**Applications of DFT to a better understanding and design of industrial catalysts in refining and petrochemistry**

**Dr. Herve' Toulhoat**

IFP, France

The main specificities of heterogeneous catalysts will be first recalled, as well as the typical conceptual gaps hampering the rational design and synthesis of these key materials for production of fuels and chemicals.

A wish list of the basic requirements for an adapted computational chemistry approach follows logically. In view of this list, the specificities of density functional theory (DFT) with respect to other ways to solve the poly-electronic Schrödinger equation, combined with the sustained validity of the "Moore law", help explain why this approach became so overwhelming popular over the past two decades, in particular for addressing heterogeneous catalysis research issues.

This adequacy will be illustrated by a few examples covering, for systems of industrial significance, both detailed structural and energetic descriptions of catalytic surfaces and elementary reaction steps, and in silico screening of new materials guided by periodic trends and the principle of Sabatier.

The combined Forcefield+DFT treatment of confinement effects in micro-porous materials will be also briefly exemplified.

Finally, care will be taken to signal the main pitfalls to avoid, to discuss know limitations of DFT, and to foresee the progress to be expected for the years to come.