This project is dedicated to provide a fundamental insight into the mechanisms regarding selfdischarge and overpotential of hydrogen evolution (HER) and oxygen evolution (OER) of MXenes.

MXenes are new family of 2D layered materials that have gained a lot of attention since their discovery. Especially for energy storage devices, MXene electrodes can provide a high capacitance and a high power density. However, they are suffering from a high self-discharge and low working voltage. The inferior stability performance of MXenes can be connected to their irrational design.

Therefore, this project aims for offering a rational roadmap for designing MXenes to release their maximum abilities.

The main strategy is to modify the chemical and physical/structural characteristic of MXenes. The key parameters are functional groups, surface defects, and the textural roughness of layers, which together make MXenes vulnerable to parasitic reactions. When parasitic reactions become eliminated, a pure performance from a system can be expected.

Since there was lack of attention on important electrochemical aspects, i.e., self-discharge or working voltage range, we felt an urge to shade a light into the missing knowledge regarding such key parameters.

What is more, we will put the acquired knowledge to the engineering of MXene materials that may be the future of our energy storage devices.