UNIVERSITÀ DEGLI STUDI DI TRIESTE

CONFERENCE ANNOUNCEMENT

On **WEDNESDAY MARCH 29th 2023,**
At **15:00**, in the **SALA DEL CONSIGLIO (I floor)**
of the DEPARTMENT OF CHEMICAL AND PHARMACEUTICAL SCIENCES,
University of Trieste, Build. C11, Via Giorgieri 1

Professor GIOVANNI MARIA PICCINI

RWTH Aachen University (DE)
Institute Technical and Macromolecular chemistry
will give a conference entitled:

Accelerating Catalytic Phenomena in Molecular Simulations

The Department Director

Prof. Paolo Tecilla

Accelerating Catalytic Phenomena in Molecular Simulations

G. M. Piccini

Aachen University, Institute Technical and Macromolecular chemistry

Molecular dynamics (MD) is a valuable tool for investigating the evolution of complex chemical systems. However, the exploration of relevant metastable states, such as reactants and products, can be limited due to large free energy barriers. Enhanced sampling methods, such as metadynamics, have been developed to overcome these challenges and facilitate the transitions between metastable states.

This presentation will focus on the use of enhanced sampling methods for studying realistic catalytic systems with wide application potential, with an emphasis on the rare events problem and the solutions developed to address it. Biasing methods and appropriate collective variables will be discussed.

To demonstrate the practical utility of these methods, several realistic application problems in nanoconfined catalytic reactions will be presented. These examples will include the organic synthesis of pharmaceutical interest compounds in biomimetic calixarene capsules and heterogeneous catalysis in zeolites and nanoporous materials. The presentation aims to contribute to a deeper understanding of complex chemical systems at the atomic level by showcasing the practical utility of enhanced sampling methods in the study of chemical reactions.

In this seminar, we will have an overview of Machine Learning techniques, going from classical methods to state-of-the-art. We will see how a data-driven approach can enrich the scientist's point of view and how Machine Learning is becoming a major player in many fields of science. After a short intro, we will see concrete examples of applications to all kinds of chemical problems, ranging from spectra prediction to chemical reactivity and drug design.