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Exfoliation of two-dimensional atomic crystals with automated identification

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After graphene was first isolated with a simple piece of scotch-tape in 2004, it has demonstrated a rich landscape for interesting physical phenomena and research on its promising technological potential has blossomed. By further applying the technique of mechanical exfoliation to analogous materials, new two-dimensional (2D) atomic crystals with distinct physical properties from their bulk counterparts have been discovered. However, the time-consuming manual identification of 2D flakes after exfoliation hinders practical technological applications and fundamental research. Coupling deep learning algorithms with optical microscopy can automate identification with high accuracy. However, deep learning algorithm's high computational complexities, large dataset requirements, and more importantly, opaque decision-making processes limit their accessibilities. As an alternative, we have developed physically informed, transparent tree-based machine learning (ML) algorithms to automate identification of exfoliated 2D atomic crystals under diverse optical settings. We show that the decision trees, gradient boosted decision trees, and random forests successfully classify optical images of exfoliated 2D atomic crystals with physical and transparent decisions. We also find that the tree-based methods do not suffer from extreme overfitting and large dataset requirements. We then couple these successful ML methods with mechanical exfoliation to promote scalable fabrication of large flakes.

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