UNIMORE
UNIVERSITÀ DEGLI STUDI DI MODENA E REGGIO EMILIA

Dipartimento di Scienze Chimiche e Geologiche

PhD Course

Models and Methods for Material and Environmental Sciences

PRESENTS

Molecular Modelling for Industry: Tools and Applications for Advanced R&D

Speakers Prof. A. Pedone, G. Piccini, C. Adamo, D. Avagliano, F. Muniz-Miranda

Abstract: The course offers a practical and theoretical framework for using molecular modelling to address complex industrial challenges. Through four in-depth modules, participants will explore computational methods tailored to industry-relevant materials and processes, including glass manufacturing, catalysis, and spectroscopic analysis. Each module combines a brief description of the state-of-the art methodologies used and rigorous instruction with practical examples, derived from real-world applications and the instructor's research, to equip participants with a comprehensive skill set for research and development.

Module 1: *Molecular Dynamics of Inorganic Glasses*

Module 2: Free Energy Calculations in Molecular Simulations

Module 3: DFT for Ground and Excited Electronic States

Module 4: Vibrational Properties of Molecules Across Aggregation States

By the end of the course, participants will possess the theoretical knowledge and practical skills to apply molecular modelling tools in R&D contexts across multiple industries.

16-17 June 2025

Time 10:00-13:00 & 15:00-18:00

18 June 2025

Time 9:00-12:00

Room UInt3

(DSCG – Via G. Campi, 103 – Modena)

To partecipate register at

https://forms.gle/gSCkk3KsQzRwwNs87

Host: *Alfonso Pedone* *alfonso.pedone@unimore.it*