PhD in CHIMICA INDUSTRIALE E INGEGNERIA CHIMICA / INDUSTRIAL CHEMISTRY AND CHEMICAL ENGINEERING - 40th cycle

PNRR 630 Research Field: EXPERIMENTAL INVESTIGATION OF THE PERFORMANCE OF SOLID OXIDE CELLS (SOCS) IN ELECTROLYSIS, CO-ELECTROLYSIS AND FUEL CELL MODES

Monthly net income of PhDscholarship (max 36 months)
€ 1500.0 In case of a change of the welfare rates during the three-year period, the amount could be modified.

Context of the research activity	
Motivation and objectives of the research in this field	The transition to sustainable and net zero-greenhouse gas energy systems and chemical processes is a main challenge of the Horizon Europe program and among the top priorities of the European Green Deal. Solid Oxide Cells (SOCs) stand out as prominent solutions thanks to their efficiency, reversibility and fuel flexibility. SOCs consist of three ceramic layers: a porous air electrode, a porous fuel electrode, and a dense electrolyte which transfers oxide ions O2-. In fuel cell operation, electrical power is produced via fuel electro-oxidation, typically H2 or syngas (H2/CO mixture). Gaseous O2 is reduced at the air electrode with formation of oxide ions, which migrate across the electrolyte to the fuel electrode, where they convert the fuel. In electrolysis, H2O, CO2 or mixtures of are reduced to H2 and CO at the fuel electrode producing O2- ions, which migrate to the air electrode and form gaseous O2. Electrical power is hence used to split H2O and CO2 and store energy as H2 and CO. The state-of-the-art (SoA) SOCs mount an Yttria stabilized Zirconia (YSZ) electrolyte, Ni-YSZ fuel electrodes, and air electrodes based on perovskite oxides. SOCs typically operate between 700 and 850°C at atmospheric pressure, and this high-temperature conduction challenges the long-term material stability, limits startup/shutdown cycles, and forces slow dynamics.

	Objective of the PhD project is the study of the electrochemical performances of SoA industrial SOCs under three operative modes: as steam electrolyzer for H2 production (SOEC mode); as CO2-H2O co-electrolyzer for the production of syngas; as H2 fuel cell for power production (SOFC mode), achieving high conversion of O2 and H2. Planar electrode-supported SOCs from different industrial suppliers will be tested, and their durability will be investigated under conditions relevant to industrial applications for decarbonization purposes (e.g., in combination with processes of the steel, chemical and power generation industry). The reversible SOFC/SOEC conduction will be examined, and the pressurized conduction of the SOEC will be also explored up to 30 bar. The progress of possible degradation mechanisms will be monitored in time, their consequences will be verified by application of morphologic and chemical characterization methods, and counteracted with appropriate modification of the operative parameters (temperature, gas supply composition and voltage). The possible occurrence of SOC's deactivation motivates the development of novel electrodes, which will be synthesized and manufactured inhouse.
Methods and techniques that will be developed and used to carry out the research	The experimental research activities will be carried out at Politecnico di Milano, in the Laboratory of Catalysis and Catalytic Processes (LCCP). The performance of both button SOCs (2 cm diameter) and applicative SOCs (25 cm2 area) will be studied under several operative conditions by measuring current-voltage curves (IV) and by application of electrochemical impedance spectroscopy (EIS) methods. Performance indicators, such as the maximum power density (fuel cell mode), the H2 production rate (steam electrolysis mode), the syngas production rate and the CO2 conversion (CO2-H2O co-electrolysis mode) will be derived from the IV curves. The electrocatalytic behavior of the SOCs will be investigated in detail with the EIS technique, and the variation of performance parameters such as the ohmic resistance and the polarization resistance will be studied as a function of temperature and gas supply composition. The kinetics of the most relevant electrodic processes will be

	analyzed, namely the reactions of H2 evolution, O2 evolution, CO evolution, H2 oxidation and O2 reduction. Long-term experiments (24/7 up to 1500 h or longer) will be performed on applicative-sized SOCs to verify the possible occurrence of degradation phenomena. In case of deactivation, novel electrodes will be developed with solid state synthesis methods, and deposited on half-cells with screen-printing or spin-coating methods. The IV and EIS results will be rationalized by application of mathematical models of the SOC at different level of complexity (0D and 1D models for button cells, 2D model for applicative cells) in order to extract kinetic rate equations for the electrodic reactions. Morphologic (SEM with EDX, porosimetry) and chemical characterization methods (XRD, TPO/TPR, DTA-TG) will be applied on pristine and post-mortem cells. Once the SOCs' performance parameters are measured, the kinetic parameters are calibrated, and the microstructural properties are established, the single cell models will be used for predictive purposes. The behavior of a SOCs stack will be then simulated at the plant level and the interaction with the other BOP components will be analyzed to establish the optimal operative conditions for target industrial applications.
Educational objectives	The candidate will learn and apply: •fundamental practices for testing SOCs and perform long-term experiments •state-of-the-art electrochemical measurement methods •state-of-the-art synthesis and manufacture techniques for SOCs fabrication •physical models to interpret the measured results.
Job opportunities	Opportunities in professional carriers, as specialist of solid state electrolyzers and fuel cells are found in the fields of: •energy engineering •chemical engineering •advanced hybrid power generation systems

	•materials science
Composition of the research group	1 Full Professors 2 Associated Professors 2 Assistant Professors 0 PhD Students
Name of the research directors	Proff. A. Donazzi, P. Colbertaldo, S. Campanari

Contacts
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Additional support - Financial aid per PhD student per year (gross amount)	
Housing - Foreign Students	--
Housing - Out-of-town residents (more than 80Km out of Milano)	--

Scholarship Increase for a period abroad	
Amount monthly	750.0 €
By number of months	6

National Operational Program for Research and Innovation	
Company where the candidate will attend the stage (name and brief description)	Baker Hughes – Nuovo Pignone via Felice Matteucci, 2 Firenze https://www.bakerhughes.com/baker-hughes-italia
By number of months at the company	6
Institution or company where the candidate will spend the period abroad (name and brief description)	To be defined
By number of months abroad	6

Additional information: educational activity, teaching assistantship, computer availability, desk availability, any other information
Confidentiality: since this is a thematic scholarship, the management of Confidential Information, Results and their publication is subordinate to the restrictions agreed upon with the funding company. Upon acceptance of the scholarship, the beneficiary must sign a specific commitment. **Individual budget for research** (about 6.000 euro): 1st year: 2.000 euro; 2nd year: 2.000 euro;

3rd year: 2.000 euro

Teaching assistantship (availability of funding in recognition of supporting teaching activities by the PhD student): there are various forms of financial for activities of support to the teaching practice. The PhD student is encouraged to take part in these activities within the limits allowed by the regulation.