DIPARTIMENTO DI SCIENZE
E INGEGNERIA DELLA MATERIA,
DELL'AMBIENTE ED URBANISTICA

Water and Waste Environmental Engineering LAB

SEMINAR ANNOUNCEMENT

July 23rd, 2024, 15:00, Aula 155/8

Dr. A. Rabdel Ruiz-Salvador

Universidad Pablo de Olavide

Sevilla, Spain

Atomistic modeling of nanoporous materials

Dr. Ruiz-Salvador studied physics in University of Havana, where also got his PhD in developing computational methodologies for the structural studies of zeolites (1999). In parallel to computational work, he contributed to structural and spectroscopy experimental studies of zeolites. In 2003 he started working on metal-organic frameworks (MOFs), combining modelling and experiment and incorporating method developments for in-silico material design. In 2009 published the first automatic approach for MOF design based on topology (JACS) in connection to the synthesis of new materials. He moved to Spain in 2013, to the University Pablo de Olavide in Seville, being only working in modelling. In 2018 he got a permanent position as a professor and recovered the combination of experiment and modelling research. Currently, he is part of the VALZEO European project that involves UNIVPM together to Universities Autonoma de Barcelona and Havana, and research centres or companies from Spain, Ireland, UK and Cuba to study water treatments and biodiesel production. A list of his publications can be accessed via ORCID http://orcid.org/0000-0002-2004-687X

Abstract

Crystalline nanoporous materials, typified by zeolites and MOFs, are subject of intense research due to their performance in diverse applications, such as catalysis, ion exchange, adsorption and molecular separation among the most significan. This seminar will show examples of recent studies on the use of atomistic modeling for the study and design of these materials in connection to applications.