# Supervisor Expression of Interest
**MSCA-IF Marie Skłodowska Curie Action-Individual Fellowship 2020**

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<tr>
<th><strong>Supervisor name:</strong></th>
<th>Matteo Maestri</th>
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<tr>
<td><strong>Email address:</strong></td>
<td><a href="mailto:matteo.maestri@polimi.it">matteo.maestri@polimi.it</a></td>
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<tr>
<td><strong>Link pagina docente:</strong></td>
<td><a href="http://www.shape.polimi.it/people/matteo-maestri-cv/">http://www.shape.polimi.it/people/matteo-maestri-cv/</a></td>
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<tr>
<th><strong>Department Name:</strong></th>
<th>Dipartimento di Energia</th>
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<tr>
<td><strong>Research topic:</strong></td>
<td>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)</td>
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<tr>
<th><strong>MSCA-IF Research Area Panels</strong></th>
<th>CHE_Chemistry</th>
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<tr>
<td></td>
<td>ECO_Economic Sciences</td>
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<td>ENG_Information Science and Engineering</td>
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<td>ENV_Environmental and Geosciences</td>
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<td>LIF_Life Sciences</td>
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<td>MAT_Mathematics</td>
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<td>PHY_Physics</td>
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<td>SOC_Social Sciences and Humanities</td>
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<th><strong>Politecnico di Milano Areas:</strong></th>
<th>Cultural Heritage</th>
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| **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](http://www.energia.polimi.it)). The ERC group SHAPE ([www.shape.polimi.it](http://www.shape.polimi.it)) is hosted at the Department of Energy in the Laboratory of Catalysis and Catalytic Processes ([www.lccp.polimi.it](http://www.lccp.polimi.it)). The group has strong expertise in multiscale modeling of chemical processes ([www.catalyticfoam.polimi.it](http://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. |


**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. The great challenge consists of the ability of nano-designing catalytic materials and processes based on functional understanding rather than empirical testing. Multiscale analysis based on microkinetic modeling 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. First-principles multiscale modeling is currently one of the most emerging and challenging topics in modeling catalysis. The possibility of modeling the surface chemistry in detail and at the fundamental level enables the consolidation of fundamental knowledge about a catalytic process under different operating conditions [1].

In this context, key-aspects to be considered and addressed via a specific project proposal are among others:

a) the need of accounting for the explicit effect of the active site in multiscale simulations by means of atomistic calculations (e.g., size and shape effects, confinement effects in voids of molecular dimensions, …) [2-4].

b) analysis and assessment of solvation effects with a specific focus on electrocatalysis

c) coupling between operando-experiments and theoretical investigation of the catalytic phenomenon [5]

d) CFD simulations of reacting flows at surfaces [6,7]

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 relevance for **energy applications** (e.g., CO₂ reduction, dry-reforming of methane, …) in the context of thermal-catalysis or electrocatalysis.
