POLITECNICO DI MILANO

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

PNRR 630 Research Field: DECARBONIZATION OF CHEMICAL PROCESSES THROUGH GREEN HYDROGEN FROM RENEWABLE ENERGY SOURCES

Monthly net income of PhDscholarship (max 36 months)
€ 1400.0 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	**Motivations and Objectives of the Research**The urgent need to mitigate climate change and transition towards a sustainable, low-carbon economy has propelled the search for innovative solutions to decarbonize industrial processes. The chemical sector, responsible for approximately 7% of global greenhouse gas emissions, presents a significant opportunity for emissions reduction. This research focuses on leveraging green hydrogen, produced from renewable energy sources, as a key enabler for decarbonizing chemical processes. **Objectives**The research aims to advance the field of green hydrogen utilization in chemical processes through a multifaceted approach. The primary objective is to develop innovative methods for integrating green hydrogen from renewable energy sources into chemical processes. This goal encompasses several interconnected areas of focus, including the optimization of green hydrogen production and its seamless integration into existing chemical processes.The research will also address the economic and environmental aspects of this transition, conducting comprehensive techno-economic analyses and life cycle assessments to quantify the benefits and potential challenges of implementing green hydrogen-based solutions. Furthermore, the study will contribute to the broader understanding of system-level

	integration by developing robust models that simulate the interplay between renewable energy sources, hydrogen production, and chemical processes.Ultimately, the research seeks to generate valuable insights that can inform policy decisions and support the adoption of green hydrogen technologies in the chemical industry, thus contributing significantly to the global effort to decarbonize industrial processes and transition to a sustainable, low-carbon future. **Key Research Areas** • Green hydrogen production optimization • Process integration techniques • Techno-economic analysis • System modeling and simulation • Life cycle assessment • Policy recommendation formulation Through these areas of study, the research aims to address the complex challenges associated with decarbonizing chemical processes and pave the way for a more sustainable chemical industry. https://commission.europa.eu/strategy-and-policy/priorities-2019-2024/european-green-deal_enhttps://www.governo.it/it/approfondimento/rivoluzione-verde-e-transizione-ecologica/16703https://casale.ch/sustainable-solutions/flexigreen/https://unfccc.int/process-and-meetings/the-paris-agreement
Methods and techniques that will be developed and used to carry out the research	**Methods and Techniques for Research Implementation** The research on decarbonizing chemical processes through green hydrogen from renewable energy sources will employ a multidisciplinary approach, integrating computational modeling and systems analysis. The following methods and techniques will be developed and utilized to carry out the research. **Computational Techniques Process Simulation:** software packages will be used to model and simulate integrated chemical processes incorporating green hydrogen. These simulations will help optimize process conditions and predict large-scale behavior. Machine Learning (ML): advanced ML algorithms, including deep

	neural networks, will be employed to analyze large datasets generated from experiments and simulations, aiding in the discovery of optimal process parameters. **Systems Analysis** Techno-economic Assessment: a comprehensive techno-economic model will be developed to evaluate the economic viability of green hydrogen integration in chemical processes. This will include capital and operating cost estimations, sensitivity analyses, and scenario planning. Life Cycle Assessment (LCA): an LCA framework will be constructed to quantify environmental impacts across the value chain, from renewable energy generation to final chemical products. Energy Systems Modeling: the integration of renewable energy sources with hydrogen production and chemical processes will be analyzed using energy systems modeling tools. **Data Analysis and Validation Uncertainty Quantification:** Monte Carlo simulations and sensitivity analyses will be conducted to assess the robustness of model predictions and identify key sources of uncertainty in the integrated system. Validation Studies: experimental results will be systematically compared with model predictions to validate and refine computational approaches. By combining these methods and techniques, the research aims to comprehensively understand the challenges and opportunities in decarbonizing chemical processes through green hydrogen.
Educational objectives	1. Develop advanced expertise in green hydrogen production technologies and their integration into chemical processes. 2. Gain proficiency in computational modeling and simulation techniques for complex chemical systems and energy integration. 3. Cultivate a deep understanding of techno-economic analysis and life cycle assessment methodologies for sustainable process development. 4. Acquire interdisciplinary knowledge spanning renewable energy systems, chemical engineering, and environmental science. 5. Enhance research skills, including experimental design, data analysis, scientific writing, and effective

	communication of technical concepts to diverse audiences. https://www.bath.ac.uk/corporate-information/institute-for-sustainability-research-theme-sustainable-chemical-technologies/ https://www.nrel.gov/hydrogen/ https://www.nrel.gov/analysis/lca.html
Job opportunities	1. Research and Development Scientist in renewable energy companies or chemical industries focusing on green hydrogen integration and process optimization. 2. Process Engineer specializing in sustainable chemical production and decarbonization strategies for industrial applications. 3. Energy Systems Analyst in consulting firms or government agencies, providing expertise on the transition to hydrogen-based technologies. 4. Academic Researcher or Professor in chemical engineering, environmental science, or sustainable energy departments at universities. 5. Technology Innovation Manager in clean-tech startups or established companies developing green hydrogen solutions for various sectors.
Composition of the research group	0 Full Professors 1 Associated Professors 1 Assistant Professors 1 PhD Students
Name of the research directors	Prof. D. Manca - Dr. R. Ostuni

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	700.0 €
By number of months	6

National Operational Program for Research and Innovation	
Company where the candidate will attend the stage (name and brief description)	CASALE SA Via Giulio Pocobelli, 6 – 6900 Lugano, Switzerland https://casale.ch/
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 5.700 euro):
1st year: 1.900 euro;
2nd year: 1.900 euro;
3rd year: 1.900 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.

Additional information:
Ph.D. students at Politecnico di Milano follow a few mandatory courses to amplify and enhance their cultural and professional background in Chemical Engineering and Industrial Chemistry Ph.D. students may support the supervisor in their teaching activities in both bachelor's and master's degree courses.
There is a dedicated office for the Ph.D. candidate with a desk and a desktop workstation with double monitors and a phone.
The affiliation to Politecnico di Milano opens access to a plethora of software packages and process simulators.