IDENTIFICATION OF BOROPHENE ALLOTROPES FROM STM IMAGES BY MACHINE LEARNING: FROM THE DEVELOPMENT OF A NEURAL NETWORK INTERATOMIC POTENTIAL TO BUILDING THE IMAGE CLASSIFICATION TOOL

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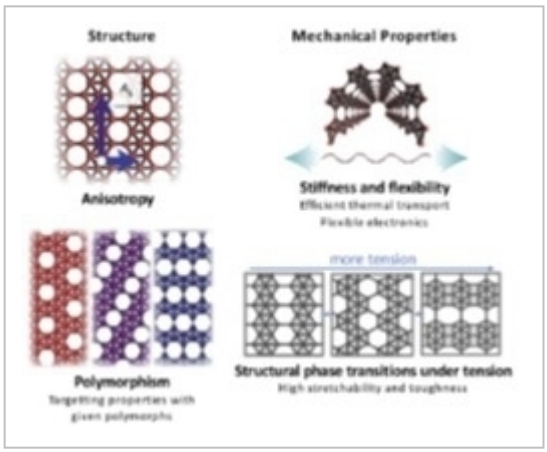
SCIENTIFIC CONTEXT :



Single layer materials have drawn a lot of attention due to their particular physical properties (opto-electronic properties, high conductivity, flexibility . . .). In particular, it has been predicted that boron could exist as a single atomic layer in distinctive crystallographic configurations (allotropes), called borophene – in reference to the carbon equivalent, graphene. Borophene is one of the only 2D material with metallic behavior, among other interesting properties [1]. Recent studies have focused on the synthesis of such material under various allotropic forms, the obtained allotrope depending on the substrate used and experimental parameters such as synthesis temperature [2–5]. Once synthesized, characterizing the produced sample is generally done through STM imaging. However, identifying the obtained allotrope is made difficult by the substrate-borophene interactions as well as possible surface corrugations [6], so that there is no direct way to identify the allotrope from an STM image. The only way to clearly identify the imaged allotrope is to compare the experimental STM image to a simulated one from a known structure. The endgame of this project is to develop an interactive tool to facilitate the recognition of the obtained allotropes from experimental STM images. This tool will be based on image classification, one of the numerous aspects of machine learning.

MISSIONS :

To generate this simulated STM images database, the strategy is to perform DFT electronic calculations on a variety of physically sound structures.in order to get the simulated STM images by computing the electronic structures from the configurations database. The generation of the database of physically acceptable structures will be performed through classical molecular dynamics (MD) simulations using a precise and flexible classical atomistic potential able to provide realistic conformations of borophene allotropes over various substrates. For this purpose, Neural Network Potentials (NNP) [7, 8] have already been trained and tested for single layered borophene on silver [9]. The purpose of this internship is to:
• Perform classical MD simulations using the NNP to generate a database of physically sound structures of borophene on various substrates.

• Compute the simulated STM images from the obtained structures.
• Build the image classification neural network.
• Train and test the neural network.
• Develop an interactive tool based on streamlit to classify experimental STM images.

OUTLOOKS :

The internship held in an dynamic environment in between iLM and LMI, may be followed by PhD.

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