DEVELOPMENT OF MACHINE LEARNING TOOLS FOR EFFICIENT MODELING OF 2D MATERIAL ON METALLIC SUBSTRATES

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LEVEL : M2
TEAM(S) : THEOCHEM

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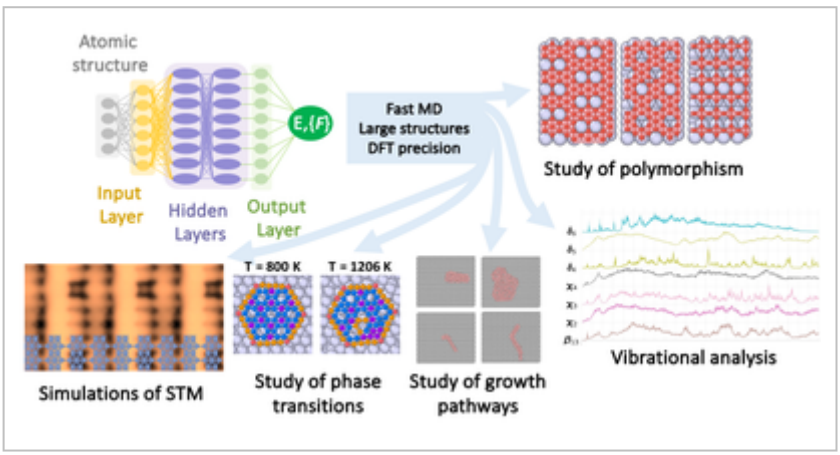
SCIENTIFIC CONTEXT :



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]. The use of atomistic simulations is thus necessary to understand the allotropes behaviors and identify their structural properties.

MISSIONS :

The purpose of this internship is to develop a Machine Learned Interaction Potential (MLIP), i.e. a classical interatomic potential trained with Machine Learning based on DFT calculations for Ag and other metallic substrates. The general workflow for such a development was established in a previous work [7] and will be used various neural networks frameworks (n2p2 and deepMD). Various analysis tools will then be employed to characterize the efficiency and accuracy of the obtained NNPs. Once validated, the NNPs may be used to perform various MD studies of borophene-on-substrate samples as well as to produce simulated STM images.

This is a purely computer-based internship. The training will be provided to the use of dedicated tools: python, bash, LAMMPS [8], VASP [9] ... although a first experience with any of these is a plus.

The paid internship is planned for 5 to 6 months from February 2025 and will take place in a warm and dynamic atmosphere at the Institut Lumière Matière (iLM) in Lyon. It includes computer facilities and access to computing clusters.

OUTLOOKS :

The intership may be followed by a PhD thesis.

BIBLIOGRAPHY :

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[5]Sci. Adv. 7 (2021),eabk1490

[6]Nano Lett. 16 (2016), 6622–6627

[7]Int. J. Quantum Chem. 115 (2015), 1032–1050

[8]Phys. Rev. Lett. 98 (2007), 146401

[9]“High-dimensional neural network potential for borophene on silver surfaces”, P. Mignon, A.-R. Allouche & C. Bousige, submitted (2023)

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