## Project 3.2 High-Performance Nano-Structural Electrode Materials for Li-S battery

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## Background:

Lithium-sulfur (Li-S) batteries are a promising candidate for next-generation energy storage systems due to their high theoretical energy density (2600 Wh kg -1), low cost, and environmental friendliness. However, the problems related to the electrode processes at the cathode of these batteries, namely the dissolution of the polysulfides (LiPSs) and the shuttle issues, cause a severe deterioration in efficiency, hindering their practical use. In the present project, multi-functional materials that can firmly trap LiPSs and accelerate the kinetics of the LiPSs redox reaction will be studied. In particular, new nanostructured electrode materials based on (a) nitrogen-enriched 2D graphitic carbon, g-C3N4, (b) active porphyrin sites covalently embedded in conductive polymer, poly(Th-por), and (c) surface-modified CNTs with ionic liquid-like polymer, CNTs@plL will be investigated.

The electrocatalytic properties of these nanostructured materials, tested by cyclic voltammetry (CV), linear sweep voltammetry (LSV), multi-cycling galvanostatic charging/discharging, and electrochemical impedance spectroscopy (EIS), will be correlated with (i) AFM imaging in PeakForceQNM and Kelvin probe mode, and (ii) microgravimetric measurements using electrochemical quartz crystal microbalance (EQCM). DFT calculations will support the experimental studies explaining structure-reactivity correlation in Li-S batteries using g-C3N4, poly(Th-por), and CNTs@plL.

## Aim:

The main research goal of the present project is to develop molecular electrocatalysts based on graphene-like surfaces designed to possess parameters adapted to the sulfur redox reaction in operating Li-S batteries. The proposed nanostructured materials will be used to fabricate the Li-S battery prototype.

## **Requirements:**

- Master's degree in chemistry or physics or related field,
- advanced English language skills