High-dimensional neural network potential for borophene on metallic surfaces

Colin BOUSIGE[1]
Pierre MIGNON[2]
1 – Laboratoire des Multimatériaux et Interfaces, CNRS, Université Lyon 1, Villeurbanne, France
2 – Institut Lumière Matière, Université Lyon 1, Villeurbanne, France
colin.bousige@cnrs.fr

Single layer materials have drawn a lot of attention due to their peculiar 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 behaviour, 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].

To identify and assess borophene allotropes synthesised on metallic substrates, we propose to produce an extended database of simulated structures and their corresponding STM images, allowing a facilitated allotrope identification from experimental STM imaging using image classification. For that purpose, one needs a large database of accurate extended models comprising several units cells of substrate and borophene – such large models are needed to allow describing Moiré patterns and/or borophene corrugation. In the first stage of this work, we have developed a new atomic potential using a machine learning approach [6–8], which allows us to explore multiple structural arrangements of borophene allotropes on metal substrates. The developed potential presents the advantage of performing fast simulations with a level of accuracy comparable to ab initio calculations [9] – moreover, no classical potential pre-existed for this type of system.

Here, we will present the methodology to develop this machine learning potential as well as the various borophene allotropes that have been simulated on Ag surfaces. We will also show how structural properties of given allotropes can be retrieved from their STM images.

References

[1] A. Mannix et al., Nat. Nanotech **13** (2018), 444–450
[2] A. Mannix et al., Science **350** (2015), 1513–1516
[3] B. Kiraly et al., ACS Nano **13** (2019), 3816–3822
[4] B. Feng et al., Nat. Chem **8** (2016), 563–568
[5] M. Cuxart et al., Sci. Adv. **7** (2021), eabk1490
[6] J. Behler & M. Parrinello, Phys. Rev. Lett. **98** (2007), 146401
[7] J. Behler, Int. J. Quantum Chem. **115** (2015), 1032-1050
[8] A. Singraber et al., J. Chem. Theory Comput. **15** (2019), 3075–3092
[9] A. Singraber et al., J. Chem. Theory Comput. **15** (2019), 1827–1840