hugo Garcia Aguilar [1]

[1]*Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and The Barcelona Institute of Science and Technology, Campus UAB, 08193 Bellaterra, Catalonia, Spain.*
[2]ICREA — Institució Catalana de Recerca i Estudis Avançats, 08010 Barcelona, Spain
andrei.tomut@icn2.cat
josehugo.garcia@icn2.cat

Open science databases like C2DB Jarvis and others provide access to thousands of 2D structures. Using this material as fundamental building blocks in creating new materials by stacking allows development of amazing new materials with properties that may be completely different from those of the components.
However exploring the new space comes with two bottlenecks. Firstly, the new space of combinations is vast since the resulting stacked material's properties depend not only on the constituent materials but also on the stacking method. Secondly, evaluating the properties of new materials is challenging with classical methods such as DFT and other techniques. As a first step in addressing this problem, we created Latmatcher, a tool that allows you to stack 2D structures while minimising the supercell size and predicting the properties of the new material using a set of machine learning algorithms. Such a tool can be further integrated into other machine learning pipelines, such as genetic algorithms or reinforcement learning, to expedite the evaluation step.

References

[1] Haastrup et. all, 2D Materials, 5 (2018) page (Century Gothic 11) Indicate references with sequential

Figures

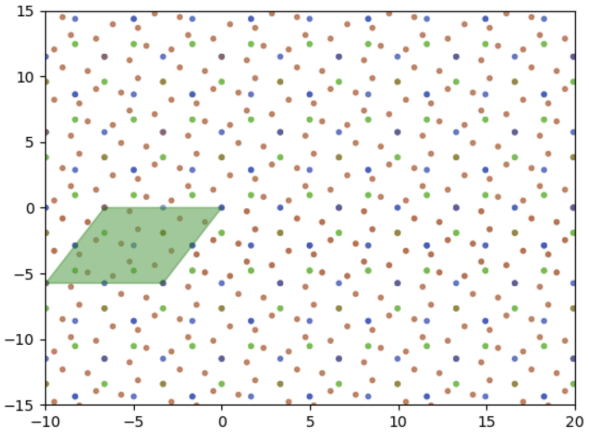

Figure 1: Supercell generated by stacking elements WSe2 on top of graphene, with the supercell delimited with green .

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