

## PARTNER PRESENTATION AND INTEREST IN HORIZON EUROPE PARTICIPATION

Name of the organisation	NATIONAL INSTITUTE FOR RESEARCH AND DEVELOPMENT OF ISOTOPIC AND
	MOLECULAR TECHNOLOGIES - ITIM
Country	Romania
Type of organisation	NATIONAL INSTITUTE FOR RESEARCH AND DEVELOPMENT
Short description	The Molecular and Biomolecular Physics Department is a multidisciplinary scientific research entity (fundamental and applicative) in the field of physics and molecular and biomolecular systems' technology. The department has some of the most modern and performant RDI equipment and highly trained research personnel. The mission of the department targets RDI activities aiming sustainable economical growth, development of novel molecular technologies with applications in medicine, bioeconomy, eco-technologies and emerging bionanotechnologies.
Laboratory/	"Molecular and Biomolecular Technologies" research team
Faculty Department	
Contact person	Dr. Ioan Turcu
Phone	+40731030063
E-mail	ioan.turcu@itim-cj.ro

### Short description of research team involved

*"Molecular and Biomolecular Technologies"* research team is involved in advanced research that explores and develops novel micro/nanostructured systems targeting emerging technologies, theranostic biomedical applications, biomimetics, molecular and biomolecular sensors, molecular electronics etc.

http://en.itim-cj.ro/research/research-teams/molecular-and-biomolecular-technologies/

#### **Research topics:**

- Molecular recognition and self-association processes, intra and inter-molecular interactions
- Supramolecular structures with controlled architecture and functionality
- Bioinspired intelligent micro/nanostructures with applications in medicine, industry and counter-fitting
- Real-time identification and detection of microorganisms using ultrasensitive spectroscopy techniques
- In silico investigation of molecular systems layed onto metallic surfaces, quantum transport processes, and of biomolecular complexes

- Identification of novel antimicrobial and anticancer peptides
- Transport mechanisms through membrane models, protein channels, biological and solidstate nanotubes/nanopores
- Development of exozome-based innovative platforms for theranostic biomedical applications

### Expertise

- Fabrication of molecular structures with controlled architecture and functionality, using of molecular beam epitaxy (MBE) in ultra-high vacuum, and of micro-/nano-structured surfaces, using nano-imprint lithography (NIL), for applications in molecular sensory and molecular electronics
- Nanoscale topographical characterization of surfaces using microscopic scanning techniques (STM and AFM) in ultra-high vacuum
- Microorganisms detection by means of Raman and surface-enhanced Raman spectroscopies (SERS), and their differentiation through multiple chemometric analyses (PCA, LDA, PCA-LDA on vibrational spectra)
- Rational design, generation and characterization of short antimicrobial/anticancer peptides
- Atomic to molecular scale (coarse-grained) molecular modelling and simulation of complex biophysical systems (proteins/short peptides, DNA/RNA, bacterial and mammalian membrane models) by means of molecular dynamics and quantum chemistry
- Development of "tight-binding" and ab-initio models for various molecular systems
- In silico computation of free energy profiles/PMFs for transmembrane molecular transport, (self)association, membrane affinity, by means of equilibrium (Umbrella Sampling), nonequilibrium (FR method), flat-based histrogram ((MW)2-XDOS method), molecular docking (affinities)
- Characterization of biomolecules (with therapeutic/pharmaceutical potential, biomimetical, proteins involved in molecular signalling associated to cancer, oxidative stress/neuro-degenerative diseases) by means of computational simulations (molecular dynamics, molecular docking); biochemical and biophysical methods: SEC-MALS, spectroscopic techniques (UV/Vis, fluorescence, Raman), immunodetection (Western Blot), electrophoresis and gel densitometry; biochemical and microbiological methods: antibacterial activity (MIC/MBS and diffusometric method), testing for cellular viability (IC50), enzymatic activity (TTC), metabolic activity (MTT), membrane integrity (LDH), antioxidant activity (SOD, CAT, GPx, GSH), inflammatory markers
- Bacterial cellular growth; Proteins' expression in E. coli (cloning in expression vectors, PCR, point mutation genesis, DNA segment assembly cloning); Protein purification (sonication, centrifugation, chromatography techniques); Structural characterization by means of X-ray crystallography of proteins, small molecules, biomolecules

### Involved persons. Short CV

**Dr. Ioan Turcu (**<u>https://www.brainmap.ro/ioan-turcu</u> ) - Senior researcher I / Head of "Molecular & Biomolecular Physics" Department; **Areas of Interest:** 1) Self-assembled supramolecular systems; 2) Molecular recognition and self-organizing processes, molecular devices, molecular electronics; 3) Fabrication and characterization of supramolecular structures with controlled architecture and functionality. **Dr Ioan Turcu** coordinated as Project Director or Project Responsible interdisciplinary, research projects (many of them carried out in partnership with other high qualified research teams) focused on developing new emerging molecular technologies based on micro/nanostructured systems with biomedical applications. It is also worth mentioning that Dr. Turcu was the director of an important infrastructure investment project: "Modernizing of the Department of Molecular and

Biomolecular Physics", 2008 - 2012. Value: 6 500 000 EURO. The aforementioned project allows us to acquire high performance scientific equipments dedicated to research and technological developments in the field of supramolecular self assembled structures, molecular devices, molecular electronics, etc. He coordinated as a project manager or project responsible more than 10 projects dedicated to research activities or investment in research facilities accumulating a value which exceed 8 000 000 EURO.

Dr. Daniel Marconi (https://www.brainmap.ro/sorin-daniel-marconi) joined INCDTIM in 2012 on a research scientist position and since then he focused on the fabrication of thin films using MBE technique in UHV, and on the structural characterization of the grown film's surfaces, using STM and AFM. The scientific experience of the project leader is highly relevant for the proposed theme of the project, as in the last years he have been working on micro / nanofabrication techniques, surface science and biophysics. He used the NIL technique to fabricate nanopaterned surfaces used to fabricate flexible, high resolution three-dimensional (3D) QR codes with selective and reflective properties, suitable as anti-counterfeiting and fabrication and characterization of gold-coated nanopost arrays, their use as refractometric sensors, and their optimization through photonics simulations. He accumulated experience on the deposition of thin films, especially of metallic films deposited by MBE deposition technique. He have come to be able to optimise the deposition parameters to fabricate gold films using molecular beam epitaxy technique onto Si(1 1 1) 7 x 7 substrates. The most recent results was to develop and validate an experimental demonstrator in the form of a miniaturized, microfluidic platform and nanopillars for the label-free SERS detection of pathogens within less than 15 minutes. The high international visibility of research carried out to date in Physics, Micro / Nanofabrication Techniques, Surface Science and Biophysics, is confirmed by the international recognition in ISI publications.

Dr. Alia COLNIȚĂ (UNGUREAN) (https://www.brainmap.ro/alia-colnita) physicist has been working at the National Institute for R & D of Isotopic and Molecular Technologies Cluj-Napoca from 2012 as a Research Assistant and since 2014 as Scientific Researcher. Her research interests and activities are in the fields of Surface Science, Nanomaterials and Biophysics. During the last 7 years, Dr. COLNIȚĂ has been involved as a Postdoctoral Researcher or Key Researcher Member in 11 (eleven) Research Projects, among which in 6 (six) Research Projects, she used her thin film and nanostructured surfaces fabrication by MBE and NIL and characterization using STM and AFM expertise for (i) the fabrication of new hybrid organic-inorganic diodes (AlZnO/ZnO/FePc/Au and NdZnO/ZnO/FePc/Au) on flexible/solid substrates using MBE technique; (ii) the fabrication and characterization of high quality flat metallic (Au, Ag) and nanostructured, pillar-based Si surfaces using MBE and scanning probe microscopy - SPM for the development of highly efficient molecular sensors; the results were published in 3 scientific articles; (iii) the fabrication of high quality, micrometer-sized Au/Ag/glass interdigitated electrodes using a newly developed UV irradiation system; (iv) the fabrication of a new reflective gallium optical modulator; (v) the fabrication of circular interdigitated microelectrodes, microfluidic channels and nanotrenches on flexible substrates using NIL; (vi) the optimization of NIL process to fabricate nanostructured quick response codes on flexible substrates as anti-counterfeiting elements. The results of her work have been summarized in a number of 13 ISI and 2 non-ISI articles (6 of them involving MBE thin film deposition and STM characterization), 4 book chapters, 2 pending national patents, 7 oral presentations to international/national conferences and more than 35 poster presentations to international/national conferences.

**Dr. Andra-Sorina TĂTAR** (<u>https://www.brainmap.ro/andra-sorina-tatar</u>) joined the Molecular & Biomolecular Physics Department at INCDTIM in March of 2022, after obtaining her PhD in Physics in 2019 with summa cum laude honours, following a Master's degree in Molecular Biotechnologies and two Bachelor's degrees: in Physics and Biochemistry. After earning of her PhD, she proposed and won two national projects (a Young-Teams project and a Post-Doctoral project) and one intra-university project (from the Babeş-Bolyai University) with a total amount of almost 131 000 Euros. Since the beginning of her PhD years, she was also a member in 6 other national projects, with objectives regarding cancer theranostics via various nano-technological approaches. Overall, her research focus

is the synthesis and characterisation of gold nanoparticles of different shapes (nanospheres, nanostars, nanourchins) and sizes, and their (bio)functionalisation for biomedical applications. Thus, Andra-Sorina's main research interests and expertise are aimed at theranostics, Raman/SERS imaging, smart/controlled drug delivery, and most recently SERS/LSPR sensoristics for biomarkers detection. This is made possible through the use of different cargos with therapeutic molecules or contrast agents, of various types of polymers and the employment of specific recognition elements such as antibodies and/or aptamers. Her work is summarized in 15 poster presentations and 3 oral presentations at international conferences, and 7 ISI publications, out of which all but one are in Q1 journals, attesting to the quality of her research.

# If you are interested in a particular call, please indicate the Reference of the call/ Topic of interest—potential contribution.

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