ACTIVE SITES AND KINETICS PROPERTIES OF HETEROGENEOUS CATALYSTS IN REACTIVE ENVIRONMENT: INTERPLAY BETWEEN EXPERIMENTS AND ATOMIC SCALE MODELING

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Most efficient heterogeneous catalysts used industrially are generally very complex systems. Far away from perfect crystallinity and well-defined oriented surfaces at low coverage, they involve structural disorder, heterogeneous site distribution with variable coordination and structural dependence upon the chemical environment. Unraveling their atomic-scale structures and understanding their roles in the catalytic reaction are not easy tasks, as the respective contributions of each type of site to the spectroscopic or catalytic responses are generally convoluted. Computational chemistry is of great help to address these issues, but very often, simple structural models are proposed to understand catalytic reactions. In the present talk, we will show how Density Functional Theory (DFT) calculations provide original information about the structure for active sites of complex catalytic systems of industrial relevance, as a function of their environment, to assign spectroscopic observations and to quantify the kinetics of multi-step reactions they can catalyze. We will also show how *ab initio* thermodynamic and kinetic information can be introduced in kinetic models, to access macroscopic predictions thanks to a multiscale approach. Heterogeneous catalysts involved in industrial applications such as refining, petrochemistry, biomass conversion and pollution abatement will be chosen as examples. The synergy with experimental spectroscopic[1-3] and kinetic [4] investigations will be illustrated in each case.

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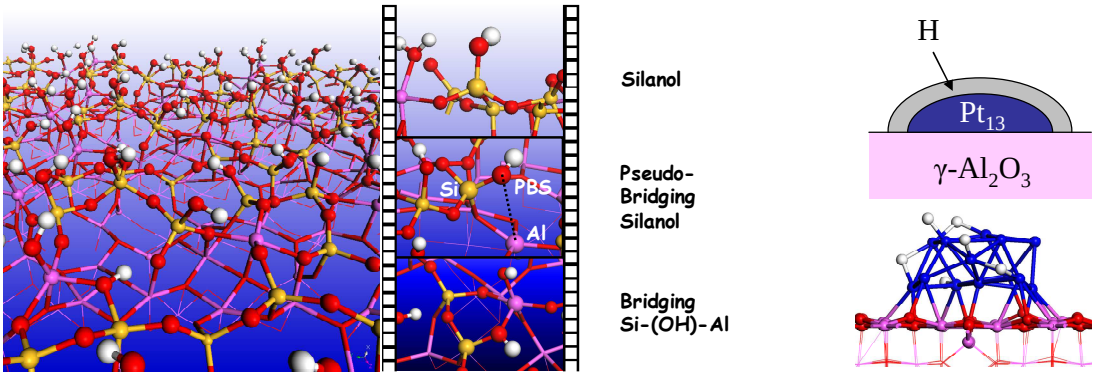

Fig. 1 Some examples of models for industrially relevant systems: amorphous alumino-silicates and supported platinum particle in the presence of hydrogen.

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