



MORE-MXenes



Magnetically-Ordered Rare Earth MXenes

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- Participants: - Néel Institute (CNRS, UGA) Grenoble, France (J. Coraux)
- Université Catholique de Louvain (UCL), Belgium (B. Hackens)
- Linköping University (LiU), Sweden (J. Rosen)

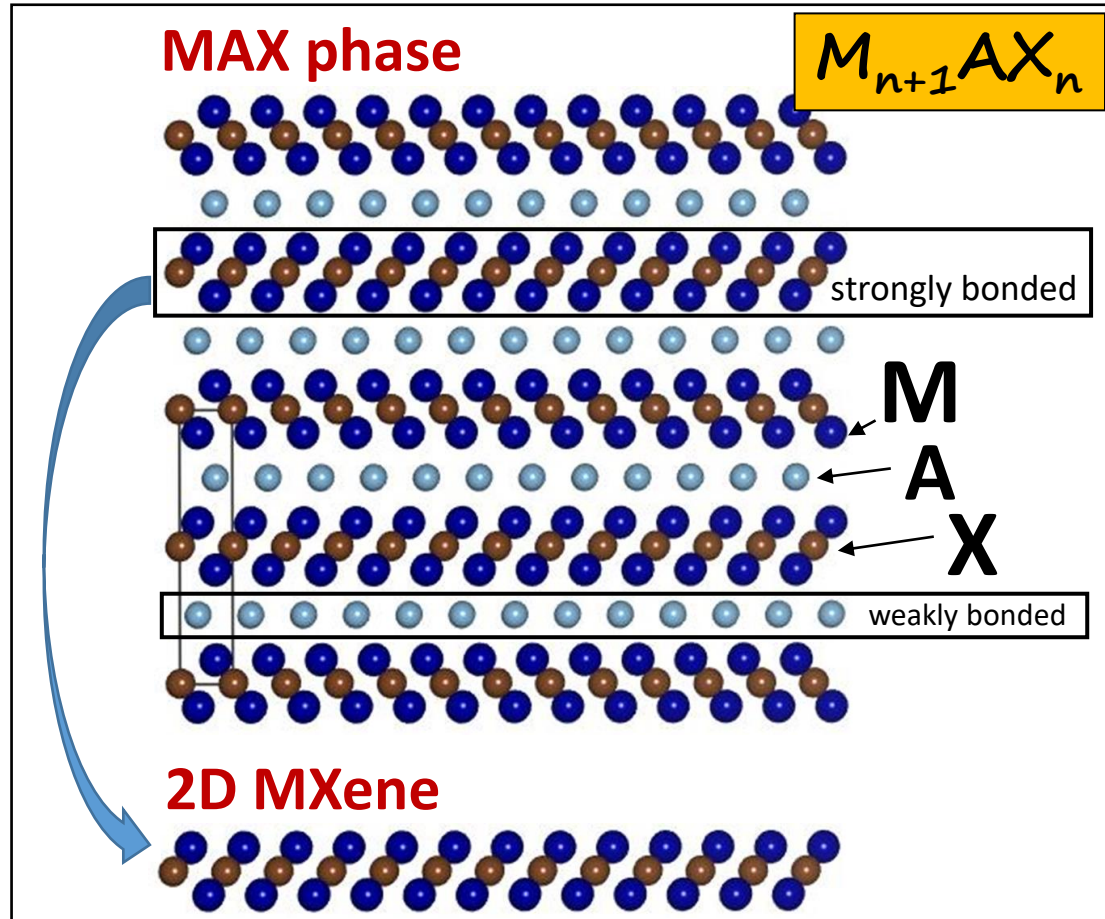
Novel Magnetic MAX phases

→ Two-dimensional ferromagnetic MXenes potentially useful for spin injection.

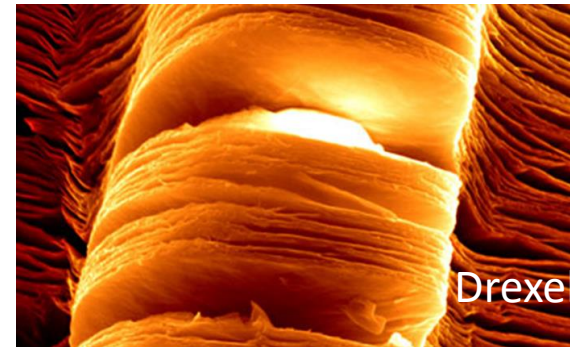
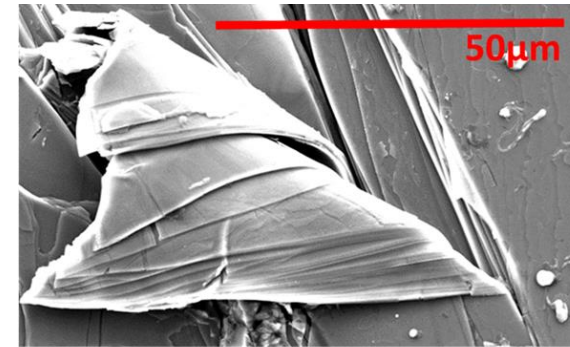


Introduction

Our books are called MAX phases.



Our pages are called MXenes.



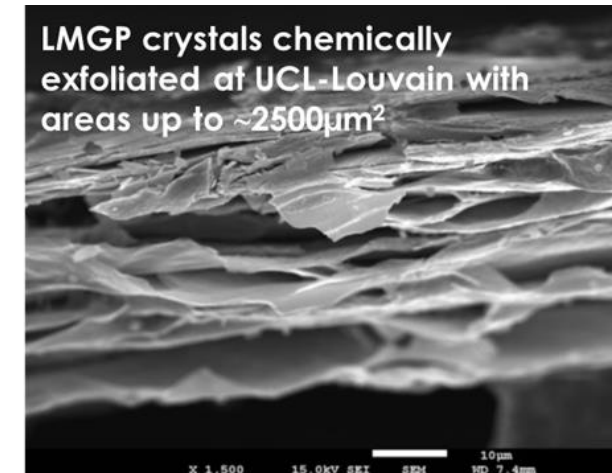
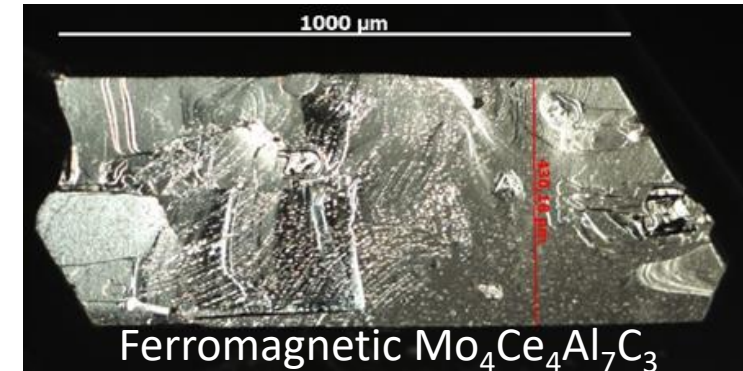
All MXenes reported to date are hydrophilic 2D metals with a high DOS at E_F .

Our specificity is to start from:

1/ both single crystals and powders.

2/ novel magnetic, nanolamellar phases.

Entirely new family discovered and identified at LiU, Linköping, in 2017 (those phases can incorporate any element from the lanthanide row).



Our objectives

- Understand, at a fundamental level, the electronic and magnetic properties of a new family of magnetic nanolamellar phases in order to fabricate 2D magnetic systems.
- Determine practical ways to produce magnetic MXenes and assess their properties (*e.g.*, can the RE's be used to control the spin of the *d*-electrons at E_F ?).

Initial task sharing

LMGP: Crystal growth, chemical exfoliation on crystals, crystal structure, material characterization, physical properties+ coordination...

LiU: Powder synthesis, TEM Microscopy, chemical exfoliation on powders, new phases' stability, crystal structure...

UCL: *Ab initio* DFT and DFPT calculations, magneto-transport, clean room processes, device fabrication...

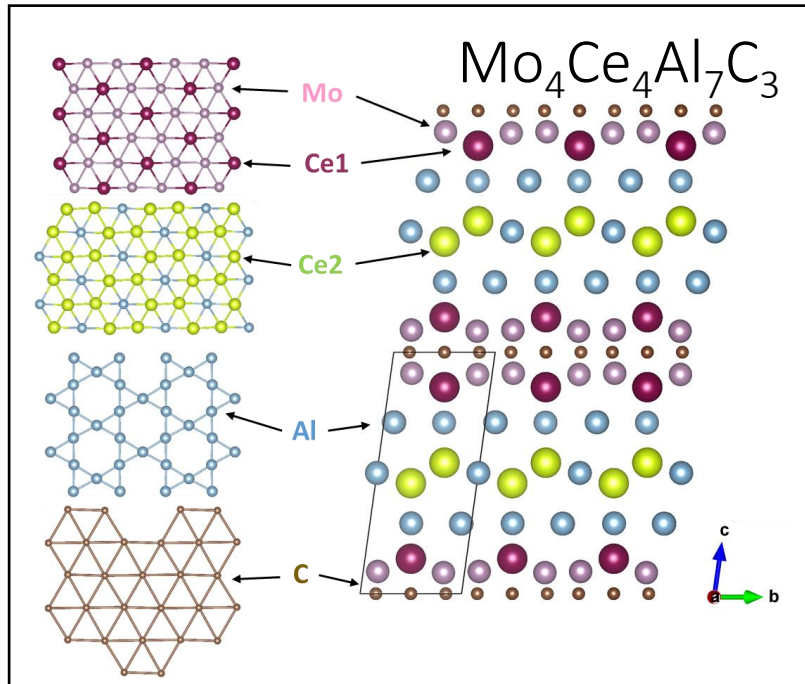
NEEL: Mechanical exfoliation, clean room processes, surface functionalization, magnetism, XPS, STM, MOKE, device fabrication...

+ Strong interaction with Drexel (M.W. Barsoum).

+ Intensive use of Large scale Instruments:

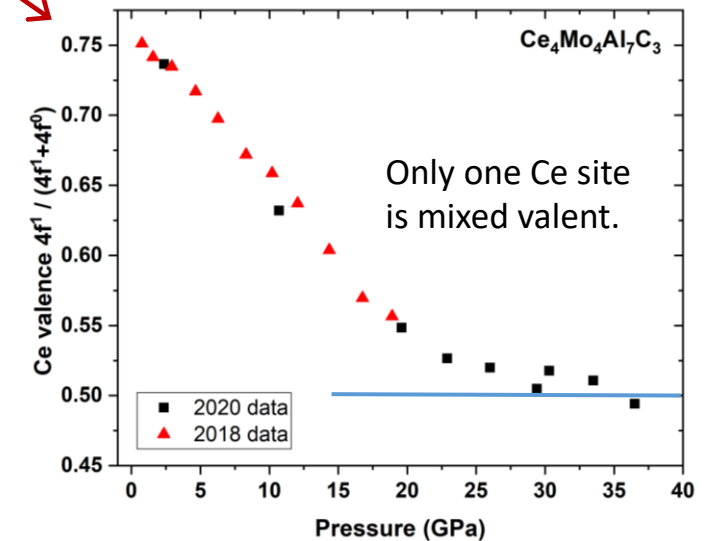
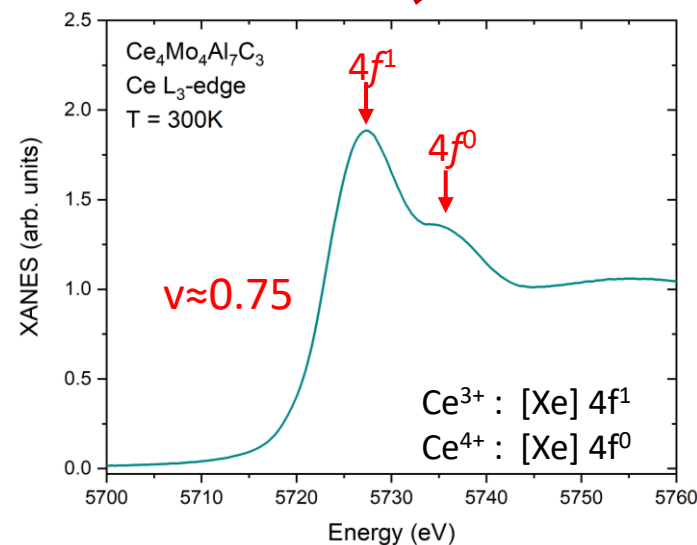
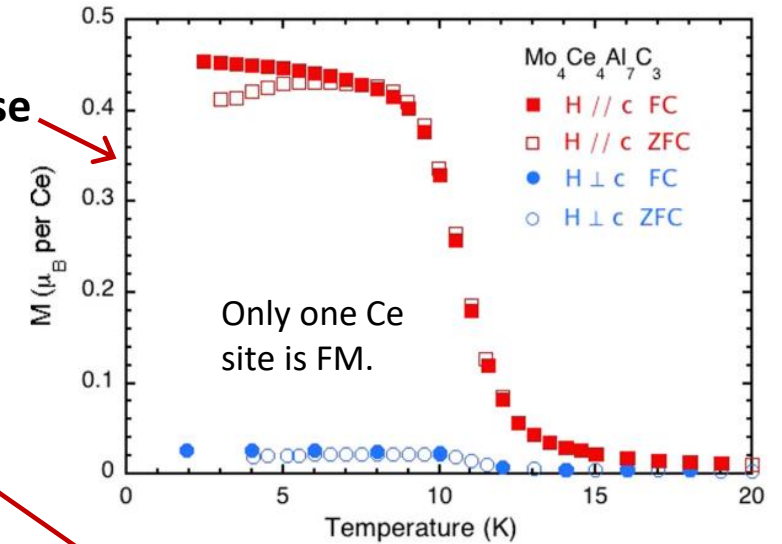
- ILL for powder+single crystal neutron diffraction (LiU+LMGP, local contact C. Colin & E.Ressouche).
- ESRF for magnetic dichroism/ Xray absorption (LMGP, local contact F. Wilhelm).
- Aichi Synchrotron Research center & Nagoya University for ARPES (LMGP, local contact T. Ito).
- Synchrotron SOLEIL (LMGP, local contact F. Bertran).

Physical properties of the nano-lamellar phases: focus on $\text{Mo}_4\text{Ce}_4\text{Al}_7\text{C}_3$

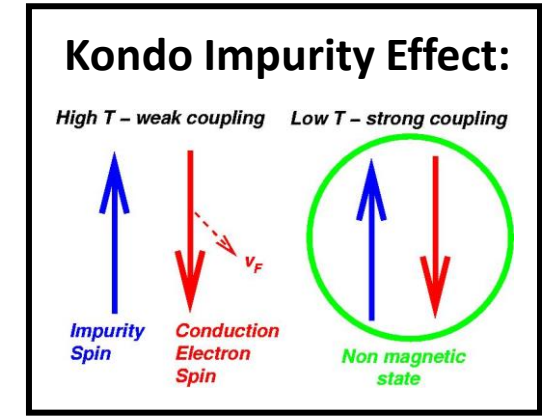
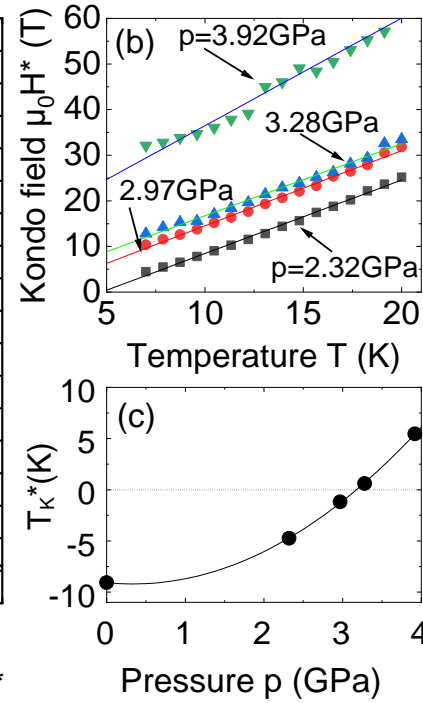
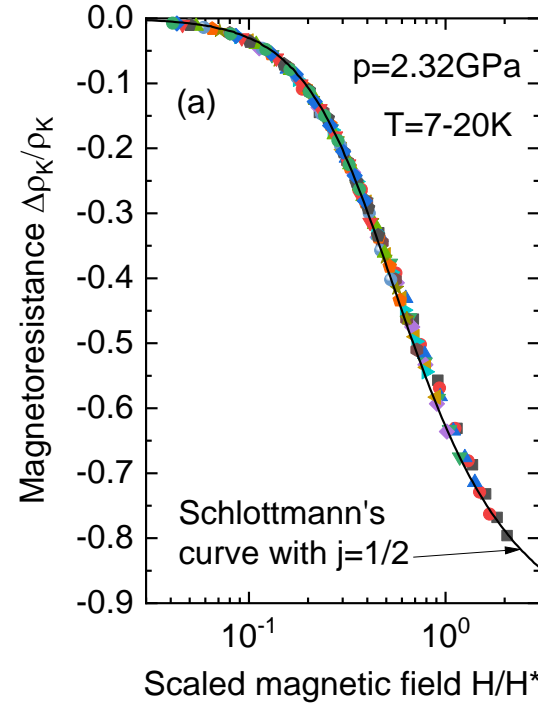
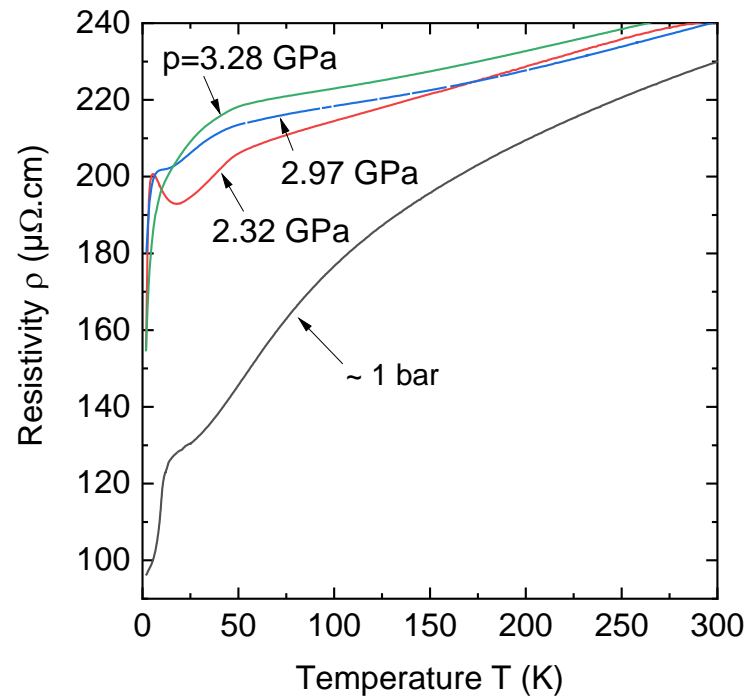


Nanolamellar Ferromagnetic phase

Mixed valence of the Ce's

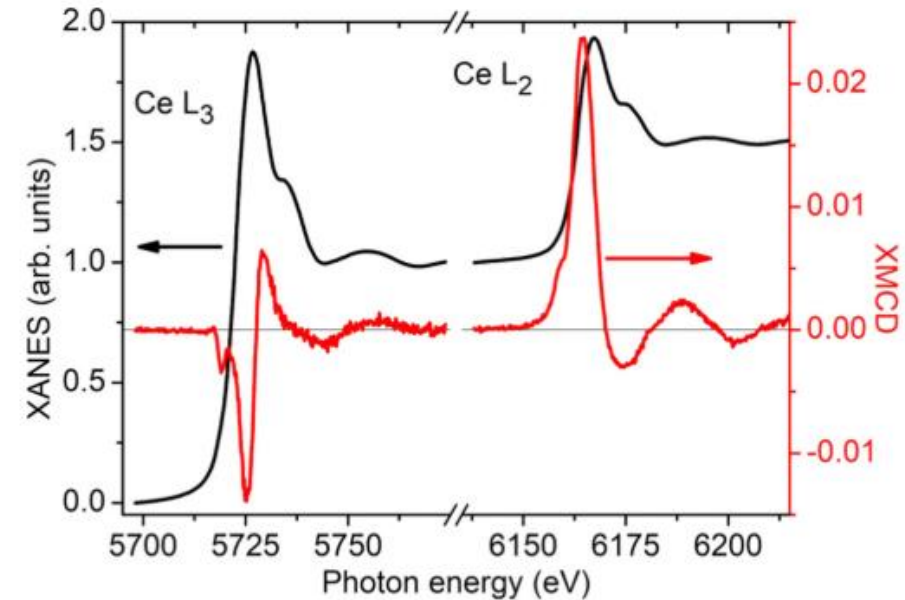
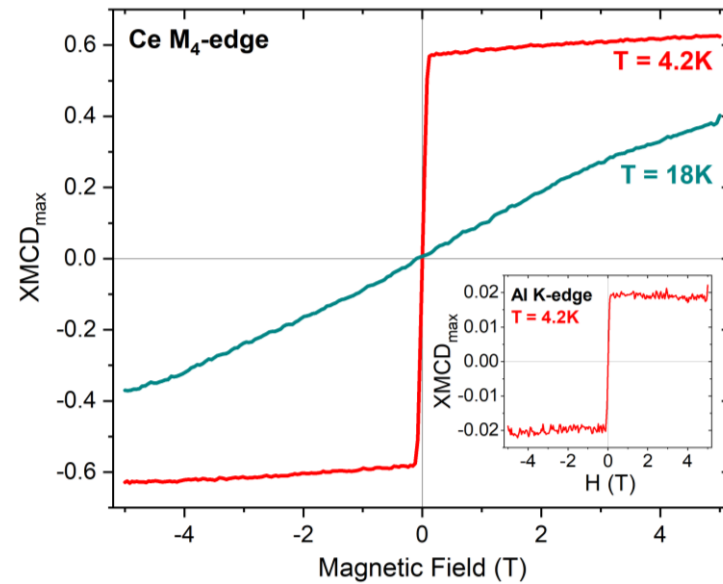
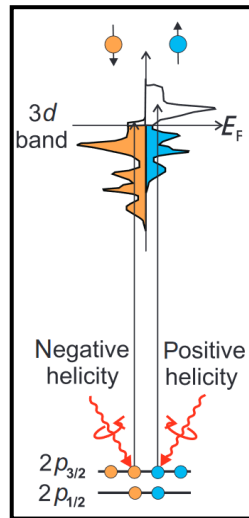


Physical properties: Focus on $\text{Mo}_4\text{Ce}_4\text{Al}_7\text{C}_3$



Ferromagnetic Kondo lattice: Competition between Kondo and FM interactions (rather unusual system).

Physical properties: Focus on $\text{Mo}_4\text{Ce}_4\text{Al}_7\text{C}_3$

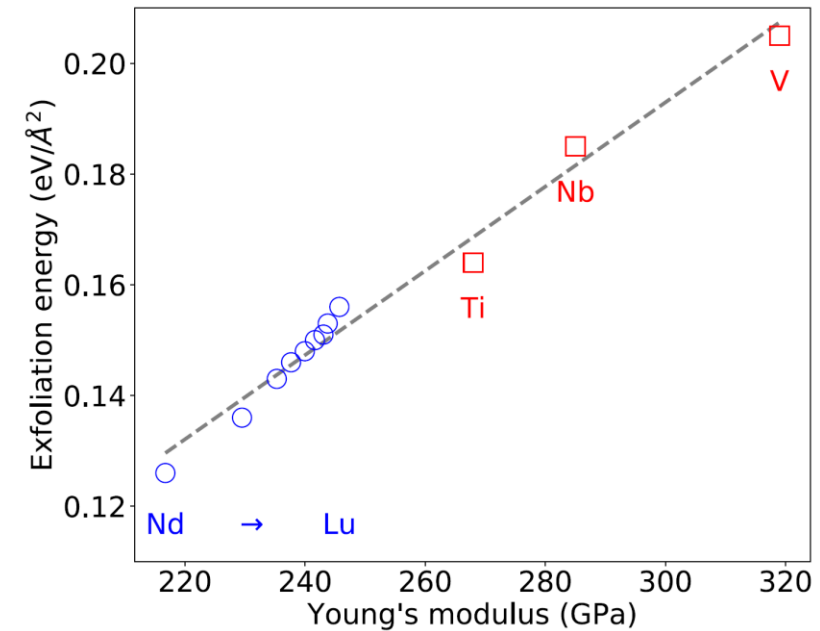
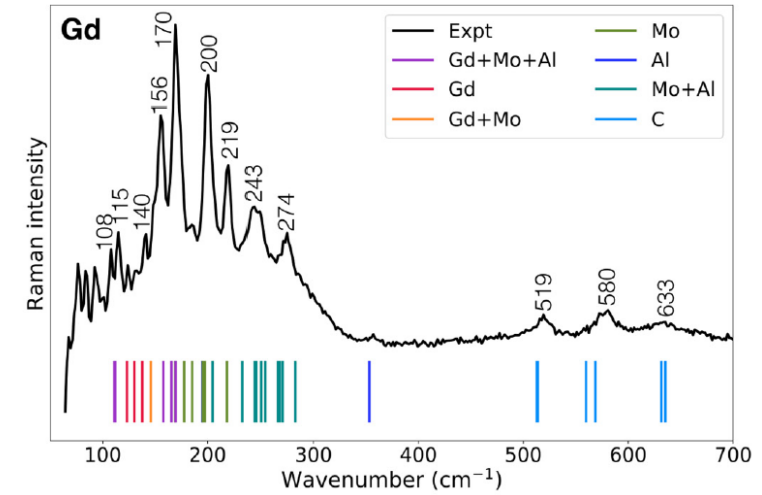
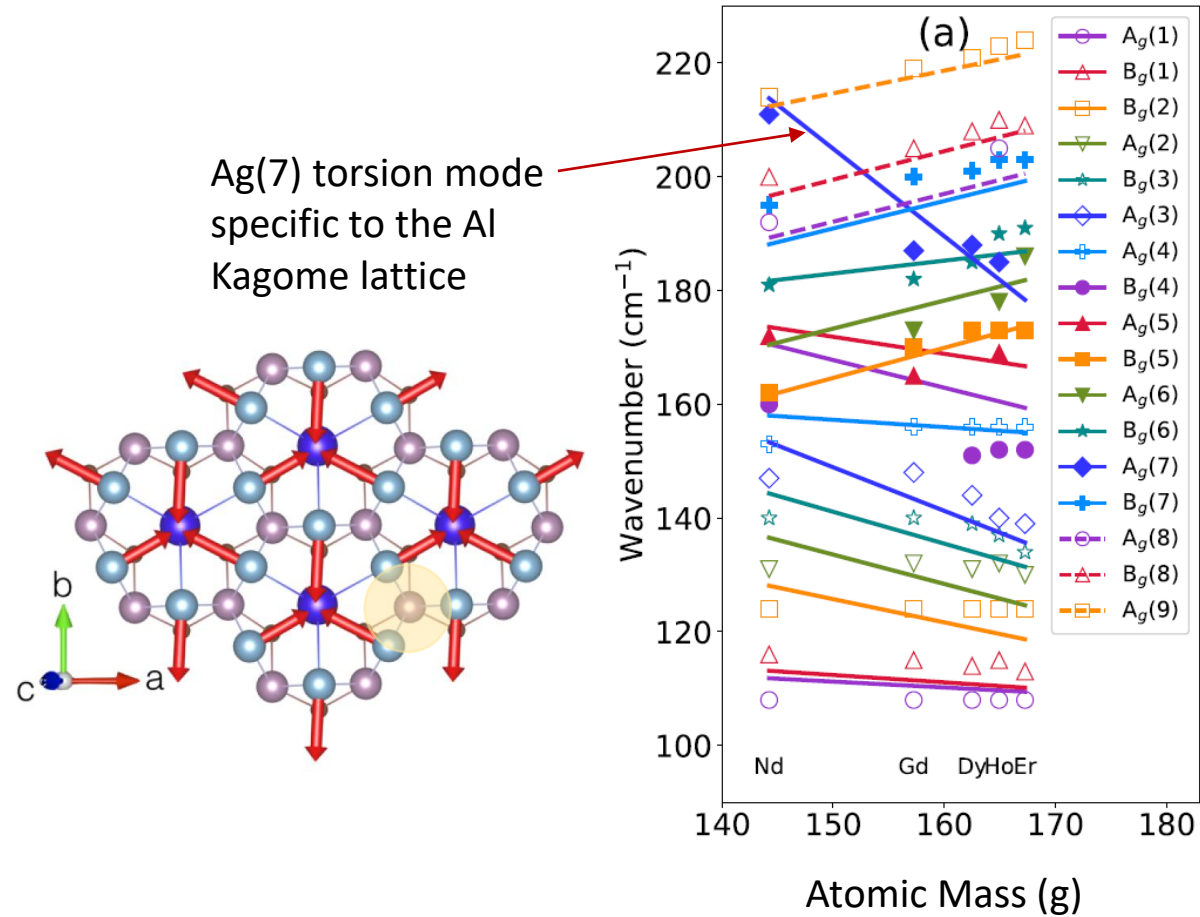


X-ray absorption measurements (each element may be probed individually!).

- Only the Ce $4f^1$ Ce sites are FM.
 - FM is only induced on Al sites, and not on Mo and C sites.
- Ferromagnetism originates from the Ce atoms embedded in the Al layers.
 → Mixed valence is due to the Ce sites in the Mo layers, and those Ce's are just PM.

➡ We need to keep the Al layers ➡ For this phase, mechanical exfoliation is required!

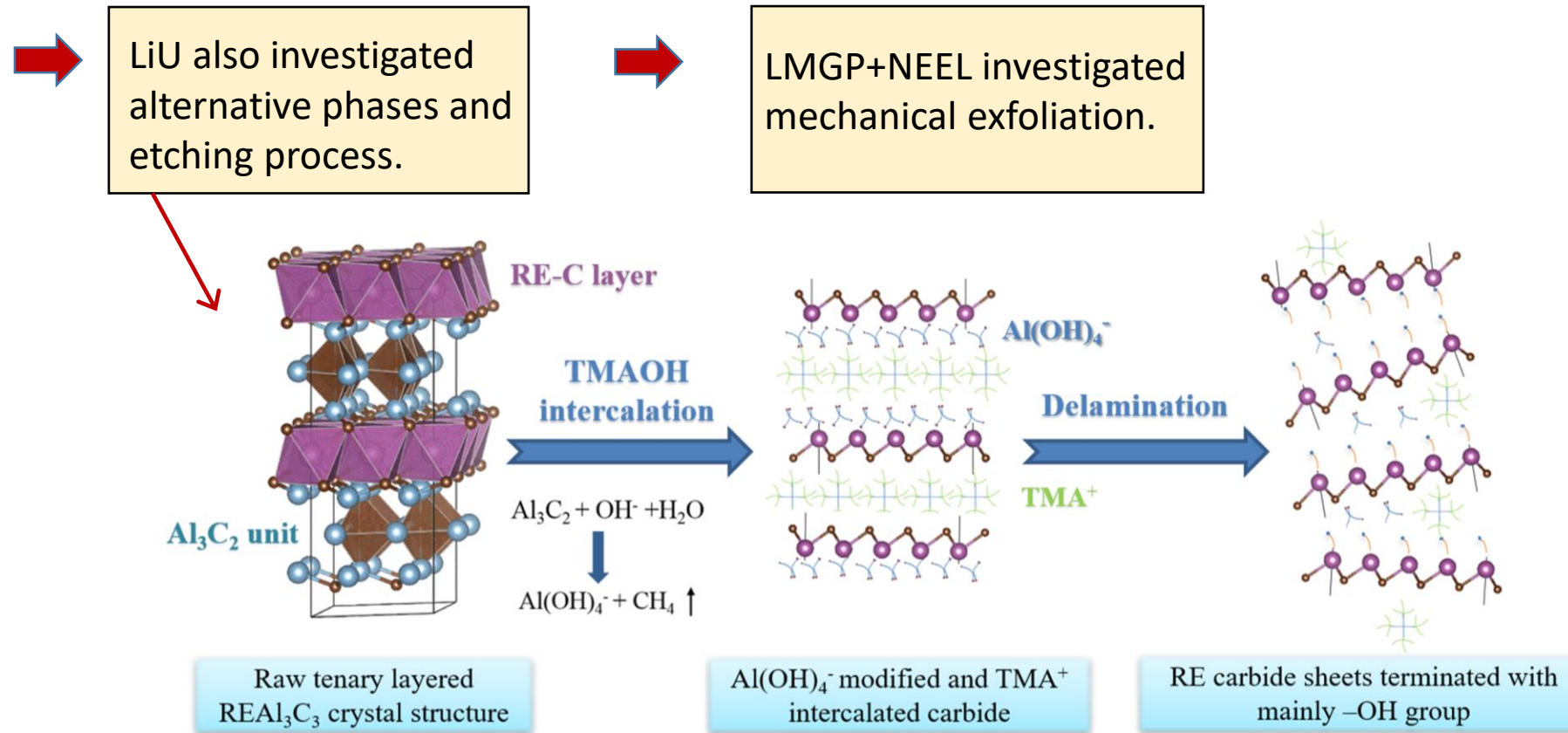
From mechanical properties to chemical exfoliation



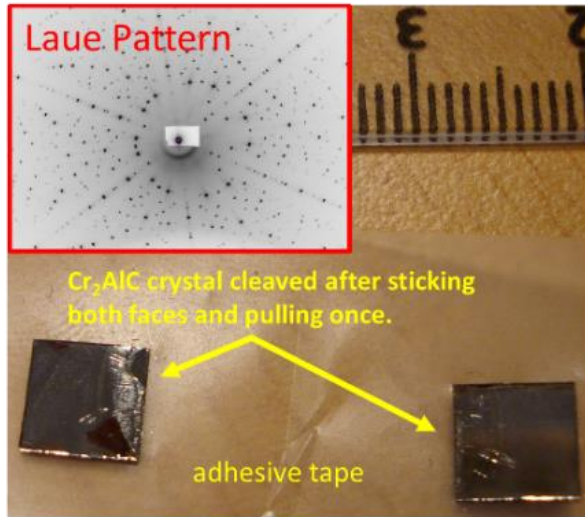
RE-based i-MAX phases predicted to be easier to exfoliate.

Chemical exfoliation

Chemical exfoliation of the RE-based i-MAX phases with HF and/or LiF+NaCl turned out to be quite difficult, since the RE's are also etched.

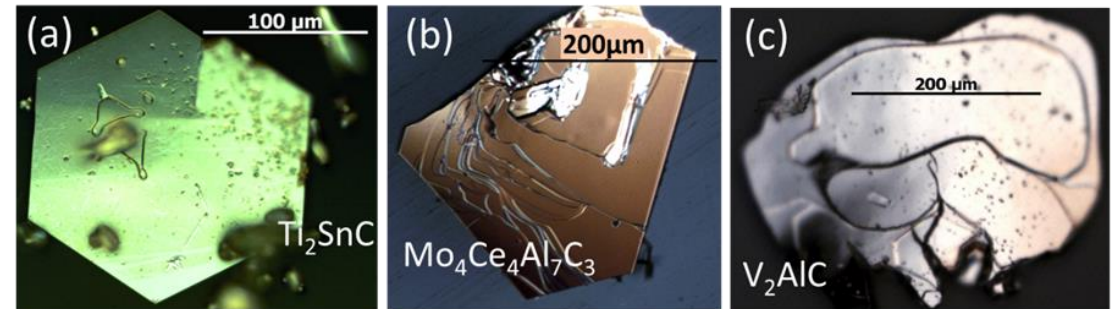


MAX phase mechanical exfoliation



« Big » crystals cannot be mechanically exfoliated down to very thin layers (roughness increases too much after a few exfoliation steps).

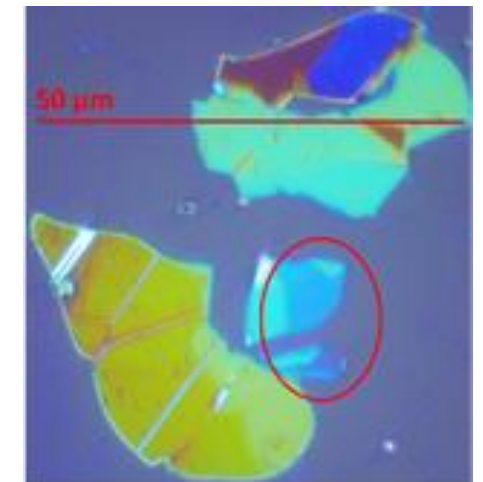
Increase nucleation and synthesize small, thin crystals



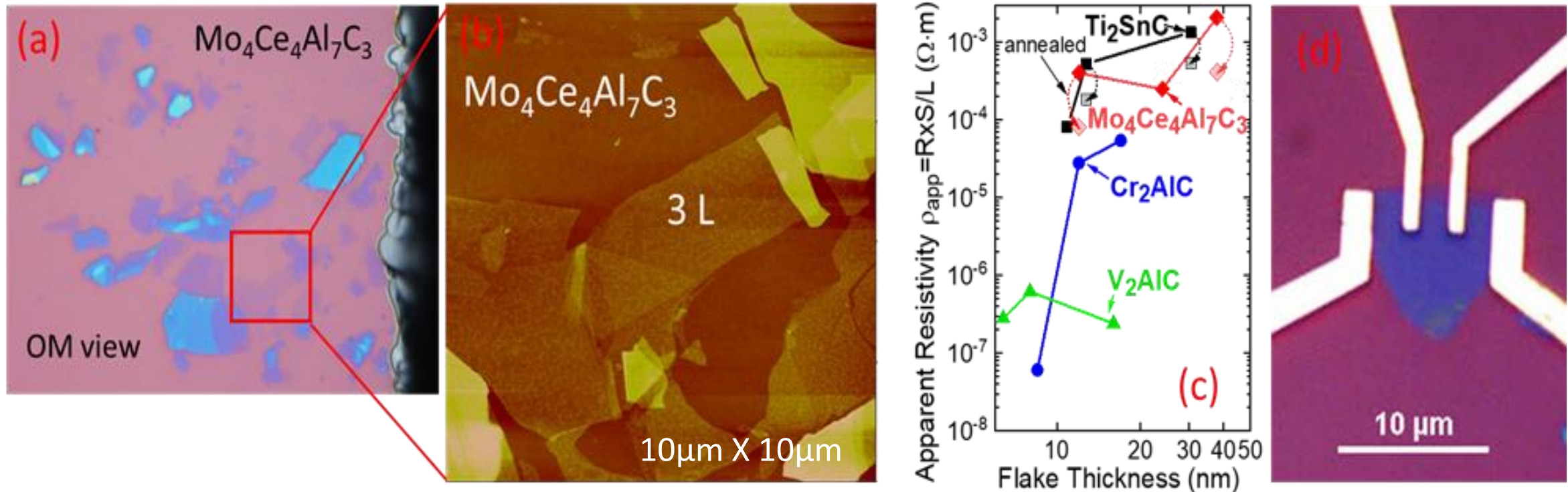
Select crystal size by sieve shaking

Exfoliate thin crystals with 100 μm -300 μm lateral size (adhesive tape method)

Report them on SiO_2/Si substrates



Mechanical exfoliation and first electron devices



The events of the last and present years prevented us from measuring the magnetism of the flakes. This is planned in 2021 at ESRF.

Targets met and targets missed; prospects

Targets met:

- 1 A whole new family of nanolamellar magnetic phases discovered and investigated.
- 2 Magnetic properties of all RE-based iMAX phases fully deciphered.
- 3 First mechanically exfoliated devices successfully processed and measured.

Targets only partially met or missed:

- 1 Quite hard to keep the RE's using chemical exfoliation.
- 2 Magnetism of individual, exfoliated flakes yet to be measured.

Prospects:

- 1 XMCD of magnetic, exfoliated flakes planned at ESRF in 2021.
- 2 New magnetic phases with higher transition temperatures currently investigated.

Responsible Research and Innovation (RRI) aspects

- **Public engagement:**

- Basic research project, somewhat difficult to identify precise applications directly related to RRI objectives.

- **Gender, etc.:**

- Postdoc directly funded by the project: 2 women, 1 man.
- PhD students directly funded by the project: 1 woman.
- PhD students working directly on the project with another funding: 2 men, including 1 with disability status.

- **Open access:**

- All publication summaries were uploaded on a free access website, where access to the full text of the publications can be obtained upon private request.

- **Science Education:**

- Participation to the Cargèse lectures in Physics.