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Supervisor Expression of Interest
MSCA-IF Marie Sklodowska Curie Action-Individual Fellowship

Supervisor name:	Prof. Matteo Maestri
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Department Name: Research topic: (https://www.polimi.it/en/scientific-research/research-structures/departments/)	Dipartimento di Energia Chemical Technologies and Processes (PE4_10 heterogeneous catalysis; PE4_12 chemical reactions: mechanisms, dynamics, kinetics and catalytic reactions; PE4_13: theoretical and computational chemistry; PE8_2: Chemical Engineering, technical chemistry)
MSCA-IF Research Area Panels	X 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 X Smart Cities ☐ Territorial Fragilities ☐ Health ☐ Industry 4.0
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 ERC group SHAPE (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 a strong expertise in multiscale modeling of chemical processes (www.catalyticfoam.polimi.it). Experimental and computational facilities are available to the group. SHAPE is an ERC project focusing on the development of an experimental and theoretical methodology for structure dependent microkinetic models in heterogeneous catalysis.

POLITECNICO
MILANO 1863

Brief project description: **(max 1 page)**	The worldwide rapidly growing demand for more efficient exploitation of energy and material resources strongly urges upon the scientific and industrial communities the development of new and improved catalytic processes. In particular, the required extreme targets on activity, selectivity and stability under very demanding operating conditions represent a great challenge and call for the ability of nano-designing catalytic materials and processes based on functional understanding rather than empirical testing. Multiscale analysis based on microkinetic modelling is acknowledged to be the essential key-tool to contribute to this quest, thus providing fundamental insights into the functional-based understanding of a catalytic process. The last decade experienced steadily growing progress in the way how predictive-quality theory and simulation can be quantitatively applied to address this task. First-principles multiscale modelling is currently one of the most emerging and challenging topics in modelling catalysis. The possibility of modelling the surface chemistry in detail and at the fundamental level enables the consolidation of fundamental knowledge about a catalytic process under different operating conditions. Despite its attractive potential, the application is still strongly limited by the inherent complication and complexity of the problem, which make such an approach limited and prohibitive for most of the processes of technological interest [1]. In this context, key-aspects to be considered and addressed via a specific project proposal are, among others: a) need of accounting for the explicit effect of the active site in multiscale simulations (e.g., size and shape effects, confinement effects in voids of molecular dimensions, ..). b) incorporation and detailed modeling of diffusion effects at the meso-scale in multiscale simulations c) development of methodologies based on a hierarchical approach to overcome the complexity of the problem (scale-coupling; propagation errors; …) The proposal has to elaborate one or more of the previous points by considering also the application of the multiscale microkinetic approach to processes of industrial relevance for energy applications (e.g., methanol-to-olefins, direct conversion of methane to fuels and chemicals, CO_2 hydrogenation to chemicals, …) [1] M. Maestri, Chem. Commun., 2017,53, 10244-10254