UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

SYLLABUS DEL CORSO

Introduction to gas sorption and diffusion in porous material

2526-116R-M03

Title

Introduction to Gas Sorption and Diffusion in Porous Materials.
Experimental and Computational Analysis of Gas Capture and Separation for Industrial Applications.

Teacher(s)

Dr. Jacopo Perego
Dr. Charl X. Bezuidenhout

Language

English

Short description

Porous materials are key players in various industrial applications, from catalysis to gas separation and purification. The course provides a fundamental description of sorption and diffusion phenomena in porous materials, offering a combined experimental and computational approach. The course introduces the theory of gas sorption and diffusion in porous media, both from an experimental and computational approach. It will be highly interactive, complementing theory with practical sessions of data analysis and computer simulations.

MODULE A Physics of sorption in porous materials. Experimental techniques and data analysis.
The relevant theories describing sorption and diffusion of gaseous species in porous materials will be introduced and discussed. Gas sorption theory, thermodynamics of gas-solid interactions and gas diffusion in confined media will be briefly introduced. (2h)
Basic and advanced experimental techniques to characterize gas-solid interactions and separation processes will be presented in detail: gas sorption analysis, calorimetric methods and continuous flow measurements ("breakthrough" experiment) will be discussed and illustrated using a "hands-on" approach through the analysis of data collected on state-of-the-art instrumentation. (2h)

Module B Computational modelling and simulation of gas sorption processes
The second part of the course provides a foundational understanding of gas sorption simulations in porous materials. Participants will learn basic techniques for simulating pure and mixed gas sorption using Grand Canonical Monte Carlo (GCMC) simulations. This will introduce Grand Canonical ensembles and Monte Carlo simulations, especially for gas sorption simulations. Analyses of GCMC results for determining the active sorption sites, gas competition, and gas selectivity for multicomponent gas mixture simulation. (2h)
Finally, the participants will perform breakthrough simulations using the state-of-the-art RUPTURA software, comparing simulated and experimental data and assessing the selectivity of porous materials with a combined approach. (2h)

CFU / Hours

1 CFU/8 hours

Teaching period

January 26-29, 2026.

10:30-12:30, Seminar room.

Sustainable Development Goals

AFFORDABLE AND CLEAN ENERGY | INDUSTRY, INNOVATION AND INFRASTRUCTURE | CLIMATE ACTION