



Towards the nano-engineering of the catalytic processes



The Shape project fine-tunes a theoretical and experimental methodology

Heterogeneous catalysis plays a crucial role both in the production of important chemicals (for instance, ammonia, the basis for production of fertilizers), energy applications (for example, fuel production) and environmental protection (for example, pollution abatement from vehicles). Peculiar to heterogeneous catalysis is the interaction between the reactants and specific functional materials (“the catalysts”), which allows for the selective enhancement of the rate of elementary reactions. The Shape project, funded by the European Research Council for the period 2016-2021 and coordinated by Prof. Matteo Maestri (Politecnico di Milano, Italy), aims at establishing an experimental and theoretical methodology for the development of structure-dependent microkinetic models. This allows prediction of structural changes of the catalyst during reaction by achieving an atomistic-level description of the structure-activity relation. The potential contribution of Shape on catalysis science and technology is very high by making possible the engineering of the chemical tran-

sformation at the atomic level. The possibility to predict the catalyst structure under reacting conditions has a direct impact on the fundamental analysis and design of the structure-activity relation, thus paving the way towards the nano-engineering of the catalyst structure and composition to tailoring activity and selectivity for advanced process intensification in applications of technological relevance.

