PHYSICS

MUR DM 118 - Development of bimetallic materials for efficient CO2 electrochemical valorization

Funded By	MINISTERO DELL'UNIVERSITA' E DELLA RICERCA [P.iva/CF:97429780584] Dipartimento DISAT
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Context of the research activity	The conversion of CO2 through electrochemical means holds great promise in addressing the challenges associated with the adoption of carbon-neutral energy sources. It offers a convenient and high energy-density approach to store renewable electricity. CO2 represents the most stable oxidized state of carbon from a thermodynamic perspective. Consequently, any attempts to reduce CO2 require substantial energy input to overcome thermodynamic barriers. Therefore, it is crucial to identify suitable catalysts that can enhance the conversion kinetics and improve product selectivity. The primary objective of this PhD research is to achieve a significant breakthrough in the development of an electrochemical CO2 conversion pathway for the production of valuable chemicals. Progetto finanziato nell'ambito del PNRR - DM 118/2023 - CUP E14D23001640006
	This PhD project focuses on investigating the surface physics and chemistry of novel bimetallic Cu/M catalysts to enhance their performance for the carbon dioxide reduction reaction (CO2RR). By synthesizing and characterizing these catalysts using different methods, the project aims to achieve a comprehensive understanding of their physical and chemical properties. Through an in-depth exploration of surface phenomena, the project aims to tune the catalysts' activity, selectivity, and stability for efficient CO2 conversion. Project objectives: 1. Synthesis of bimetallic Cu/M materials with designed properties: The project will synthesize a series of novel bimetallic Cu/M catalysts with controlled chemical composition and morphology. The focus will be on exploring the surface physics and chemistry of these catalysts, aiming to optimize their CO2RR performance. Various secondary metals and Cu:M atomic ratios will be investigated to understand their effects on the catalysts'

Objectives	surface properties. 2. Investigation of surface physics and chemistry: Advanced surface characterization techniques, such as scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), and infrared spectroscopy (IR/Raman), will be employed to probe the surface physics and chemistry of the Cu/M catalysts. The objective is to gain insights into surface species, active sites, and their interactions with CO2 molecules, enabling a deep understanding of the underlying mechanisms influencing catalytic performance. 3. Correlation between surface properties and CO2RR performance: The project will establish correlations between the surface physics and chemistry of the Cu/M catalysts and their CO2RR performance. By examining surface morphology, crystal structure, composition, electronic structure, and surface active sites, the aim is to identify key surface properties that influence activity, selectivity, and stability. This will contribute to the rational design and optimization of catalysts for efficient CO2 conversion. 4. Optimization of catalyst surface properties: Based on the insights gained from the surface physics and chemistry investigations, the project will focus on optimizing the surface properties of the selected Cu/M catalyst. By modifying synthesis parameters, such as temperature, precursor concentration, and reaction time, the aim is to tailor the surface characteristics, including surface area, morphology, and active site density, to further enhance CO2RR performance. Methodology: • Catalyst synthesis and characterization: Bimetallic Cu/M catalysts will be synthesized different chemical/physical deposition methods, followed by comprehensive surface characterization using advanced techniques such as SEM, XPS, and IR/Raman spectroscopy. This will provide detailed information about surface morphology, composition, chemical state, and adsorption behavior. • Surface physics and chemistry investigations: The synthesized catalysts will undergo extensive investigations to explore surface physics and chemistry. This will involve probing surface reactions, surface species identification, and studying the influence of surface phenomena on catalytic activity and selectivity. • Correlation analysis: The obtained surface characterization data will be correlated with CO2RR performance results, enabling the identification of key surface properties that dictate catalyst performance. Computational modeling may also be employed to gain a comprehensive understanding of the surface-activity relationships. • Optimization of catalyst surface properties: Based on the identified surface-property-performance correlations, the project will focus on optimizing the catalyst surface properties. By modifying synthesis parameters, the aim is to fine-tune the surface characteristics to achieve enhanced CO2RR performance, including improved activity, selectivity, and stability. Expected Results: (i) Comprehensive understanding of the surface physics and chemistry of novel bimetallic Cu/M catalysts for CO2RR. (ii) Identification of key surface properties, such as morphology, composition, and active site density, influencing catalyst performance. (iii) Correlation between surface properties and CO2RR performance, providing insights into the underlying mechanisms. (iv) Optimization of catalyst surface properties through synthesis parameter modifications, leading to enhanced CO2 conversion efficiency.

Skills and competencies	Knowledge of surface physics and chemistry. Elementary electrochemistry.

competencies for the development of the activity	Knowledge of experimental techniques to characterize the structure, morphology and physical properties of surfaces. Knowledge of physical and chemical techniques to synthesize nanostructure.