Distributed chemicals and fuels production from CO_2 in photoelectrocatalytic devices

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The abatement of CO_2 emissions is one of today's big challenges to keep the planet temperature below a specific dangerous threshold. A great opportunity arises from the exploitation of the chemical reduction of CO_2 into value-added chemicals and fuels. However, the reduction of CO_2 is both thermodynamically and kinetically challenging, requiring powerful catalysts to favour the process with good efficiency and product selectivity. In the framework of CO_2 reduction, the use of solar light as the energy source to trigger the CO_2 fixation is the most desirable route, whereby heterogeneous semiconducting materials can be designed to absorb the visible light, undergoing charge separation and so activate the multi-step CO_2 reduction sequence. In particular, heterogeneous catalyst design is today flourishing in the field of multi-phase materials, where correctly tuned interfaces hold the key for enhanced performance by exploitation of synergistic effects. A current frontier is represented by the incorporation of carbon nanostructures (CNS) in the catalyst final composition, giving rise to carbon-inorganic nano-hybrid catalysts with unique properties. The goal is to interface carbon and inorganic (i.e. metal oxides) semiconductors to achieve improved visible-light response, better charge separation with longer lifetime, suitable potential energy of the valence band and conduction band, and tailored material surface to aid CO_2 diffusion and binding to the active site.
The research activity of this project will focus on the design of nanohybrids consisting of carbon nanostructures and inorganic semiconductors, opportunely interfaced and chemically and/or structurally modified in order to: 1) form ad hoc junctions (p-n junctions or Z-Scheme) for improved charge separation and redox ability, 2) improve the catalyst stability for continuous CO_2 reduction, 3) tailor the superficial properties of the two phases by heteroatom doping (metal ions, metal nanoclusters or non-metal dopants) or controlled defectiveness (e.g. vacancy distribution, controlled porosity, covalent functional groups) for boosting activity and selectivity.
The PhD student will trained on classic and state-of-the art synthetic methods for nanomaterials and nanohybrids, will gain fundamental and deep knowledge of heterogeneous photocatalysis, and will have the opportunity to learn the theory and practice of many characterization techniques, such as electron microscopy (TEM, SEM, EDX), atomic force microscopy (AFM), spectroscopy (Raman, FT-IR, XRD, XPS) and determination of textural properties of material, as well as basic principle of electrochemistry. The research activity will be performed in the frame of a European Project H2020-H2020—RIA-CE-NMBP-25 Program-Grant No. 862030 - DECADE and in collaboration with academic and industrial experts for advanced photo-electrocatalysis and functional nanomaterials.

References: Melchionna, M.; Bonchio, M.; Paolucci, F.; Prato, M.; Fornasiero, P. "Catalysis-Material Crosstalk at Tailored Nano-Carbon Interfaces", Chapter 6 in Making and Exploiting Fullerenes, Graphene, and Carbon Nanotubes, M. Marcaccio and F. Paolucci Editors, Springer Link, 2014, pp. 139-180.