

PARTNER PRESENTATION AND INTEREST IN HORIZON EUROPE PARTICIPATION

Name of the organisation	National Institute for R&D in Microtechnologies- IMT Bucharest
Country	Romania
Type of organisation	Research Organization
Short description	<p>IMT-Bucharest (www.imt.ro) is an important actor in Romania and Eastern Europe in its field of activity. The research is oriented to micro and nanoelectronic devices; micro and nanophotonics; nanotechnologies; advanced materials.</p> <p>At European level, in this moment (2023) IMT run as partner 6 Horizon Europe Projects and 1 as coordinator. IMT was involved in 11 H2020 projects.</p> <p>IMT infrastructure IMT-MINAFAB is a facility for design, simulation, Micro-nanofabrication of electronic devices, sensors and systems, nanotechnologies and Carbon based nanomaterials.</p> <p>IMT-MINAFAB addresses the whole value chain starting with design and simulation to micro-nanofabrication, microphysical characterization and reliability tests, with relevance to ICT, Space, Health, Environment and Energy areas.</p>
Laboratory/ Faculty Department	Simulation, Modelling and Computer-Aided Design Laboratory
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Short description of Laboratory involved

The Laboratory is involved in research, development and applications of simulation, modelling and design techniques of micro-electro-mechanical MEMS and microfluidic systems focused on collaborative research projects, education, services (specific design solutions, models, experiments) and consultancy (design/optimization) in the field of micro-nano-bio/info technologies. Also, the laboratory is developing techniques for rapid prototyping from micro to macro scale, micro-sensors and MOEMS and MEMS actuators. Furthermore, we investigate within the Density Functional Theory (DFT) new classes of advanced materials and heterostructures with applications in nanodevices and oxide electronics.

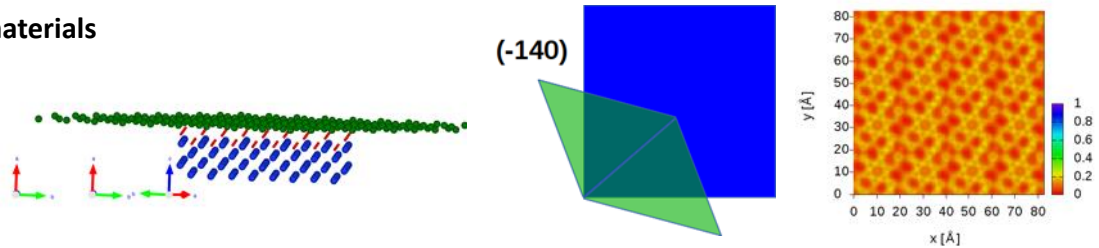
Main software facilities: ANSYS Multiphysics 2022 R2., COMSOL M 6.1, COVENTOR 2014, Materialise Magics 26.0; electronic structure codes: Quantum ESPRESSO, SIESTA, FPLO, VASP, visualization and post processing software.

Scientific computation facilities: High Performance Computing cluster consisting of one Windows node with two Intel(R) Xeon(R) E5-2670 v3 processors, 24 cores, 256 GB RAM, and 10 Linux nodes 10 x 2 CPUs Intel(R) Xeon(R) CPU E5-2670 v3, 240 cores, 256 GB RAM/node.

Expertise

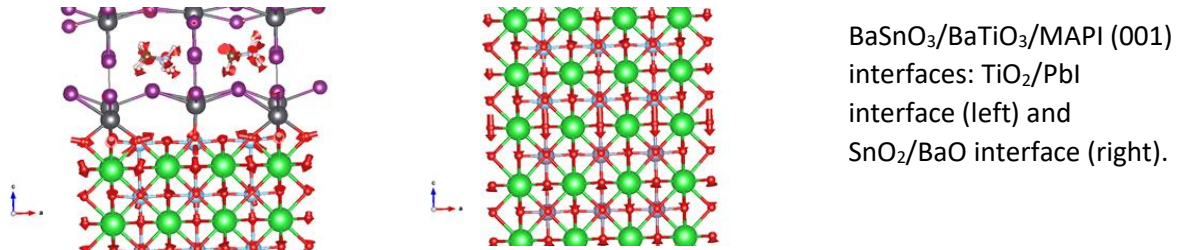
- *First principles* calculations of electronic structure and materials modeling at atomic scale.
- Applications of theory and finite element methods in quantum mechanics for continuum medium physical phenomena simulations.
- Modelling and simulation of multiphysics phenomena: mechanical, thermal, electrical, electromagnetic, piezoelectric, coupled field analysis: static and transient.
- Fabrication of multilevel heterostructures with (ultra)thin layers by advanced technological processes for multifunctional devices.
- Analysis of the physical phenomena at surfaces and interfaces in metal-oxide-semiconductor heterostructures. Modeling their properties for multifunctional devices.

2D materials



Silicene on hydrogenated (100) silicon substrate: structural model (left), silicene layer (-140) orientation on the substrate (middle), SCF charge density (right).

Ferroc Surfaces and Interfaces



BaSnO₃/BaTiO₃/MAPI (001) interfaces: TiO₂/PbI interface (left) and SnO₂/BaO interface (right).

Involved persons. Short CVs.

Dr. Neculai Plugaru, C.S.I, PhD in Physics, Babes-Bolyai University, Cluj, Romania. Expertise in simulation and modeling of material properties from *first principles* electronic structure, using DFT methods.

Dr. Rodica Plugaru, C.S.I, PhD in Physics, Institute of Atomic Physics, Magurele, Romania. Expertise in design and fabrication of advanced heterostructures and the analysis of their optical and electrical properties.

Dr. Titus Sandu, C.S.I, PhD in Physics at Texas A&M University, USA. Expertise is in the field of electronic structure and optical properties of materials with ab-initio and empirical methods, quantum transport in nanostructures, molecular dynamics, electromagnetic response, plasmonics, and dynamical systems.

Phys. Catalin Tibeica, C.S. III: Expertise in the field of modeling and simulation of MEMS, optical, microfluidic and semiconductor devices by using FEM-based simulation tools, in the range of mechanical, thermal, electro-magnetic, optical, and complex coupled field analyses.

Topics of interest. Potential contributions.

HORIZON-CL4-2023-DIGITAL-EMERGING-01-12: Adaptive multi-scale modelling and characterisation suites from lab to production (RIA)

- Develop integrated methodologies of multi-scale and multi-technique characterisation, combined with respective multi-scale modelling and machine learning:
 - developing complex structure-property correlations in advanced materials.
- Integrate modelling and characterisation:
 - developing modelling methods that provide the capabilities to virtually characterise materials and enhance the interpretation of the results of particular characterisation methods in order to guide and refine experiments;
 - developing accurate, validated physics-based models, in areas where these capabilities are a bottleneck, by utilising a combination of characterisation and machine learning to generate material and application specific parameters and equations.

HORIZON-CL4-2023-DIGITAL-EMERGING-01-33: 2D materials of tomorrow (RIA)

- Modeling high-quality 2DM and hetero-structures platforms by exploiting most promising emerging 2DM and/or discovering new ones, and combining them in functional systems and hetero-structures.
- This should be achieved by pushing the boundaries of growth, characterisation methods, deposition and layer-by-layer assembly of atomically thin crystals supported by multiscale theoretical modelling of materials and devices. Multidisciplinary research and innovation activities.
- Coupled atomistic/continuum modelling.

Have you already participated in an EU funded project? If so, provide some references/ results.

H2020: BIONANOPOLYS -Open Innovation Test Bed for Developing Safe Nano-Enabled Bio-Based Materials and Polymer Bionanocomposites for Multifunctional And New Advanced Applications, Call: H2020-NMBP-TO-IND-2020-two stage, Contract nr. 953206, 2021–2024, IMT **Partner Leader: Dr. Oana Tatiana Nedelcu**