Supervisor Project Idea

Supervisor

Insert a brief CV and/or external link, the total number of publications, the ORCID link, 5 of the most significant/recent publications, and a list of funded projects and awards. max 300 words

External link to the CV:
https://www.univpm.it/Entra/Ingegneria_1/docname/idsel/794/docname/EMILIANO%20LAUDADIO;
68 publications in peer-review journals; H index 20; 836 citations.
ORCID link: https://orcid.org/0000-0002-8053-6539;

Most recent publications:
Colloids and Surfaces A: Physicochemical and Engineering Aspects; 10.1016/j.colsurfa.2023.131388; https://doi.org/10.1016/j.colsurfa.2023.131388
Results in Physics 57 (2024) 107415; https://doi.org/10.1016/j.rinp.2024.107415
Journal of Physics and Chemistry of Solids 185 (2024) 111755; https://doi.org/10.1016/j.jpcs.2023.111755
ACS Omega 2023, 8, 50, 48292–48303; https://doi.org/10.1021/acsomega.3c07637
Nanomaterials 2023, 13(8), 1319; https://doi.org/10.3390/nano13081319

Funded projects and awards:
- H2020 project entitled “Nano-scale Development of Plasmonic Amplifiers Based on 2D Materials” (**PLASNANO**)” The European Innovation Council (EIC), ID: 101099552 (2023-2026).
- H2020 project entitled “Wideband optical antennae for use in energy harvesting applications” (**GreEnergy**)” SOCIETAL CHALLENGES - Secure, clean and efficient energy, ID: 101006963 (2020-2024).
- H2020 project entitled "Nanomaterials enabling smart energy harvesting for next-generation Internet-of-Things (**NANO-EH**) "EXCELLENT SCIENCE - Future and Emerging Technologies (FET) ID: 951761 (2020-2023).
- Innovation, digitalisation and sustainability for the diffused economy in Central Italy – **VITALITY**” (MUR D.D. n. 3277/2021) (July 2022-May 2023).
- Adrion Master On Circular Economy and BioEconomy (**AMOCEAB**)" (January 2023-September 2023).
- CINECA-ISCRA C: “Anticancer agents derived from Epigallocatechin-gallate targeting EGFR/HER2 in non-small-cell lung cancer therapy” (code: **HP10CMPMGP**) (2020);
- CINECA-ISCRA C: “Design of new non covalent EGCG based inhibitors targeting EGFR to overcome T790M and C797S resistance in advanced non-small-cell lung carcinoma” (code: **HP10CRPVH2**) (2021).
-CINECA-ISCRA C “Nanoscale predictions of semiconductor materials' electrical properties: an efficient in silico approach to design new prominent nanomaterials.” (code: **HP10CK3EZ0**) (2022).
-CINECA-ISCRA C “Atomistic simulations of nanoscale devices based on HfO2, MoO2, and VO2 (code: **HP10CEE3EH**) (2023).

Research Group Description

Provide the name the reference department and a brief description of the research group, including external links, and available instrumentations and infrastructures. max 300 words

The Research group is composed by E. Laudadio (*https://www.univpm.it/emiliano.laudadio*), P. Stipa (*https://www.univpm.it/pierluigi.stipa*), and S. Sabbatini (*https://www.univpm.it/simona.sabbatini*) from the Department of Science and Engineering of Matter, Environment and Urban Planning (SIMAU).
Materials design and analysis will be carried out by means of atomistic simulation techniques based on ab-initio, Density Functional Theory (DFT), Semiempirical methods, and Molecular Dynamics (MD) Simulations using four workstations with 16-core central processing unit (CPU) of type Intel I9 10900K. The whole research field is based on the use of different software and tools, as Quantum Atomistic Toolkit (QATK), QuantumEspresso (QE), GaussView (G), LAMMPS, NAMD, and Gromacs. For extremely onerous and time-consuming simulations, the Research group uses the high-performance computing system located at CINECA Supercomputing Center (https://www.cineca.it/).
The research group also makes use of chemistry laboratory for the synthesis and development of possible new materials with the aim to verify the computational results. Lab facilities: a Perkin Elmer Spectrum GX1 Fourier Transform Infra-Red (IR) spectrometer, equipped with DTGS detectors and Attenuated Total Reflectance (ATR) attachment with a zinc selenide (ZnSe) crystal; Bruker EMX/Xenon Electron Paramagnetic Resonance (EPR) spectrometer system equipped with a microwave frequency counter and an NMR Gauss meter for field calibration in X band, variable temperature with the possibility of "in cavity) direct light irradiation Nuclear Magnetic Resonance spectrometer as well as Mass Spectrometer will be soon available. NMR Bruker Fourier 80, Shimadzu LCMS-2050 liquid chromatograph single quadrupole mass spectrometer.

Title and goals

Provide the title of the topic and a short summary of the project idea. max 200 words

The title of this topic is: **development of novel sustainable materials and complexes for biomedical and industrial 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 industrial 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.

Contact details (*including email address of the supervisor*)

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