Deciphering the atomic structure of surfaces and interfaces

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With the raise of 2D physics, the interface is more than ever the device [1] in modern materials science. This points to the need of efficient computational tools to analyse STM topography that are not always straightforward to decipher from experiments. In this paper, I will present two different examples connected to graphene science. The first example addresses the atomic scale level with the (3x3) surface reconstruction that occurs at the SiC surface when graphene is grown. Based on an intensive DFT-based exploration [2], we find that this reconstruction comes from an ordered all-silicon over-layer adopting a honeycomb-kagome lattice. We further characterize this model by means of STM simulation including an explicit tip. This allows us to refine the model, showing that a disorder substitution is at play below the over-layer. The combination of the two reconstruction levels makes this surface reconstruction unique among other semiconductors, explaining why it took decades to decipher its atomic structure. The second example links both atomic and moiré scale for graphene grown on Rh by coupling in-operando STM with multi-scale atomistic simulations [3] of grain boundary formation during nuclei coalescence. The simulations and experiments reveal a mechanistic model that supports moiré engineering techniques [4]. We apply our technique to in-operando STM micrographs to showcase the atomic structure of grain boundaries from the moiré scale.

References

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Figures

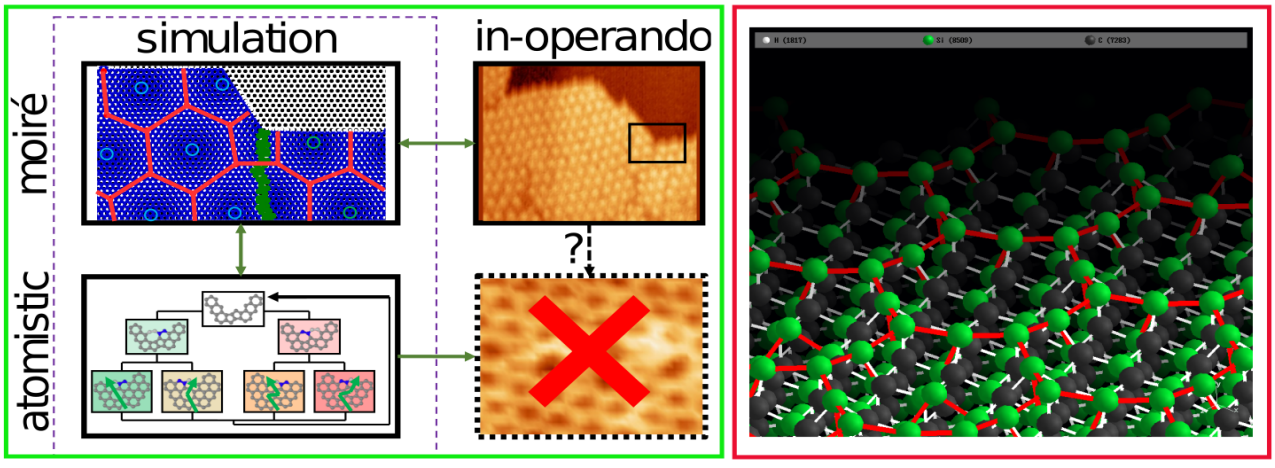

Figure 1: Right: the silicon over-layer on SiC [2]. Left: our moiré engineering technique [3].