PhD scholarship - 2021-2024

Functionalization of 2D transition metal carbide sheets (MXenes) using ion-implantation: structural modifications and properties.

Supervisors	Vincent Mauchamp	Marie-Laure David	Philippe Moreau
Starting	Sept./oct. 2021		
Application deadline	March, 30th 2021		
Gross Salary	~ 2000 €/month (funded by the Labex Interactifs)		
Key words	MXenes	Functionalization	Implantation
	Aberration-corrected transmission electron microscopy	Electronic properties	Electron energy-loss spectroscopy

Description of the research topic

Background: MXenes are two-dimensional (2D) transition metal carbides which were discovered in 2011.[1] Due to their original properties, they are studied for a large range of applications including energy storage, catalysis, optoelectronic or gas sensors.

This research project is part of a general scientific issue aiming at controlling the MXenes' surface functionalization to modify their intrinsic properties.[2] Usually, the nature of the functionalization groups, T, is determined by the chemical exfoliation process used to obtain the sheets (see figure 1a for the $Ti_3C_2T_x$ system). If the relative content between the different T-groups can be modified when changing the etchant,[3] the complete control of the functionalization is generally difficult. There is thus a huge interest for the development of new functionalization strategies for this large class of 2D materials.

In this context, we have recently shown that ion implantation is a promising approach to extend the possibilities for MXenes' functionalization.[4] This technic is based on the introduction in the sheets, or between the sheets for multilayers, of new atomic species which are accelerated in a controlled way. The control of the induced structural damages, together with the possibility to introduce new atomic species, opens very large and original functionalization possibilities in order to modify and control the MXenes sheets properties.

PhD project: This three years PhD project, funded by the Labex Interactifs, will be conducted in the framework of a collaboration between two French laboratories: the Institut Pprime (UPR 3346 CNRS –University of Poitiers) and the Institut des Matériaux Jean Rouxel (UMR 6502 –University of Nantes). The aim is to further develop implantation approaches, together with the corresponding characterization protocols, in order to modify in a controlled way, the electronic properties of MXenes. These properties will be investigated from the macroscopic scale, focusing on the optical/transport properties of MXene spin coating thin films, down to the single sheet and atomic level using high resolution aberration corrected and monochromated transmission electron

microscopy. Potential related applications are, among others, transparent conductive thin films and supercapacitors.

The PhD program will notably include:

(i) the optimization of implantation conditions using a combination of simulations and structural characterization.

(ii) the analysis of the induced structural modifications in the MXene sheets in order to promote new functionalization sites.

(iii) the controlled implantation of atomic species in order to develop new functionalization groups on the MXene sheets.

(iv) the investigation of the role played by these new functionalization opportunities on the electronic structure of the MXenes sheets combining optical spectroscopies and cutting-edge high-resolution electron spectroscopies in transmission electron microscopy. The rationalization of these data will involve DFT simulations.[5-7]

For more information about the project please email vincent.mauchamp@univ-poitiers.fr

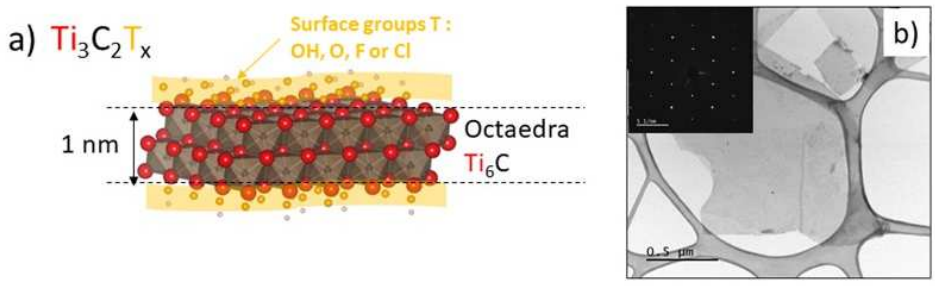

Fig. 1 : a) Structural model of a $Ti_3C_2T_X$ MXene sheet showing the usual T functionalization groups. b) TEM micrograph and related energy filtered electron diffraction pattern obtained on a MXene multilayer.

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

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Application process. Please submit applications by email at vincent.mauchamp@univ-poitiers.fr and philippe.moreau@cnrs-imn.fr in the following format:

- A CV
- Application letter
- Master 1 and 2 marks
- One or two academic references

References: (1) M. Naguib*et al.*,Adv. Mater. 2011, 23, 4248 - (2) V. Kamysbayev *et al.*, Science 2020, **369**, 979-983 – (3) M. Benchakar*et al.*, Applied Surface Science 2020, **530**, 147209 – (4) H. Pazniak *et al.*, ACS Nano 2021, accepted – (5) D. Magné *et al.*, Physical Chemistry Chemical Physics 2016, **18**, 30946-30953 – (6) D. Magné *et al.*, Physical Review B 2015, **91**, 201409(R) – (7) V. Mauchamp *et al.*, Physical Review B 2014, **89**, 235428.