Deciphering the atomic structure of glassy-like 2D materials: from SiC surface reconstruction to borophene

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In the current state of the post-graphene field, more and more new 2D materials are synthesized by MBE or CVD. In both cases, a 2D film is epitaxially grown on a substrate surface. However, removing the film from this support for its further characterization is not an easy task. This constrain is also encountered in the field of surface reconstructions for which STM is the method of choice for characterizing the structures. Despite its success, STM technique suffers from intrinsic limitations, since the analyses of the film is restricted to a few atoms of the surface. A striking example of this is the long time between the observation of the (7x7) reconstruction of silicon and the complete understanding of the underlying atomic model. The situation is more critical for the (3x3) reconstruction of the carbon-face of hexagonal silicon carbide, which remains unknown to date. Indeed, even though the surface cell is smaller than for the (7x7) case, the complexity arises from the possible alloying at the surface that cannot be derived from experimental data. This specific case illustrates well the issue of deciphering a surface relying solely on a restricted top view of the surface atoms. Moreover, as we will show, its intrinsic glassy-like character also biases the exploration of the surface PES. Nowadays, there is no exhaustive tools to handle this kind of PES. In view of these limitations, we made an extensive manual search, mainly driven by user intuition and comparison spanning over a large range of concentration, and managed after several years to decipher this surface reconstruction [1]. In this presentation, I will present three cases of 2D glassy-like surface ranging from pure surface reconstruction to pure 2D materials, namely borophene [2] and considering ultrathin silica [3] as an intermediate case. The comparison of their PES and the implication for their full characterization will be analyzed.

References

[1] Machado-Charry *et al.* under review (2019).
[2] Mannix *et al.* Science, **350** 1513 (2015).
[3] Kremer *et al.* ACS Nano **13** 4720 (2019).
[4] Alvarez-Quiceno *et al.* submitted (2020).

Figures

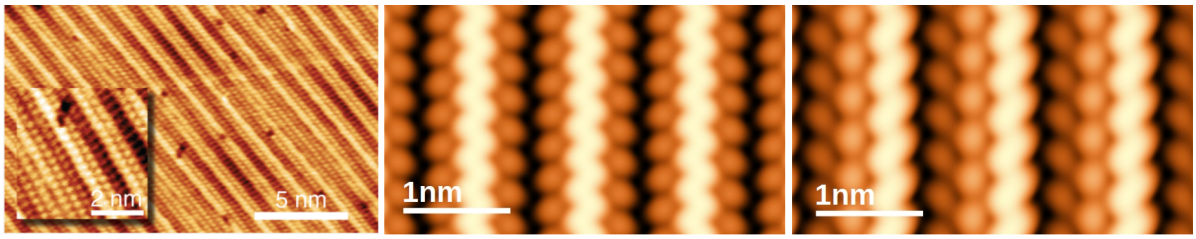

Figure 1: Comparison of the borophene stripped phase [2] with two of our proposed models [4].