Brief description of the training project (2)

- **Title of the Training Project:**
  Development of magnetic catalysts for electrified dehydrogenation reactors

- **Description of the scientific and educational objectives:**

The electrification of reactors, i.e. the use of energy from renewable sources instead of fossil fuels to produce the heat necessary for the operations of industrial reactors, is an important goal from an industrial point of view to reduce the carbon footprint of the chemical industry (emissions of greenhouse gases) and dependence on fossil fuels. This is particularly important for reversible endothermic reactions such as those of dehydrogenation.
This technological change also offers significant opportunities for innovation, to reduce inefficiencies related to limitations on heat transport that reduce both the productivity and energy efficiency of the process and therefore strongly determine costs. In current industrial reactors where the heating takes place outside the reaction tubes in which the catalyst is contained, interphase transfers are present which severely limit the overall heat transfer process.
By introducing a new heating technology that allows heat to be generated in direct contact with the catalyst, these limitations are drastically reduced. Furthermore, it is possible to create a temperature gradient between the surface of the catalyst and the fluid phase, allowing a rapid cooling of the products as they desorb from the catalyst, allowing an improvement in the control of secondary reactions and the formation of carbon, therefore an improvement in the selectivity and of stability.
Therefore, technological change offers considerable possibilities for improving the process and its cost-effectiveness, as well as a drastic reduction in CO_2 emissions.
However, a redesign of the catalyst is needed to take advantage of these opportunities.
One of the possibilities of generating the reaction heat directly in contact with the catalyst is by introducing nanomagnetic elements into the catalyst, which through the application of an external magnetic field, generate the heating of the nanomagnet.
The heating of the magnetic particles caused by changes in the magnetic field can occur through different mechanisms, the main one is to generate heat losses due to induced eddy currents, but in nanoparticles, the heat is generated by the thermal energy dissipated through the domain inversion process magnetic occurring in ferromagnetic material. By realizing a structure of the core-shell catalyst, where the nanomagnetic material is in the core of the nanoparticle and the catalyst in the outer layer, a new concept of catalysis can therefore be developed where heat (for the endothermic reaction) is generated (through the application of a modulated magnetic field) directly inside the catalytic nanoparticle. The further advantage of this technology is the possibility of externally inducing fluctuations in the temperature that allows operating in periodic transient conditions that can allow for improvements in the catalytic behaviour.
It is therefore a highly innovative technology that allows not only to significantly reduce CO_2 emissions but also to significantly improve the process itself, thus allowing an increase in industrial competitiveness.
The topic addressed will therefore allow the creation of a highly qualified figure, on the issues of i) development of innovative processes for the electrification of chemical processes, ii) reduction of the carbon footprint in industrial reactors, iii) preparation and testing of nanocatalysts, iv) improvement of catalytic dehydrogenation processes, v) advanced characterization of nanomagnetic and core-shell catalysts, vi) reactors heated by

magnetic induction and their engineering. The study provides for the multidisciplinary integration of various skills, focused on industrial chemistry, but which extends from the study of the physics and chemistry of materials and their characterization to the engineering of devices and industrial development. The proposed study is therefore perfectly consistent with the themes of the ACCESS PhD, which is centred on the development of innovative solutions for the industry that uses renewable energy by replacing the current methodologies that use fossil fuels.

The proposed research is fully consistent with the needs of the country, in terms of i) reduction of dependence on fossil fuels and ii) greenhouse gas emissions, iii) promotion of the use of renewable energy, iv) increase of innovative capacity and the competitiveness of industry, v) promotion of human capital. It is also fully consistent with the territories involved in the program (Sicily), as there is a) the promotion of human capital, b) the development of the renewable energy chain, c) the reduction of greenhouse gas emissions and d) the development of innovative solutions for the electrification of reactors in chemical processes. The technologies developed to allow an increase in the resilience of the territory and represent new innovative possibilities for the development of sustainable and integrated chemistry with the territory, which also represents an industrial recovery plan for the crisis areas present in the region following the closure of many production lines in the chemical area.

- **Company Supervisor:** Dr. Angelo Ferrando (Versalis spa)

- **Methods of carrying out training and research activities:**

  The training and research activities will be integrated into the context of the ACCESS International and Industrial Doctorate which provides for a series of training and educational activities, which are coherently integrated with the proposed research activity. The interaction with other PhD students, the possibility of interaction and collaboration with other national and international PhD students, the training activities (from seminars to schools and meetings) and the additional skills that are provided (from training to work in the industrial sector, to aspects of confidentiality and patents, to the increase of computer and linguistic skills, as well as to work in teams) are an added value compared to the typical training in Doctorates. The additional added value is represented by a period, from 6 to 12 months, at Versalis to further increase the ability to operate in the field of industrial development.

  The research activity, apart from the period at Versalis, will be carried out at the CASPE (Catalysis for Sustainable Production and Energy) Laboratory of the University of Messina which has experience of several decades in the development of innovative heterogeneous catalysts for industrial and on process innovation and electrification to reduce the carbon footprint in industrial processes. This centre, therefore, has the skills, staff and equipment that allow the PhD student to operate with maximum efficiency in achieving the aims of the project.

  The study will address the various elements necessary for complete training of the PhD student, from the preparation of the catalysts and other necessary materials to their characterization using a combination of experimental techniques, to the study of their behaviour, and to the development of the reactors and devices necessary for the study. , including aspects of scale-up and industrial development, depending on the results obtained.

- **Effects and expected results with particular emphasis on promoting economic development and the production system:**

The study combines both fundamental and applicative aspects, as the goal is the development of technology applicable from an industrial point of view, with therefore considerable attention to all aspects that allow a quick transition from laboratory results to industrial application.
The expected results are the development of knowledge for a new catalytic dehydrogenation technology in magnetically heated reactors with renewable energy and the innovative nanomagnetic catalysts required for this technology. The study represents the first element that will have to be further developed at higher TRL to arrive at the development of the new process.
The results, therefore, represent the first element in the development of a new catalytic dehydrogenation technology to arrive at a new process with a low carbon footprint and greater efficiency, based on the use of renewable energy. This will therefore make it possible to achieve the objectives of climate change mitigation and innovation at the basis of the PNRR and of economic development and the production system..

Company name: Versalis S.p.A.
Website: https://versalis.eni.com
Country: Italy
The aforementioned company will host the PhD student beneficiary of the scholarship financed on the resources of Ministerial Decree 352/2022 for a period of 6 months during the course of the doctorate.

Period abroad for a period of 6 months at the following institution:
Technische Univ. Munich (TUM, Germania)