POLITECNICO
MILANO 1863

Supervisor Expression of Interest
MSCA - Marie Sklodowska Curie Action - (PF) Postdoctoral Fellowship 2022

Supervisor name:	Matteo Pelucchi
Email address:	matteo.pelucchi@polimi.it
Link *"Pagina docente":*	https://tinyurl.com/44yxhr2c
Department Name:	Department of Chemistry, Materials and Chemical Engineering "G. Natta"
Research topic:	PE4_12 Chemical reactions: mechanisms, dynamics, kinetics and catalytic reactions PE8_2 Chemical engineering, technical chemistry PE8_9 Production technology, process engineering PE4_1 Physical chemistry
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 X Industry 4.0
Brief description of the Department and Research Group (including URL if applicable):	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 for modelling aspects in energy conversion processes such as pyrolysis, gasification and oxidation on fossil and renewable energy sources, chemical recycling of wastes, biomass conversion and carbon nanomaterials chemistry. The group is constituted by 6 professors, 1 postdoc fellow and 8 PhD students, and has a consolidated experience in the multiscale modeling of

POLITECNICO
MILANO 1863

	reactive flows (homogeneous and heterogeneous) with detailed chemical kinetics, and in the field of physical-chemistry. http://creckmodeling.chem.polimi.it/
Title	**Automated chemistry models development for the energy transition and for a sustainable chemical industry**

Brief project description:
(max 1 page)

The imminent decarbonization of the chemical and energy industries and the transition to a circular economic model urge upon the scientific and industrial communities aiming for the development of new or improved processes for energy conversion, materials (e.g. carbon materials), chemicals (e.g. syngas) and energy vectors/fuels production (e.g. H_2, bio-fuel/bio-oils) or utilization.
The development and deployment of flexible, reliable and automated approaches coupling the fundamental knowledge of **physical chemistry** and **chemical reaction engineering** aspects with new frontiers of science such as **data analytics** and **machine learning** can pioneer the automated generation, development and validation of accurate kinetic models of use for industrial reactor design and optimization, thus supporting the large-scale accomplishment of the required technology change.
Despite the great recent advances of automated theoretical and model generation frameworks in the area of homogeneous gas-phase processes such as hydrocarbon and renewable fuels pyrolysis and combustion, condensed and multi-phase processes of current industrial relevance have not been tackled yet in a similar bottom-up fashion.
This can be justified by many different reasons such as: 1) intrinsic complexity of multiphase, multicomponent and multi scale phenomena limiting the availability of purely kinetic experimental information, 2) dominance of phenomenological simplified models of limited general validity, and 3) computational time limitations inhibiting the applications of high-level theoretical methodologies (ab initio molecular dynamics, density functional theory models).
In this context, key processes that should be considered and addressed via a specific project proposal are: 1) **biomass conversion** with pyrolysis and gasification, 2) **plastic wastes recycling** with pyrolysis and gasification, 3) **carbon material and hydrogen synthesis** from the catalytic pyrolysis of hydrocarbons.
Key-aspects (**one or more**) to be targeted in relation to **one** of the above processes of interest in the energy and circular economy transition scenarios are:

a) Development of **automated computational chemistry** tools for the determination of model parameters (i.e. kinetic rate constants, thermodynamic and transport properties);
b) Development of **automated** tools for kinetic **model generation** using cheminformatics and machine learning methods;
c) Development of **automated model analysis**, assessment and design of experiments tools