Supervisor Expression of Interest
MSCA - Marie Sklodowska Curie Action
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Link pagina docente:	Institutional web-page / Research group web-page
Department Name:	Department of Chemistry, Materials, and Chemical Engineering “G. Natta”
Research topic: (https://www.polimi.it/en/scientific-research/research-at-the-politecnico/departments/)	PE8-11: Environmental engineering, e.g. sustainable design, waste and water treatment, recycling, regeneration or recovery of compounds, carbon capture and storage; PE8-2: Chemical Engineering, technical chemistry; PE4-12: Chemical reactions: mechanisms, dynamics, kinetics and catalytic reactions
MSCA-PF Research Area Panels:	☐ CHE_Chemistry ☐ ECO_Economic Sciences X ENG_Information Science and Engineering ☐ ENV_Environmental and Geosciences ☐ LIF_Life Sciences ☐ MAT_Mathematics ☐ PHY_Physics ☐ SOC_Social Sciences and Humanities
Politecnico di Milano Areas:	☐ Cultural Heritage ☐ Smart Cities X Horizon Europe Missions ☐ Health ☐ Industry 4.0
Title and brief description of the Department and Research Group (including URL if applicable):	**Title** Turning plastic waste into hydrogen and chemicals: a physico-chemical description of the gasification process The Department of Chemistry, Materials, and Chemical Engineering "Giulio Natta" joins together different skills to identify safe, cost-effective, and sustainable solutions to current challenges in multi-disciplinary fields such as environment, renewable resources, energy, industrial processes and health. The CRECK Modeling Lab is a worldwide reference in pyrolysis, oxidation, and combustion of fossil and alternative fuels. The group has a strong experience in the numerical modeling of homogeneous and heterogenous reactive flows with detailed kinetics. Internationally recognized expertise in thermal treatment of biomasses and plastics and computational facilities are available in the group, which is the ideal host for a successful MSCA applicant. URL: http://creckmodeling.chem.polimi.it/

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Brief project description

More than 150 million tons of **plastic waste** are generated in the world every year (26 million in EU only), and less than 10% are collected for recycling[1,2]. Despite the cumulative plastic waste generation is increasing continuously, only a small amount of collected plastic waste (especially PET/PE packaging) gets actually recycled[3,4]. Composite, mixed plastics, and dirty materials are mostly incinerated[5].

Chemical recycling via gasification is a promising alternative to mechanical recycling[6]. The huge potentiality of this process resides in its ability to convert the polymer structure into high added-value products, such as **hydrogen** and chemicals. In particular, the resulting syngas (a H_2/CO mixture) forms the basis for the production of synthetic hydrocarbons, methanol, ammonia and transportation fuels, to name just a few. Thanks to the methanol-to-olefin process (MTO), gasification products can be eventually converted to light olefins and then to **new polymers in the context of a circular economy**[7].

The main obstacle to the application of gasification at the industrial scale is the **poor level of knowledge** about the chemical processes governing the thermal degradation of plastics during the gasification itself. In particular, there is no clear understanding of how the composition of the resulting syngas is affected by the plastic waste composition (which is inherently variable)[6]. This serious limitation prevents the possibility to control the quality of gaseous products.

The proposed project intends to bring new insights into gasification of plastic waste, filling the gap in our current knowledge of chemistry (and its interaction with transport phenomena) governing the thermal degradation of in the context of gasification. More specifically, the project has the ambition to develop and implement a **multi-scale/multi-physics numerical platform** to model the gasification process at the reactor scale, with detailed description of pyrolysis, partial oxidation, and gasification reactions. The final goal is to pave the way to the application of modeling-driven approach for **design and optimization of real-scale gasifiers for plastic treatment** (with emphasis on the quality of gasification products), as a mean to enabling a circular economy in the process industry.

In order to reach this goal, the research activities will require a multi-disciplinary approach, including in particular: i) development of detailed mechanisms for thermal degradation of most common polymers[8]; ii) formulation of chemically reduced-order-models (or meta-model) via machine-learning to be applied at the reactor-scale[9]; iii) implementation of multi-scale/multi-physics models for real-scale gasifiers (with different fidelity levels and computational costs), specifically conceived for plastic waste treatment.

References

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