# Abstract

## Exploring new frontiers in modeling complex chemical transformations in nanoporous materials

**Veronique Van Speybroeck**
**Ghent University**

Chemical transformations in nanoporous materials are vital in many application domains, such as catalysis, molecular separations, sustainable chemistry,.... Model-guided design is indispensable to tailoring materials at the nanometer scale level. At real operating conditions, chemical transformations taking place at the nanometer scale have a very complex nature, due to the interplay of several factors such as the number of particles present in the pores of the material, framework flexibility, competitive pathways, entropy effects,... The textbook concept of a single transition state is far too simplistic in such cases. A restricted number of configurations of the potential energy surface is not sufficient to capture the complexity of the transformation. In this contribution first principle molecular dynamics methods are used to simulate complex chemical transformation in nanoporous materials, capturing the fully complexity of the free energy surface. Advanced sampling methods will be used to explore the interesting regions of the free energy surface and the number of guest molecules present in the pores of the material is properly taken into account.

**Back to Machine Learning for Many-Particle Systems**