CHEMICAL ENGINEERING

ENEA - Green H2 production via a Perovskite-based device for sunlight-driven water splitting

Funded By	ENEA - Agenzia Nazionale per le Nuove Tecnologie, l'Energia e lo Sviluppo Economico Sostenibile [P.iva/CF:00985801000]

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Context of the research activity	The aim of this PhD fellowship is to develop a novel photo/electrochemical reactor integrating perovskite-based photovoltaic cells and low-cost and scalable electrodes for green hydrogen production driven by sun energy.

	Context of the research activity The EU energy system is 80% based on fossil fuels, which cause 80% of EU GHG emissions, and about 53% of the energy consumed in the EU is imported from outside countries. Exploiting sustainable technologies to produce green fuels like hydrogen by using renewable resources offers an opportunity to preserve the environment. It will contribute to reducing greenhouse gases, in line with the commitments agreed in the 2021 Glasgow Agreement signed during the United Nations Climate Change Conference (COP26). Indeed, hydrogen is an energy vector that provides a possible solution to our needs for sustainable fuel for future transport requirements and an approach to large-scale energy storage. More than 95% of this H2 comes from fossil fuel (steam methane reforming) feedstock using high temperatures. Sunlight-driven water electrolysis is a promising technology for green hydrogen production. It avoids the consumption of fossil fuels and CO2 emissions because it uses a highly abundant renewable energy source and just water as feedstock. Another positive aspect is that the produced hydrogen has a high purity of >99.9%. In this context, in the framework of the National Recovery and Resilience Plan (PNRR) ENEA will fund this PhD fellowship to develop to develop a novel photo/electrochemical reactor integrating perovskite-based photovoltaic cells and low-cost and scalable electrodes for green hydrogen production. The electrochemical device will be based on an efficient zero-gap water electrolyzer with an anion exchange membrane, to be able to use novel and low-cost electrodes not based on noble metals, as it is required for current PEM-based water electrolyzers (using IrO2 and Pt catalysts). The fundamental knowledge we have acquired in previous EU and industrial projects will be implemented to accomplish the goal.

Objectives	Objectives: The main objective of this PhD is to develop a photo/electrochemical reactor consisting of an integrated system with 3rd-generation photovoltaic cells (hybrid organic-inorganic metal halide perovskite cells) and an anion exchange membrane (AEM)-based electrolyser using low-cost scalable electrodes to produce green hydrogen using solar energy as the sole energy source. The experimental activities will be performed in part at Politecnico di Torino and in part at ENEA facilities. The expected outcomes of the studies that will be performed are: • Developing new low-cost noble-metal-free catalysts modified with ionic liquids (ILs) for the hydrogen evolution reaction (HER) exploiting scalable synthesis techniques based on wet chemistry. • Chemical-physical and electrochemical characterisation of the developed catalysts. • Kinetic analysis in different electrolytes (basic and neutral media) for comparison with a benchmark HER catalysts. • Developing a half membrane-electrode-assembly (MEA) integrating the best-developed HER electrocatalysts and an anion exchange membrane (AEM). • Investigating the half-MEA performance in a zero-gap electrochemical reactor and optimising the process conditions (flow rate, pressure, temperature, applied potential, current density, etc.) to reach high stability and faradaic efficiency at industrially relevant current density values. • Development and characterisation of morphological, optical, and electrical properties of perovskite-based solar cells with different gap energies to be used as an external power supply of the zero-gap electrocatalytic reactor to produce H2. • Exploring the possibility of using the best perovskite-based photo/electrodes to be integrated and tested with the best-developed electrocatalyst to bring the basis for the development of a photo/electrochemical (PEC) reactor. • Demonstrating the Sun-driven water splitting and H2 production in a new-designed integrated photovoltaic-electrochemical (PV-EC) reactor combining the best-developed materials and optimised operative conditions. Different instruments and characterization techniques (FESEM, XRD, XPS, among others) available at PoliTO-DISAT and CREST Group https://www.disat.polito.it/it/la_ricerca/gruppi_di_ricerca/crest (e.g. Solar-Fuels Lab) will be exploited for the study of the chemical-physical properties and electro-catalytic performance of the device. An electrochemical test bench designed and manufactured in the framework of the CO2 Circle Lab (https://co2circlelab.eu/) will be used for the electrochemical activity tests and long-term stability studies. Product analysis will be performed using analytical instruments, e.g., HPLC, GC-MSD with head-space, and micro-GC. To accomplish this goal, we will implement the fundamental knowledge we acquired in previous EU (e.g., SunCOChem, Artiphyction, ECO2CO2, Solhydromics), national and industrial projects of POLITO and ENEA.

Skills and competencies for the	- Knowledge of chemical engineering, materials science, physics are preferred. - A good background or previous studies in photocatalysis, catalyst synthesis, photo/electrochemistry, and electrochemical reactions are valuable. - Know-how and/or willing to learn electrochemical characterization techniques, electrocatalyst and electrode’s preparation methods.

development of the activity	- Good knowledge of standard practices and previous experience in chemical laboratories are desirable. - Ability to set priorities, work in a multicultural and multidisciplinary team, plan the work and respect deadlines are important. - Availability for a full-time position and for mobility in Italy between Torino, Casaccia and Portici is mandatory.