MX-OSMOPED

MXene-organic semiconductor blends for high-mobility printed organic electronic devices

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Partners

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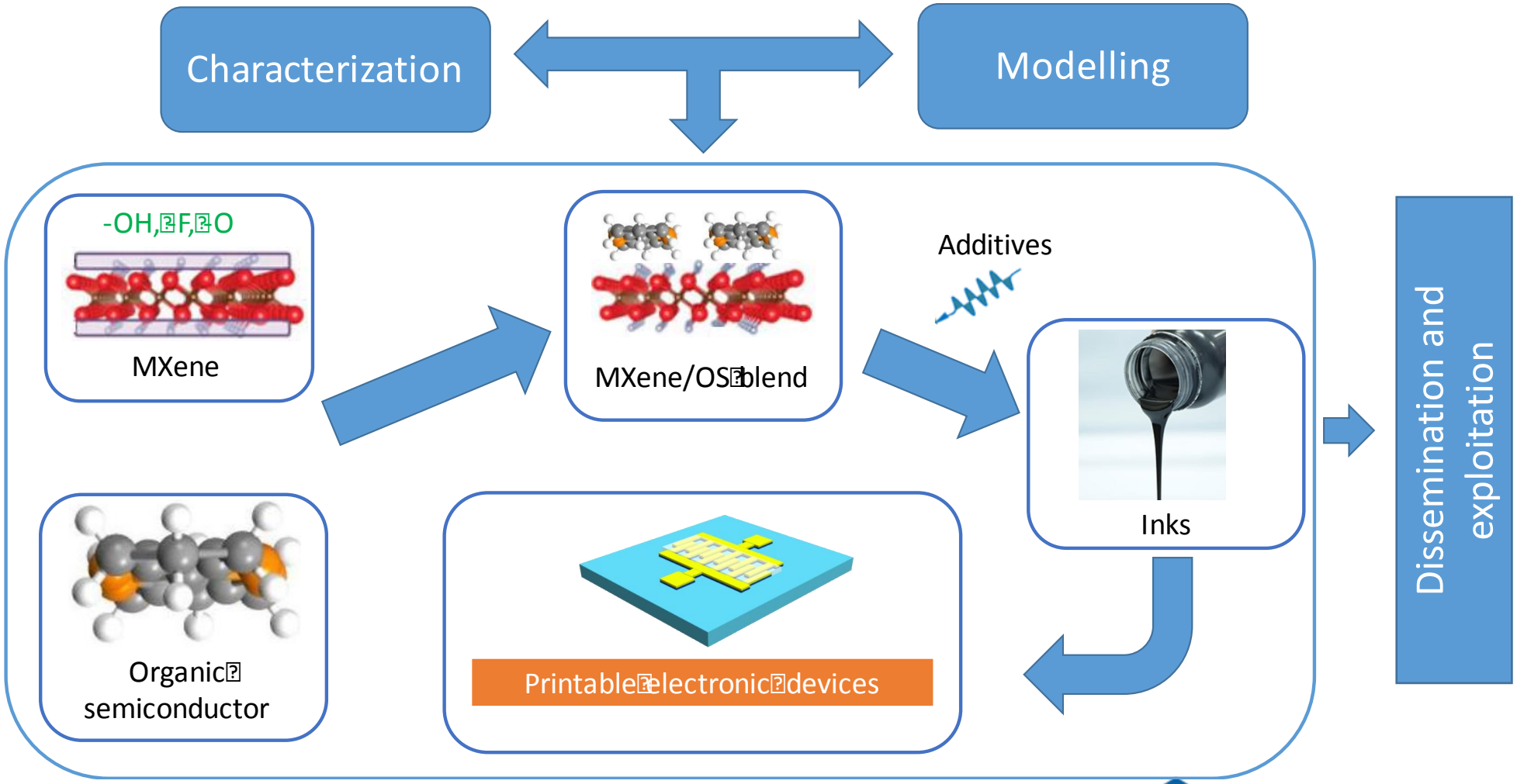
- *Institute of Supramolecular Science and Engineering*, University of Strasbourg, France
- *Department of Chemistry and Food Chemistry*, Dresden University of Technology, Germany

Goals

- The development of environmentally friendly etching methods (no HF) to obtain high-quality MXenes.
- Formulation of a MXene/OS ink capable of delivering organic thin film transistors with $\mu > 50$ cm^2/Vs and on/off ratios $>10^5$.
- Devise a protocol for device fabrication by printing on flexible substrates.

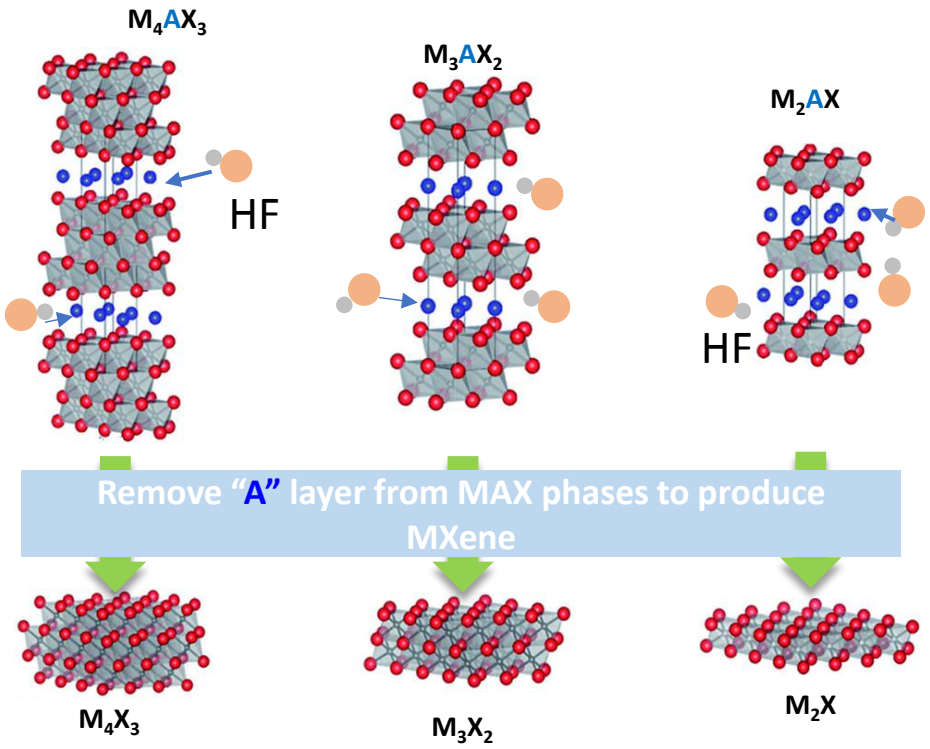
Workflow


Characterization
Modelling
-OH, F, O
MXene
MXene/OS blend
Additives
Inks
Organic semiconductor
Printable electronic devices
Dissemination and exploitation

MXene synthesis and blend preparation

Responsible partner: **TUD**

- Source materials:
  - Ti_3AlC_2, Nb_2AlC, and V_2AlC
- Preparation of blended inks with organic semiconductors, e.g.:
  - [1]benzothieno[3,2-b][1]benzothiophene (BTBT)
  - dinaphtho[2,3-b:2',3'-f]thieno[3,2-b]thiophene (DNTT)



Structure and morphology of thin films

Responsible partner: **ISIS**

- Methods
  - High-resolution Electron Microscopy
  - Atomic Force Microscopy
  - Kelvin Probe Force Microscopy
  - Grazing Angle X-ray diffraction
  - Fourier Transform Infrared Spectroscopy
  - X-ray photoelectron spectroscopy
  - Thermal Gravimetric Analysis

- Thin film preparation, all liquid-based:
  - drop casting
  - spin coating
  - spray coating
  - ink-jet printing

Modelling

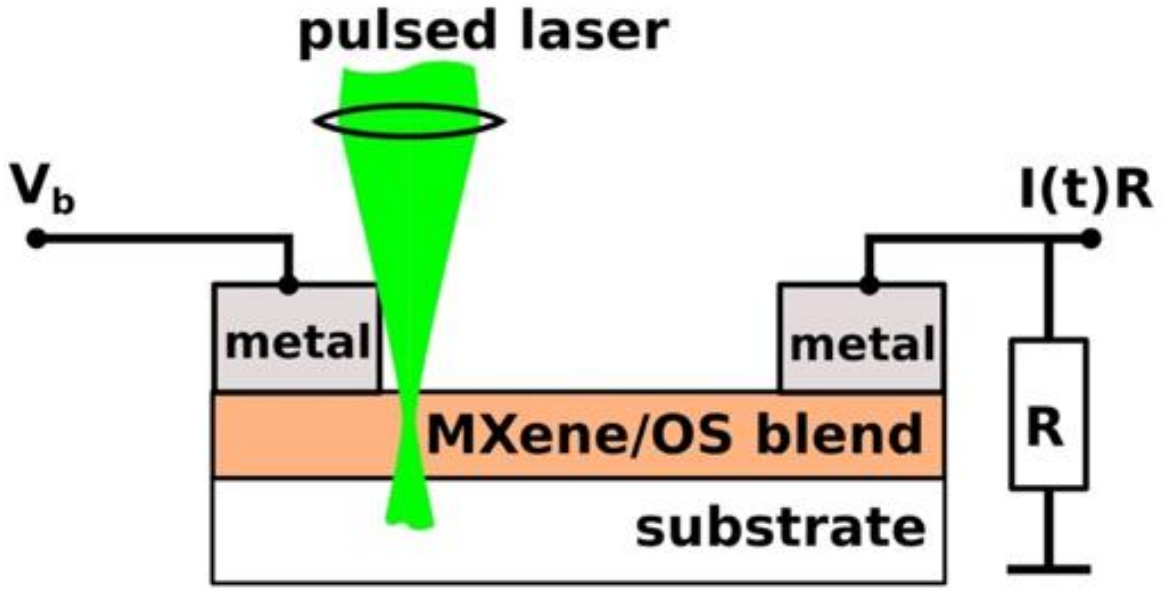
Responsible partner: **UMONS**

- Structural and electronic reorganization at MXene:OS interfaces.
  - Heterojunctions will be modeled by merging slabs of MXene and OS
  - Use of van der Waals corrected Density Functional Theory (DFT) calculations implementing periodic boundary conditions
- Charge transport simulations in MXenes:
  - OS hybrid materials parameterization of Tight-Binding (TB) models against DFT electronic structure calculations for:
    - MXenes and OS in their pristine state and in presence of defects
    - the corresponding hybrid materials.

Charge transport characterization

Responsible partner: **LOMP**

- Methods:
  - Current-voltage measurements in organic thin film transistors
  - Time-of-flight photocurrent measurements



Connection to Flagship work packages

- WP 13 Functional Foams and Coatings (main) 
  - contribution in the area of electronics, flexible electronics, and supercapacitors.
- WP 1 Enabling research 
  - modelling protocols of electronic properties of MXene/OS blends, charge transport properties of blended thin films.
- WP 3 Enabling materials 
  - understanding of the relationship between synthesis parameters and properties in 2D materials
- WP 9 Flexible Electronics 
  - printing properties of inks whose formulation is based on different concentrations of 2D materials (MXenes) and OSs.