The importance of a synergistic theoretical and experimental approach to design efficient electrochemical CO_2 reduction catalysts

Francesca RISPLENDI - *Polytechnic University of Turin*

In the last decades, due to the progressive industrial development and the improvement of the living standard, the anthropogenic emission of carbon dioxide (CO_2) has drastically increased to a level that it may catastrophically impact the environment in the near future. This problematic scenario has received great attention by the scientific communities, and new technologies for CO_2 capture and reuse are currently at an explorative research level. Among them, the electrochemical CO_2 reduction (CO_2RR) to value-added chemical compounds is one of the most promising strategy towards carbon recycling and atmospheric CO_2 content mitigation. Despite major progress in synthesizing and discovering of efficient electrocatalysts, the interpretation of their electrochemical behavior (such as the selectivity toward specific products and the corresponding efficiency) and the design rules for new catalytic materials are often difficult to derive based only on experimental evidence.

As known, theoretical approaches based on Density Functional Theory (DFT) have played and still are playing important role in interpreting and complementing experiments in different research fields and they also provide insights that may lead to the formulation of rules to design efficient and high selective electrocatalysts.

Therefore, the combination of experimental and theoretical efforts enhances the discovery process and technological innovation in the CO_2RR. This interplay is necessary to understand, predict and, eventually, design the complex materials and environments involved in these electrochemical processes.

During this talk, recent studies related to different classes of CO_2RR electrocatalysts based on bimetallic and organometallic materials will be presented by means of a combined theoretical and experimental approach. This synergistic theoretical and experimental approach elucidates the origin of high performance in CO_2 reduction to specific products highlighting its importance to design of the CO_2RR electrocatalysts.