



ALMA MATER STUDIORUM  
UNIVERSITÀ DI BOLOGNA

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## **MATERIALS MODELLING**

*A powerful tool supporting research and development of new materials and manufacturing processes. Materials Modelling provides key information about material systems, avoiding time and resource consuming experimental campaigns, thus speeding up their design and characterization.*

The research on Materials Modelling of the University of Bologna bases on a multidisciplinary approach crossing different areas and scales, from science and engineering, computational fluid dynamics, combustion, mechanical analysis, plasma physics, to computational chemistry, structural analysis and electromagnetism. The research on Materials Modelling of the University of Bologna covers several issues:

- Transport processes in polymeric, materials and membranes
- Electromagnetic characterization of materials
- Soil-structure interaction and structural analysis of historical and archaeological constructions
- Electronic models for spectroscopic characterization of molecules of biological, medical, pharmacological and astrochemical relevance
- Molecular and coarse-grained models for liquid crystals, polymers, membranes, proteins and other soft materials in the bulk or nanoconfined
- Modelling electronic processes and chemical reactions of light-induced events in complex molecular, nano-structured and biomaterial systems
- Atomistic modelling of nano-systems, self-assembled and soft molecular materials, including electronic processes and interaction with external stimuli
- Orthopaedic biomechanics
- Plasma processing and synthesis of materials
- Modelling for set-up and verification of technological processes (e.g. plastic deformations, extrusion, casting, structural analysis) and material testing
- Modelling of internal combustion engines and real-time process control
- Modelling catalysed processes in organic chemistry and within bio-systems

## HIGHLIGHTS

The University of Bologna is an active partner of the **European Materials Modelling Council (EMMC)**, aimed to bring materials modelling closer to the demands of industry and to **elaborate the Materials Modelling Roadmap as recommendation for the EC strategies**. The University of Bologna is also involved in several research projects financed at European level, contributing with Materials Modelling expertise: H2020-[SimDOME](#): Digital Ontology-based Modelling Environment for Simulation of materials.

H2020-[OntoCommons](#): Ontology-driven data documentation for Industry Commons.

H2020 - [OntoTRANS](#): Ontology driven Open Translation Environment.

H2020 - [DOME4.0](#): Digital Open Marketplace Ecosystem 4.0.

H2020-[NANODOME](#): Nanomaterials via Gas-Phase Synthesis: A Design-Oriented Modelling and Engineering Approach.

H2020-[EXTMOS](#): EXTended Model of Organic Semiconductors.

H2020-[EMMC-CSA](#): European Materials Modelling Council.

H2020-[INSPIRED](#): INdustrial Scale Production of Innovative nanomaterials for printEd Device.

FP7-[ERC-STRATUS](#): Structure and dynamics of biomolecules by two-dimensional ultraviolet spectroscopy.