

INSTITUT DES MATÉRIAUX DE NANTES JEAN ROUXEL

PhD scholarship – 2025-2028

Defect engineering in two-dimensional transition metal carbide layers (MXenes): structural and chemical modifications for the control of properties.

| Supervisors | Pr. V. Mauchamp | Pr. M-L David | Pr P. Moreau |
|----------------------|--|---------------|--------------------|
| Starting | October 2025 | | |
| Application deadline | May, 15 th 2025 | | |
| Gross Salary | ~ 2200 €/month (funded by the 2Dfects ANR project) | | |
| Labs | Pprime Institute (Poitiers) & IMN (Nantes) | | |
| Key words | MXenes | Defect | Ion and electron |
| | | engineering | Irradiation/ Ion |
| | | | Implantation |
| | Aberration-corrected | Electronic | Optical properties |
| | transmission electron | properties | |
| | microscopy | | |

Description of the research topic

Background: MXenes are two-dimensional (2D) transition metal carbide layers discovered in 2011 (see Fig. 1-a).¹ Due to their original properties, and very diverse chemical compositions,² they are studied for a large range of applications including transparent conducting electrodes (TCE) which are key elements in optoelectronic devices. This PhD project is part of a general research activity developed at the Pprime institute, in collaboration with the IMN lab, and aiming at manipulating properties using defect engineering **MXenes** by ion irradiation/implantation.^{3,4} These techniques are indeed very powerful tools to introduce defects or dopants in materials in a controlled and flexible way, thereby allowing significant improvements of their properties. Although such nanoscale engineering method has already demonstrated its high relevance for other 2D materials, ^{5,6} it is still largely unexplored in the MXene community. We here propose to develop this original strategy in order to deeply modify the optical and electrical properties, *i.e.*, relevant to TCE applications, of MXene multilayers. We expect this approach to bring new perspectives in the tuning of MXenes properties based on defect engineering.

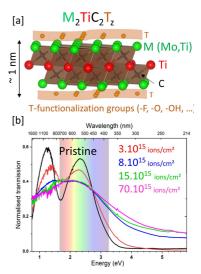


Fig. 1: [a] Structural model of a typical MXene layer with Mo and/or Ti, C and the T surface groups. [b] Evolution of the optical transmission in a $Ti_3C_2T_2$ thin films irradiated with different He⁺ fluences (in ions/cm²) at 180 kV : transmission is increased in the vis-UV range.⁴





PhD project: The PhD project will be developed in the framework of the 2Dfects ANR project, which gathers the expertise of the Pprime Institute in defect engineering and physical properties characterization of MXenes^{3,4,7} and of the IMN Lab in aberration corrected transmission electron microscopy (AC-TEM) characterizations of nanomaterials. The aim will be to develop the defect engineering strategy on MXenes combining three approaches:

- the implantation of new elements in MXenes for chemical doping.
- the irradiation of MXenes in order to induce controlled structural damages.
- the electron irradiation in AC-TEM in order to couple structural damage with *in situ* characterization.

The structural/chemical changes induced in MXene layers, as well as the corresponding modifications of their optical/electrical properties, will be characterized using a complete set of state-of-the-art characterization techniques available from the different partners of the 2Dfect project (including AC-TEM), in order to assess the role of defects on physical properties modifications.

This work will be led in close collaboration with the PhD students already working on MXenes at the Pprime Institute, and with our colleagues from IC2MP (University of Poitiers, CNRS).

[1] A. VahidMohammadi et al., Science **2021**, vol 372, eabf1581. [2] J. Zhou et al., Chemical Reviews **2023**, vol 123, 13291. [3] H. Pazniak et al., ACS Nano **2021**, vol 15, 4245. [4] A. Benmoumen et al., Applied Surface Science **2024**, vol 652, 159206. [5] L. Ma et al., Nanoscale **2017**, vol 9, 11027. [6] G. López-Polín et al., Nature Physics **2015**, vol 11, 26. [7] S. Tangui et al., Small **2024**, 2406334 (2024).

Profile:

We are looking for a highly motivated student holding a master in condensed mater physics, (nano)materials science or similar. Scientific curiosity, strong interest in experimental work and data analysis, written and oral communication skills are required. Knowledge in ion implantation/irradiation, and/or characterization technics such as optical spectroscopies or electron microscopies will be appreciated.

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<u>Labs:</u>

Pprime Institute: <u>https://pprime.fr/en/home-pprime/</u> IMN: <u>https://www.cnrs-imn.fr/index.php/en/index.html</u>