Sujet thèse / PhD subject 2025

Titre Thèse	Nanocaractérisation optique des nanomatériaux à base de MXène par transfert d'énergie de fluorescence à molécule unique et nanotechnologie de l'ADN	
PhD Title	Optical nanocharacterization of MXene nanomaterials *via* single-molecule fluorescence energy transfer and DNA nanotechnology	
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Projet phare principal		
Demande de fléchage IEMN ? (Energie / Nanocaractérisation / Technologies Neuromorphiques)	Oui ./ Non : Oui Flagship choisi : Nanocaractérisation	
Demande de labellisation Université de Lille (GREAL, labellisée)	Oui / Non : Label :	
Financement acquis Oui ☐ Non ☑ Partiel ☐	Si acquis (total ou partiel), préciser : (contrat, organisme, Université étrangère, , ….) :	
Financement demandé	Contrat Doctoral Etablissement	ULille ☐ Centrale Lille ☑ JUNIA ☐
	Région ou Autre Préciser :	Co financement (Préciser l'origine, demande en cours, et si acquis ou pas) :
		CLI et Région HdF ; demande en cours

A. Résumé / Abstract :

Context and motivation:

The discovery of graphene caused an explosion of interest in 2D materials, leading to the rapid expansion of this family of materials. As the diversity and applications of 2D materials continue to grow, so does **the need for advanced nanocharacterization methods capable of probing structural and optoelectronic heterogeneities and defects at the nanoscale, key to understading structure-function in 2D materials.** Defects (holes, single atom vacancies, grain boundaries, edges and other defect types) have been extensively studied using atomic-resolution techniques.[1] However, these techniques are complex to implement on a routine quality check basis. Additionally, probing defects under conditions matching the intended applications, such as in liquid interfaces and ambient conditions, remains challenging, and necessary to advance energy and biological sensing applications of these materials.

Recent research has demonstrated the potential of **combining 2D materials with single-molecule and super-resolution fluorescence techniques, using DNA-related technologies, as a powerful tool for nanocharacterization.**[2] In this approach, we harness the energy transfer properties of 2D materials to modulate the fluorescence of single dye molecules attached to DNA nanostructures. Here, DNA nanotechnology provides precise molecular scaffolds acting as local probes to interrogate the material beneath by positioning fluorescent dyes at controlled distances and orientations from the 2D material surface. Energy transfer between the 2D material and the dye alters the dye's fluorescence intensity and lifetime, providing insights into the local optoelectronic properties of the material, defined by the heterogeneous distribution of surface chemistries, holes or defects, presence of transfer residues, etc. **Fluorescence-based single-molecule techniques enable the study of individual molecules within unsynchronized populations, uncovering molecular heterogeneities often hidden in bulk measurements and offering a high-resolution view of molecular interactions and behaviors at the nanoscale.** This approach has enabled high-resolution optical imaging of defects in 2D materials

such as graphene,[3] hBN[4] and MoS_2[5] in liquid and ambient conditions under visible excitation wavelengths *via* confocal and widefield fluorescence microscopy (**Fig. 1b-d**).
MXenes, a promising family of 2D materials composed of early transition metal carbides and/or nitrides, hold great potential for a wide range of applications. Their synthesis, primarily achieved through top-down chemical etching of MAX phases (precursors), leads to **variations in flake sizes, surface chemistries, and defects, all of which play a critical role in defining their functionality while simultaneously posing challenges for certain applications**, especially in the field of electronics. **The impact of defects and other local heterogeneities on their properties, however, remains largely unexplored.** Recently, MXene-induced energy transfer has been studied at the single-molecule level using confocal fluorescence microscopy and DNA nanotechnology,[6] yet its potential as a nanocharacterization tool has yet to be fully demonstrated.

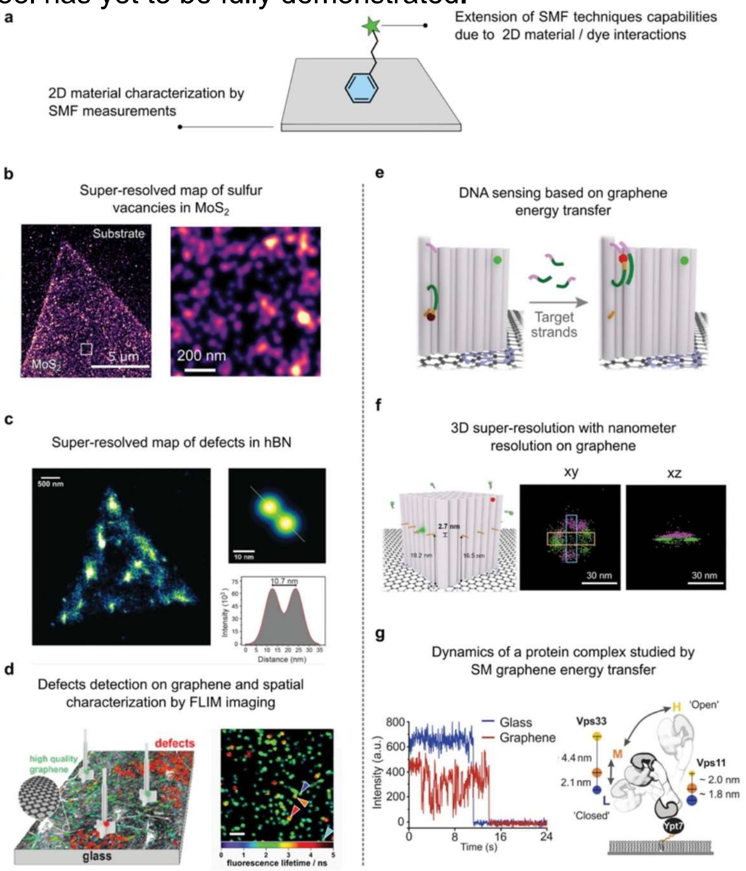

Figure 1. 1a) The combination of single-molecule fluorescence (SMF) and 2D materials offers a wide range of benefits for the study of materials (b–d), and the entities on top (e–g). Taken from Ref. 2.

Thesis project overview:

This PhD project aims to explore MXene-induced energy transfer coupled with DNA nanotechnology as a nanocharacterization tool, wherein dye-labeled DNA nanostructures, placed at precise distances from MXene flakes, will be used to characterize local defect and oxidation sites at the single-molecule level. **We hypothesize that MXene quenching properties are spatially heterogeneous around defects and oxidation sites, providing insights into intra- and inter-flake optoelectronic variations.** Furthermore, this approach can be used the other way around, that is, to characterize DNA nanostructures. In other words, instead of using DNA nanostructures to characterize MXene flakes, we can use MXene to characterize DNA nanostructures. The axial localization of dye molecules in these structures can be achieved *via* MXene energy transfer, revealing differences between various DNA nanostructure designs and experimental conditions,[7] aspects that are tightly linked to future biological sensing applications.
The PhD project involves:

- Establishing a theoretical and experimental framework for MXene energy transfer encompassing different MXene materials.
- Developing robust DNA nanotechnology-based interfaces as energy transfer calibration standards and develop MXene-specific immobilization chemistries to anchor DNA to defective sites.

- Characterizing a range of defective MXene materials to assess the capabilities of the developed nanocharacterization method under different microscopy setups and devices.
- Leveraging MXene energy transfer for the nanocharacterization of dye-labeled DNA nanostructures.

Candidate profile:
The ideal candidate will have a background (master degree) in engineering, physics, or related fields, with knowledge or experience in nanotechnology and/or fluorescence microscopy.

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