Solid Catalysts for activation of aromatic C-H bonds

Acronimo: **H-CCAT**
Call: **NMBP-01-2016 Novel hybrid materials for heterogeneous catalysis, Horizon 2020: Research and Innovation Action**
Responsabile UNIPG: **Prof. Luigi Vaccaro**

Abstract: This project intends to contribute to the definition of innovative approaches for the design of hybrid materials as support in heterogeneous catalysis. The focus of the research is towards the C-C bond formation processes via activation of inert C-H bonds and the preparation of hybrid organic/inorganic catalytic systems featuring effective recoverability and reusability that will allow to access a sustainable and environmentally-friendly chemical production.

In agreement with the specification of this Horizon2020 call, and considering the leading-edge character of the proposed research, the impact for the European industry in terms of market entry of new and improved products based on project results is expected to be in the medium to long term (5 – 10 years after project endgoals of the project).

More in details, the H-CCAT project **devises solid hybrid materials** that are superior **catalysts for C-H activation on aromatic compounds**, and develops **innovative procedures to produce and shape these catalytic materials in an economically and environmentally beneficial way**. The catalysts will allow **sustainable production of pharmaceutically relevant compounds** or other **specialty chemicals**. The targeted reactions comprise:

(i) Oxidative **C-H/C-H** couplings, in which an organic molecule is linked via its C-H bond to an aromatic reactant with another C-H bond;

(ii) Non-oxidative **C-H/C-X** couplings, in which an organic molecule with a hetero-atom (X) is coupled to the C-H bond of the aromatic reactant.

Catalysts are selected and developed starting from two material classes:

(i) **Metal-Organic Framework (MOF) materials**: these are porous, crystalline and sometimes flexible hybrid materials, made from an inorganic metal-(oxo) cluster (e.g. Zr, Al, Fe,...) and organic linkers. These MOFs will be used for **C-H/C-H coupling** and for **C-H/C-X coupling**;

(ii) **Porous hybrid silicas**, which are hybrid materials made from a silicate scaffold with organic surface groups, and which acquire porosity by templating with organic surfactant micelles. These will be used for **C-H/C-X coupling**.

The active catalytic sites will be designed in these **porous hybrid host materials** using combinations of active metals and organic ligands, all linked with robust bonds to the host matrix with **engineered porosity**. **Shaping processes** will be developed in function of **catalytic demonstration at pilot scale**. **Greening** of the reactants, solvents and processes will be

studied, strictly **avoiding toxic compounds**, and **LCA** will be performed to demonstrate the environmental benefits both in materials preparation and in pharmaceuticals production.

UNIPG research unit will lead two "working packages" including the key WP3: Catalytic testing and design of new catalytic sites. In 200 months of personnel work UNIPG will study the heterogeneous catalytic approaches to the synthesis of Rilpiverine (anti-HIV agent produced by DSM), and also will set continuous-flow reactors able to minimize the waste production.

With a budget of ca. 8 millions of euro, the project involves public research centres as CNR units of Lyon (Dr. David Farrusseng and Dr. Chloé Thieuleux) and Montpellier (Dr. P. Hubert Mutin) and 3 Universities (Leuven (Belgio), that coordinates the project with Prof. Dirk. DeVos; Goettingen (Germania), Prof. Lutz Ackermann, and Perugia (Italia), Prof. Luigi Vaccaro). In addition, the project comprises the participation of several industrial research units: AXEL'ONE (France), Johnson Matthey (United Kingdom), Fraunhofer IKTS (Germany), Johnson & Johnson (Janssen) (Belgium), Sikemia (France), ProfMOF (Norway), and the support of DSM (The Netherlands).