Title	On-Surface Synthesis of Covalent Organic Frameworks (COFs) with Tailored Organometallic Interactions for Catalytic Applications

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Place, country	El Entrego, Spain
# months (min.3)	3

Covalent organic frameworks (COFs) represent a class of porous materials with immense potential in catalysis due to their tunable structure and high surface area. Incorporating specific organometallic interactions into COFs can further enhance their catalytic performance. This project aims to synthesize COFs with tailored organometallic interactions via on-surface synthesis, focusing on catalytic applications. [1,2,3]

Objectives :

- Develop synthetic routes for COF precursors, utilizing either commercially available or custom-synthesized organic molecules through wet chemistry techniques in the laboratories of co-proponent Prof. Alessandro Moretto.
- Employ on-surface synthesis methods in the laboratories of proponent Prof. Francesco Sedona to fabricate COFs modified with organometallic interactions in ultra-high vacuum (UHV) environment.
- Investigate the catalytic activity of organometallic COFs in model reactions with small probe molecules such as O_2, CO_2, CO, and H_2 in UHV and in electrochemical environments.
- Understand the structure-function relationships of organometallic COFs through advanced spectroscopic and microscopic techniques.

Principal techniques

- Characterization of COF structures and surface properties using in UHV with Scanning Tunnelling Microscopy (STM), X-ray Photoelectron Spectroscopy (XPS), and Low Energy Electron Diffraction (LEED) at the labs of the surface supramolecular group @ unipd.
- Investigate COF interactions with probe molecules using Atomic Force Microscopy (AFM) at low temperatures with CO-functionalized tips, in collaboration with Dr. Dimas De Oteyza's laboratory (Spain).

- Electrochemical STM to investigate the catalytic properties of the tailored COF structures in electrochemical environment with high spatial resolution.
- Utilize synchrotron-based spectroscopic techniques to probe the electronic structure and chemical bonding of COF systems.

Timeline:

- Year 1: Bibliography research, synthesis and characterization of COF precursors and on-surface synthesis of organometallic COFs and initial characterization.
- Year 2: Detailed characterization of COF systems in UHV
- Year 3: Investigation of the catalytic properties of COF systems both in UHV and in electrochemical environments.

By addressing the outlined objectives, this project aims to advance the field of COF chemistry and catalysis, leading to the development of innovative materials with potential applications in energy conversion, environmental remediation, and fine chemical synthesis.

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[1] Liu, J., Abel, M., & Lin, N. (2022). On-Surface Synthesis: A New Route Realizing Single-Layer Conjugated Metal–Organic Structures. *The Journal of Physical Chemistry Letters*, *13*(5), 1356-1365.

[2] Xing, S., Zhang, Z., Fei, X., Zhao, W., Zhang, R., Lin, T., ... & Shi, Z. (2019). Selective on-surface covalent coupling based on metal-organic coordination template. *Nature Communications*, *10*(1), 70.

[3] Sedona, F., Di Marino, M., Forrer, D., Vittadini, A., Casarin, M., Cossaro, A., ... & Sambi, M. (2012). Tuning the catalytic activity of Ag (110)-supported Fe phthalocyanine in the oxygen reduction reaction. *Nature materials*, *11*(11), 970-977.