



PhD in CHIMICA INDUSTRIALE E INGEGNERIA CHIMICA / INDUSTRIAL CHEMISTRY AND CHEMICAL ENGINEERING - 41st cycle

**THEMATIC Research Field: PHYSICALLY-INFORMED DIGITAL TWINS FOR CARBON
CAPTURE AND SEQUESTRATION INTO ADVANCED MATERIALS VIA METHANE
PYROLYSIS**

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**

Decarbonizing industry requires CO₂-negative technologies that are scalable, economically viable, and compatible with renewable resources. Converting CO₂-derived methane into carbon nanotube (CNT) fibers and clean H₂ via catalytic pyrolysis can permanently store carbon while displacing CO₂-intensive metals. Process development and scale-up are currently limited by an insufficient predictive understanding of the coupled kinetics and transport processes controlling CNT formation, making reliable design difficult and often requiring computationally expensive approaches. The goal of the PhD is to develop advanced multiscale models that merge first-principles approaches with machine learning to create fast, interpretable, and robust surrogate models for both the kinetic mechanisms and reactor behavior. Close interaction with experimental campaigns carried out with international partners will enable continuous calibration and validation. The project will deliver a physically informed digital twin for CNT synthesis reactors, enabling predictive optimization, experiment guidance, and scale-up analysis toward CO₂-negative deployment.

**Methods and techniques that will be
developed and used to carry out the
research**

The project will rely on the competence, facilities, and methods of the Laboratory of Catalysis and Catalytic



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| | <p>methods of the Laboratory of Catalysis and Catalytic Processes at Politecnico di Milano.</p> <p>Herein, the student will develop the fundamental competence on the multiscale AI-aided modeling of catalytic reactors, thus building a know-how on advanced modeling techniques, machine learning, catalysis and catalytic reactors.</p> <p>The research project will be based on modelling activities, including:</p> <ul style="list-style-type: none"> •development and assessment of microkinetic mechanisms for methane pyrolysis to CNT, •multiscale modeling of pyrolysis reactors based on macroscopic models and/or computational fluid dynamics simulations, •development of physically-consistent machine learning digital twins, •assessment and validation with experimental data in collaboration with international research partners. |
| Educational objectives | To gain a high-level knowledge about catalytic processes for energy applications through advanced modeling and machine learning techniques. The candidate will develop cutting edge competences on the frontiers of the energy transition and of decarbonization strategies. |
| Job opportunities | Graduates from the Ph.D program will find abundant opportunities in research institutions, chemical industries, energy companies, consultancy companies in the field of electrification and decarbonization, catalyst manufacturers, car manufacturers. |
| Composition of the research group | 7 Full Professors 4 Associated Professors 4 Assistant Professors 15 PhD Students |
| Name of the research directors | Proff. Bracconi and Maestri |

Contacts

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| Additional support - Financial aid per PhD student per year (gross amount) | |
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| Housing - Foreign Students | -- |
| Housing - Out-of-town residents | -- |

| Scholarship Increase for a period abroad | |
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| Amount monthly | 750.0 € |
| By number of months | 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 may sign a specific commitment.

Educational activities (funding for participation in courses, summer schools, workshops and conferences) - financial aid per PhD student per year:
 1st year: around 2000 euros
 2nd year: around 2000 euros
 3rd year: around 2000 euros

Teaching assistantship: availability of funding in recognition of supporting teaching activities by the PhD student:
 There are various forms of financial of 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.