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Supervisor Expression of Interest
MSCA - Marie Sklodowska Curie Action - (PF) Postdoctoral Fellowship 2023

Supervisor name:
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Link "Pagina docente":
https://www4.ceda.polimi.it/manifesti/manifesti/controller/ricerche/RicercaPerDocentiPublic.do?EVN_PRODOTTI=evento&idugov=67311

Department Name: Dipartimento di Energia

Research topic:
MSCA-PF Research Area Panels:

- ☐ 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
- **X CHE_Chemistry**

Brief description of the Department and Research Group (including URL if applicable):
The Department of Energy (DoE) joins together different skills existing at PoliMi in various fields of engineering to provide convenient solutions to the complex problems that currently affect the energy sector (www.energia.polimi.it). The Multiscale Catalysis Group (www.shape.polimi.it) is hosted at the Department of Energy in the Laboratory of Catalysis and Catalytic Processes (www.lccp.polimi.it). The group has strong expertise in multiscale modeling of chemical processes (www.catalyticfoam.polimi.it). Experimental and computational facilities are available to the group.

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TITLE of the project:

ADVANCED MULTISCALE MODELING FOR THE INTENSIFICATION OF CATALYTIC PROCESSES FOR ENERGY TRANSITION

Brief project description:

The development and discovery of new catalysts and processes along with the optimization and improvements of the existing technologies are crucial to face the strong challenges required to reduce anthropogenic emissions. It urges to achieve higher transformation rates per unit reactor volume with concomitantly higher mass and energy efficiency improving process sustainability and reducing the human footprint. Process Intensification (PI) is playing a crucial role in addressing these challenges aiming at developing advanced catalyst, reactor and process designs fully tailored to the specific process requirements able to provide breakthrough improvements in performance. This can be achieved by a fundamental understanding of the catalyst functionality and advanced reactor design based on first-principles than on empirical testing. In the last decade, multiscale modeling has been demonstrated to provide such in-depth insights into the complex physical-chemical phenomena enabling to achieve a functional understanding and tailored process designs. First-principles multiscale modeling is currently gaining more and more importance in process intensification enabling to simultaneously account for a rigorous description of the transport phenomena along with a detailed description of the chemistry. However, the approach is inherently limited by the significant computational cost. Machine learning can be synergically employed to reduce the computational cost, while hybrid machine learning models trained with the data and enforced by physics can assist the design of unconventional but intensified reactors. The manufacturing of these unconventional systems requires adequate techniques. Additive manufacturing is showing enormous potential in this direction and their future developments are expected to make it possible to routinely fabricate intensified reactors [1].

Despite its attractiveness, the routine application is still limited by the inherent complexity and significant computational cost.

In this context, crucial aspects to be considered and addressed in a specific project proposal are, among others:

- Reduction of the computational cost of first-principles-based multiscale simulations via machine learning and artificial intelligence methods;
- Development of systematic reactor design strategies based on multiscale modeling and assisted by artificial intelligence;
- First-principles-based Modeling of the interactions between new sources of energy (e.g., microwave, electric heating) and the reaction site;
- Development of advanced multiscale models for multiphase systems (e.g., gas-liquid-solid) with detailed kinetic description;
- Advanced manufacturing for process-tailored reactors via additive manufacturing (e.g., 3D printing) and advanced testing;

The proposal has to elaborate on one or more of the previous points by focusing on the intensification of processes of extreme relevance for the energy transition and the chemical industry.

[1] M. Bracconi, , Chem. Eng. Process. - Process Intensif. 181 (2022) 109148.