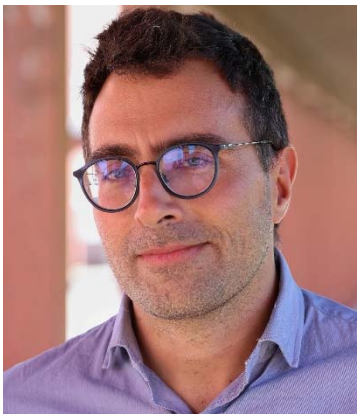
FACULTY OF SCIENCE
Charles University

School of Chemistry, Faculty of Science (FoS) would like to invite you to attend the lecture

Quo Vadis Chemie

Computation Meets Experiment: a Powerful Approach Toward Understanding Catalytic Cycles



which will be delivered by

Dr. Gabriele Manca

Italian National Council of Research (CNR)
at Istituto di Chimica dei Composti
Organometallici (ICCOM) Sesto Fiorentino

on 10.10. at 15:40

the Lecture Hall CH2, the School of Chemistry Building, FoS CU, Hlavova 8, Praha 2

Abstract: Understanding the electronic structure of intermediates and/or Transition States along a reaction pathway is fundamental for the optimization of the operative conditions and may help in looking for more sustainable alternatives with less expensive metals, low or null by-products production or shorter synthetic paths. Nowadays, modern computational techniques allow highlighting the milestones in possible reaction pathways correlating the stereochemical features with electronic structures and the energy costs. Two different examples of catalytic cycles will highlight how the experimental/computational interplay is a powerful approach for the development of new catalytic efficient processes for the synthesis of active pharmaceutical molecules using CO_2 or extended planar π-conjugated systems with potential applications in different fields of chemistry, *e.g.,* materials science or organic electronics