PhD position
At laboratoire Matériaux et Phénomènes Quantiques

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Controlling the properties of 2D materials at the atomic scale by defect engineering

The isolation of graphene in 2004 led to the rise of the field of layered two-dimensional (2D) materials that continues to foster tremendous worldwide research activities. In all 2D materials, imperfections are unavoidable. Such imperfections, e.g., vacancies or substitutional/intercalated atoms etc., when combined with the low-dimensionality and enhanced surface/volume ratio, can in principle be engineered to give desirable properties such as reactive catalytic sites, magnetism, or quantum light emission. In this context, defect engineering has recently emerged as a promising strategy to tune the properties of 2D materials.

In this PhD thesis, we will develop the generation of specific defects in selected 2D materials and investigate their structure and electronic properties at the atomic scale by scanning tunneling microscopy and spectroscopy. The targeted 2D materials are graphene, black phosphorus, and transition metal dichalcogenides (TMDs) (Figure 1). Atomic vacancies, substitutional atoms, grain boundaries, intercalated atoms will be used to tune the properties of these materials in order to reach new functionalities. The impact of defects on the density of states and ordered states such as charge density waves will be investigated. The interaction of defect sites with adsorbed molecules will be probed as well to reveal the impact of the defects on the chemical activity of 2D materials. As an example, we have recently revealed that nitrogen pairs in graphene changes the charge state of an adsorbed molecule, allowing us to directly visualized the reduction of a molecule on doped graphene (Figure 2).

This proposal is part of the ANR project DEFINE2D (2020).

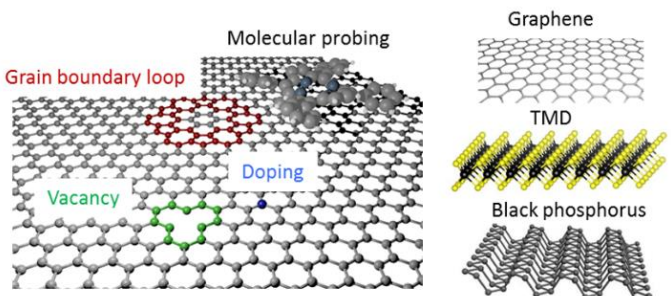

Figure 1: Defect engineering in 2D materials – defects and molecular interaction in graphene, transition metal dichalcogenides and black phosphorus

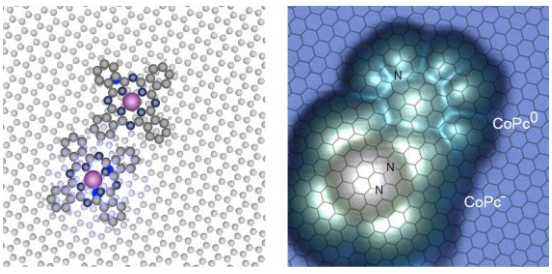

Figure 2: Scheme (left) and STM image (right), with a lateral size of 4 nm, of two CoPc molecules on nitrogen doped graphene. The molecule located above a nitrogen pair is charged while the molecule above a single nitrogen is neutral.
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