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Development of novel sustainable materials and complexes for biomedical and industrial applications

Dr. Emiliano Laudadio

Department of Science and Engineering of Matter, Environment and Urban Planning (SIMAU) - www.simau.univpm.it/

UNIVERSITÀ POLITECNICA DELLE MARCHE

Supervisor: Dr. Emiliano Laudadio
Research Group Description

Dr. Emiliano Laudadio;

Researcher in Chemistry for the Technologies

https://orcid.org/0000-0002-8053-6539

68 publications in peer-reviewed journals; H index 20; 836 citations

Link to CV:

https://www.univpm.it/Entra/Ingegneria_1/docname/idsel/794/docname/EMILIANO%20LAUDADIO

Coordinator of the **Molecular Modeling Laboratory** based in the Polytechnic University of Marche, Ancona.

Prof. Pierluigi Stipa (https://orcid.org/0000-0001-9024-0398) is a full professor in Chemistry of Technologies. He is an expert in radical systems and organic molecules with antioxidant activity. He also has deep knowledge in the use of resonance spectroscopy techniques such as nuclear magnetic resonance (NMR) and electronic paramagnetic resonance (EPR).

Prof. Simona Sabbatini (https://orcid.org/0000-0002-2383-787X) is an associate professor in Chemistry of Technologies. She is an expert in biological systems and organic synthesis. She also has deep knowledge in the use of Fourier-transform infrared (IR) spectroscopy.

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Research Group Description

Molecular Modeling Laboratory: four workstations with 16-core central processing unit (CPU) of type Intel I9 10900K for atomistic simulation techniques based on ab-initio, Density Functional Theory, Semiempirical methods, and Molecular Dynamics Simulations.

Chemistry Laboratory: Perkin Elmer Spectrum GX1 Fourier Transform Infra-Red (IR) spectrometer, Bruker EMX/Xenon Electron Paramagnetic Resonance (EPR) spectrometer. NMR Bruker Fourier 80, Shimadzu LCMS-2050 liquid chromatograph single quadrupole mass spectrometer.

- **European fundings:**
  - PLASNANO (EIC) ID: 101099552
  - GreEnergy (SOCIETAL CHALLENGES) ID: 101006963
  - NANO-EH (FET) ID: 951761

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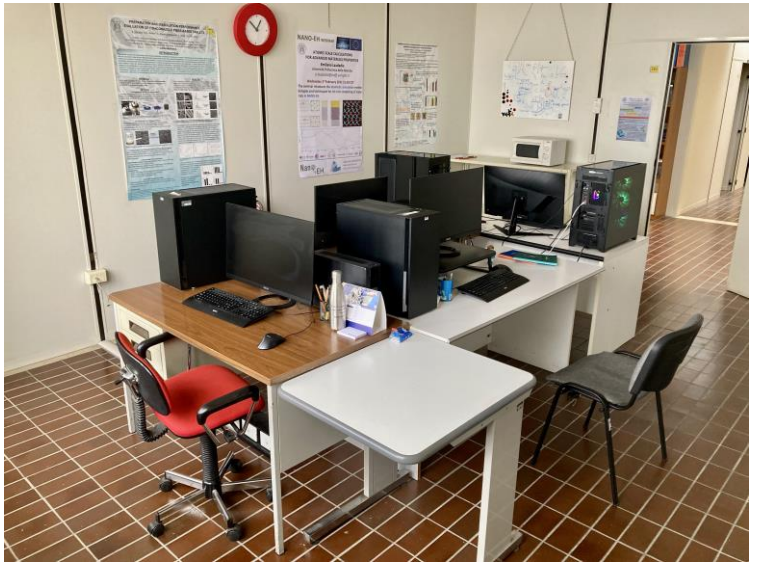
Research Group Description

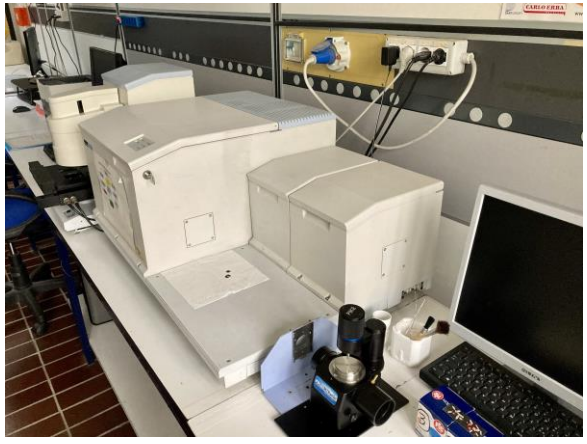
Molecular Modeling Laboratory



Bruker EPR spectrometer

Bruker NMR spectrometer

Shimadzu liquid chromatograph mass spectrometer



Perkin Elmer FT-IR spectrometer

Chemistry Laboratory

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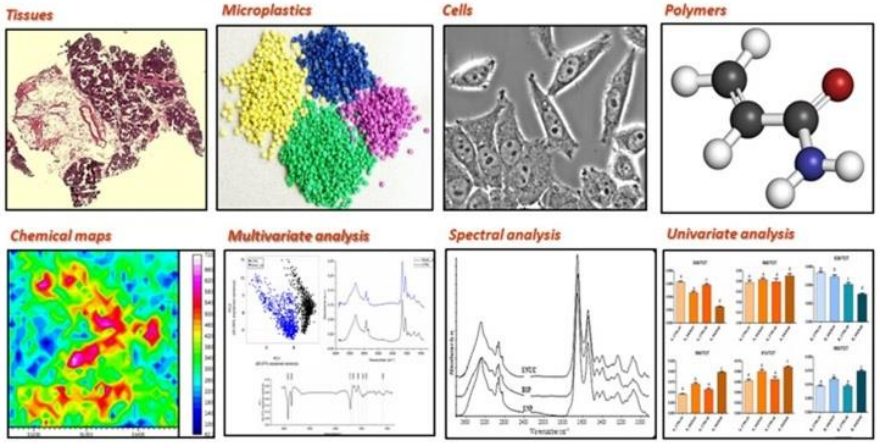
Director: Prof. Pierluigi Stipa

(http://simau.univpm.it/)

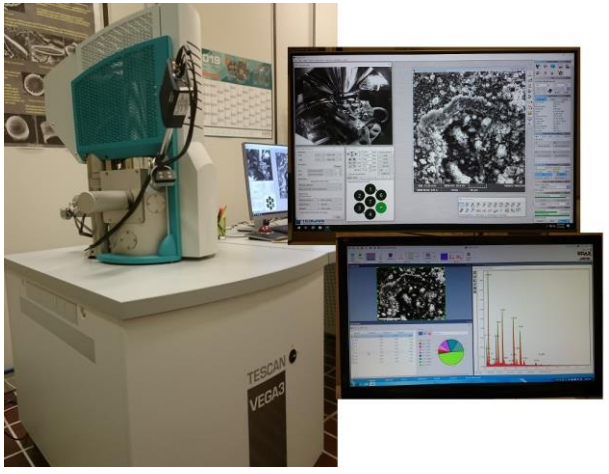
Structure in which the **confluence of different expertises** yield high-level teaching and high-profile international research in the field of **Science of Matter** and **Earth Sciences** with a special focus toward the **Environment**.

It operates within the **Engineering Faculty** offering teachers specialised in the so-called «hard sciences» (**Chemistry** and **Physics**) as well as theachers involved in more «applicative» fields, such as **Materials Engineering**, **Geotechnics**, **Geology**, **Environmental Engineering** and **Urban Planning**.

- **TECHNICAL ARCHITECTURE**
- **APPLIED GEOLOGY AND HYDROGEOLOGY**
- **ENVIRONMENTAL CHEMICAL ENGINEERING**
- **GEOTECHNICAL ENGINEERING**



Research Area



- **CHEMISTRY (ORGANIC)**
- **MATERIALS SCIENCE AND TECHNOLOGY**
- **EXPERIMENTAL PHYSICS**

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Project Idea: Development of novel sustainable materials and complexes for biomedical and industrial applications

The title of this topic is: **development of novel sustainable materials and complexes for biomedical and urban planning applications.** The first target of the present project for biomedical applications includes the study of small molecules and nanoformulations to develop optimal drug delivery systems. This step is completely focused on the atomistic simulations, which will provide many different information about the predicted physical and chemical properties of the models. Hence, systems and small molecules based on the first phase are expected to be fully studied considering the environment in which they should operate (type of solvent, number of salts, different temperatures, and pressures). The final aim is to develop the theorized formulations in laboratory to provide new strategies in specific therapies.

Regarding the industrian applications, soft and hard materials will be investigated in silico, more, interface phenomena between different properties will be considered as well as the effects of different layers on optical and electrical properties. The entire project is based on a combined computational-experimental approach able to provide all the required information to fabricate prominent devices saving costs, times, and promoting a major sustainability reducing the amount of waste.