Bayesian Neural Networks for the Predictions of the Properties of Millions of Novel 2-Dimensional Heterostructures

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There are currently more than 6000 theoretically predicted 2-dimensional (2D) van der Waals materials with properties that can be significantly different from their 3-dimensional counterparts. The combination of more than one monolayer to form heterostructures can potentially give rise to an extremely large set of structures with unique properties that will drive novel industrial applications. However, even combining only two different monolayers into bilayers, the number of possible heterostructures exceeds millions, making the analysis of the properties of this class of materials impractical from both an experimental perspective and using accurate quantum mechanical models. Here, a time and resource-efficient active machine learning approach has been used to create a database containing the functional and structural properties of millions of van der Waals layered structures. We predicted the interlayer energy, elastic constant, bandgap and piezoelectric constant of layered materials composed of two different 2D structures mainly in view of their application in energy conversion devices. Our active machine learning models can predict results of computationally expansive approaches with high accuracy.[1, 2]

[1] Fronzi, M. *et al.*, "High Throughput Screening of Millions of van der Waals Heterostructures for Superlubricant Applications" Adv. Theory Simul., 2000029. (2020)

[2] Fronzi, M.; *et al.* "Active Learning in Bayesian Neural Networks for Bandgap Predictions of Novel Van der Waals Heterostructures" Advanced Intelligent Systems, 3 (11), 2100080 (2021).