PhD thesis

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Electronic transport properties of 2D molybdenum carbide thin films (MXenes)

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	Low temperature	Magnetoresistance	Hall effect

Research topic

Context: MXenes, of general formula $M_{n+1}X_nT_x$ (where M is a transition metal, X is carbon or nitrogen, and T are the surface termination groups –O, -OH or –F, see Figure 1), are one of the widest family among the 2D materials [*Vahid Mohammadi et al., Science 2021*]. While other families like graphene or transition metal dichalcogenides are semi-metals, insulators or semi-conductors, MXene on the contrary are typically metals. Their hydrophilic character makes them easy to shape, including at the industrial scale, so that they can be envisioned in a wide range of applications such as flexible electronics, electromagnetic interference shielding, optoelectronics, or fundamental electronics. For all these applications, their electronic transport properties play a key role. It is thus of outmost importance to elucidate the transport mechanisms at stake. Indeed, these properties are determined not only by the intrinsic behavior of each bidimensional MXene sheet, but also by the coupling among neighboring sheets, as most devices comprise a stack of several 2D sheets (Figure 2). To this extent, a key tool lies in the study of the electronic transport (resistivity) at low temperature and under a magnetic field. By reducing the thermal noise, this allows to unravel the fundamental transport mechanisms. The latter evidence for example weak localization in $Ti_3C_2T_X$ [*Tangui et al., Small 2024*] – a quantum interference effect arising from the wave nature of the electrons, noticeable only at low temperature –, or Variable Range Hopping (VRH) – describing the conduction by hopping of localized electrons between adjacent sites – in solid solutions of Mo-Ti ($Mo_2Ti_2C_3T_X$, $Mo_2TiC_2T_X$ et Mo_2CT_X) [*Halim et al., Phys. Rev. B 2018*].

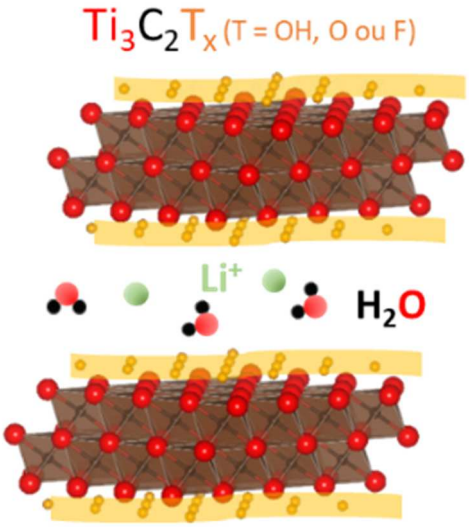

Figure 1. Structural model of $Ti_3C_2T_x$ MXene with its surface termination groups (yellow) and intercalated species (water, ions, molecules…).

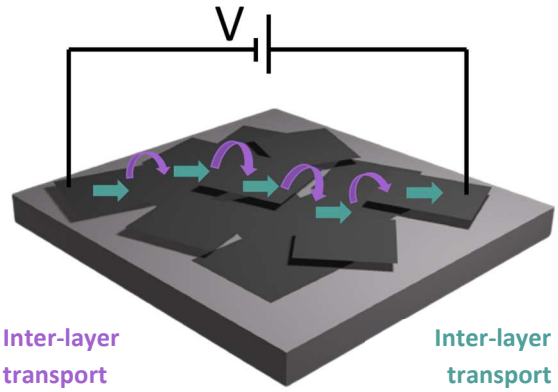

Figure 2. Scheme of the intra- and inter-layer transport mechanisms in a thin film comprising a stack of 2D MXene sheets.

Objective: The aim of this thesis is to study the transport mechanisms in MXenes, both from a fundamental point of view and for future optimization for applications in which electronic properties play a key role. MXene thin films will be fabricated by spin-coating from MXene powders elaborated by our colleagues at the Institut de Chimie des Milieux et Matériaux de Poitiers (IC2MP). The films' resistivity will be measured at low temperature (down to 2 Kelvin) and under magnetic field (up to 9 Tesla) in a cryostat (Physical Properties Measurement System, PPMS) at the Institut Pprime. These preparation and measurement methods were successfully developed as part of a previous thesis at the Institut Pprime, and were used to analyze the transport mechanisms in the reference MXene: $Ti_3C_2T_x$ [Tangui et al., Small 2024]. The aim of this new thesis is to extend these studies to other MXene families, including molybdenum (Mo)-based systems, for which magnetoresistance remains unexplained. The Hall effect in such a system also remains to be elucidated. This work can be further continued by investigating the role of various key structural and chemical parameters in the transport properties of MXene thin films. These include: (i) the role of inter-sheet coupling and (ii) the investigation of MXenes of other chemical compositions, including the V_2CT_x system, which is also promising for transparent conductive electrode applications [*Ying G. et al., FlatChem 2018*]. This work will contribute to a deeper understanding of the impact of chemical composition effects on the macroscopic properties of MXenes thin films, which underpin many applications such as transparent and conductive electrodes [*Zhang C. et al., Energy Storage Materials 2019*], among others.

Candidate profile

We are looking for a Master 2 student with a strong background in solid state physics, physics-chemistry or materials physics, with a keen scientific curiosity and good motivation to carry out all the sexperimental work, from sample preparation to characterization and interpretation.

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Applications should be sent by email to S. Hurand and V. Mauchamp including a CV, covering letter, Master's grades and two academic references.