

The Chemist's Interactions

Seminars @ the Chemistry Department



Friday, 10th February 2023

Vincenzo Busico

Department of Chemical Sciences
University of Naples Federico II (IT)



Augmenting the approach to chemical R&D

Chemistry is an empirical science and progresses mainly via trial-and-error. This fact is not likely to change in the foreseeable future. On the other hand, the impact of Digital Reality on chemical R&D is already profound. High Throughput Experimentation (HTE) has boosted chemists' ability to generate data, and HTE databases can be large enough for advanced applications of Artificial Intelligence (AI) for predictive modeling. At the same time, the latest advances in Quantum Mechanics (QM) and High Performance Computing (HPC) make in-silico screening a valid option for chemical explorations. All this represents a true revolution, that calls for multi-disciplinary research environments and competences.

This talk will highlight the new scenario taking as a case history molecular organometallic catalysis with focus on enantioselective olefin polymerization.



The event will be streamed on zoom.us
for external participants!

For registrations: marco.ortenzi@unimi.it



UNIVERSITÀ
DEGLI STUDI
DI MILANO