POLITECNICO
MILANO 1863

Supervisor Expression of Interest
MSCA - Marie Sklodowska Curie Action
Postdoctoral Fellowship (PF) 2021

Supervisor name:	Marco Mehl
Email address:	marco.mehl@polimi.it
Link pagina docente:	https://tinyurl.com/xun2rdbj | https://tinyurl.com/cc8vuspn
Department Name:	Department of Chemistry, Materials, and Chemical Engineering
Research topic: (https://www.polimi.it/en/scientific-research/research-at-the-politecnico/departments/)	PE8_2 Chemical engineering, technical chemistry, PE4_12 Chemical reactions: mechanisms, dynamics, kinetics and catalytic reactions, PE6_12 Scientific computing, simulation and modelling tools, PE8-11 Environmental engineering, e.g. sustainable design, waste and water treatment, recycling, regeneration or recovery of compounds, carbon capture and storage
MSCA-PF Research Area Panels:	X CHE_Chemistry ☐ ECO_Economic Sciences X ENG_Information Science and Engineering X 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: Enabling combustion of hydrogen at extreme conditions.** 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 recognized as a worldwide reference in pyrolysis, oxidation, and combustion of fossil and renewable energy sources, with specific focus on the mitigation of pollutants formation (e.g. particulate matter, nitrogen oxides, etc.). The group is constituted by 6 professors, 2 postdoc fellows and 8 PhD students, and has a consolidated experience in the numerical modeling of reactive flows (homogeneous and heterogeneous) with detailed kinetics, and in the field of physical-chemistry. http://creckmodeling.chem.polimi.it/

POLITECNICO
MILANO 1863

Brief project description:	**Hydrogen** (H_2) **is projected to be the energy carrier of the future**: it can be made from renewables, it can be stored, transported, and used as a fuel[1]. The elegant idea of converting renewable, but intermittent, solar and wind power into hydrogen with water electrolysis is giving rise to a plethora of hydrogen-based energy storage solutions. At the end of the chain, hydrogen **can be combusted in the existing infrastructures, with minor retrofitting, obtaining water and closing the loop**. The combustion of hydrogen does not produce greenhouse gases (e.g. CO_2) or harmful/toxic pollutants (CO, unburned hydrocarbons, particulate matter) and, thanks to its outstanding specific energy (Lower Heating Value = 120 MJ/kg) and combustion properties (e.g. high laminar flame speed, long ignition delay time), it allows high efficiency and improved stability of the combustion process. However, the **utilization of hydrogen in thermal machines** for power generation, transportation and **domestic and industrial heating is hindered by** few open challenges. One of the main challenges is safety, due to its wide flammability and explosive limits[2]. In addition, it is still not clear whether hydrogen combustion reduces the formation of **nitrogen oxides (NO_x)**[3] compared to other fuels. Many stakeholders are investigating the opportunities of **oxy-fuel combustion** of hydrogen, to prevent NO_x formation while still reaching extremely high thermodynamic efficiencies (i.e. T>2500 K). Other applications focus on highly diluted combustion or partial displacement of methane in mixtures. Particularly for these applications, it is important to resolve the issue of **combustion instabilities**[4-6], and the effects of hydrogen high diffusivity. Enabling a full exploitation of hydrogen urgently calls for a deeper understanding of combustion phenomena from microscale **thermochemical kinetics** to multi-scale **fluid-dynamics modeling with detailed kinetics**. Targeted investigations should focus on extreme conditions such as **oxy-fuel, ultra-lean conditions** and combustion in the presence of exhaust gases, for both pure **hydrogen and its blends with hydrocarbon fuels** from natural gas to diesel and jet-fuels. The proposal has to elaborate **one or more** of the points below focusing on enabling the exploitation of hydrogen in the European energy system, as in the top priorities of the European New Green Deal. 1) Development of a chemical kinetic model for the combustion of hydrogen and its mixtures with methane and other hydrocarbons, with a specific focus on NO_x formation and on mixture effects (e.g. third body colliders). 2) Development of *ad hoc* model reduction and optimization techniques for specific extreme conditions of interest for hydrogen use. 3) CFD modeling of combustion instabilities, detonation phenomena in real turbines for air transport and power production applications for improved efficiency and safety.

1. Sazali, N. *International Journal of Hydrogen Energy* (2020)
2. Zhao, M. et al. *Fuel* 275 (2020): 117986.
3. de Persis, S., et al. *International Journal of Hydrogen Energy* 44.41 (2019): 23484-23502.
4. Hosseini, S. E.et al. *International Journal of Green Energy* 17.1 (2020): 13-37.
5. Laera, D. et al. *Proceedings of the Combustion Institute* (2020).
6. Oztarlik, G. et al. *Combustion and Flame* 214 (2020): 266-276.