

Award Application

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2. Romanian Research Gala, 2024 Edition

3. Team application for the “Șerban Țițeica” Award in Physics

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6. Description of the most noticeable achievements during the last 5 years

The applicants are members of the Laboratory of Surfaces and Interfaces from the National Institute of Materials Physics, Măgurele. The group is specialized in a wealth of techniques related to surfaces, interfaces and heterostructures. The principle techniques are related to photoelectron spectroscopy (basic X-ray photoelectron spectroscopy XPS, angle- and spin-resolved photoelectron spectroscopy ARPES and SR-ARPES, photoelectron diffraction, Fermi surface mapping, etc.), *in situ* structural and compositional surface characterization techniques (low energy of reflection high energy electron diffraction LEED and RHEED, Auger electron spectroscopy), and morphology determination with atomic resolution by scanning tunneling microscopy (STM) or non-contact atomic force microscopy (AFM). Several other setups for characterization were developed, such as *in situ* electrical characterization of samples, *ex situ* magneto-optical Kerr microscopy, sample treatment at elevated pressures or temperatures, mass spectroscopy, absorption and desorption measurements etc. The setups of the group costed in total more than € 4 M (<https://infim.ro/lab-40/facilities-and-services/>) and makes them highly demanded by external users. One of the group's setups is implemented on a synchrotron radiation beamline (combined spectroscopy and microscopy on surfaces at SuperESCA, Elettra, Italy). The group publishes in average 27 papers each year and has > 100 collaborations worldwide; in the following, only research stemmed from the group will be presented.

Applied research. The group exploits actively the combined power of XPS to quantify compositions, chemical states and band bending e. g. near the ferroelectric surfaces. The samples are well characterized and surface contamination is avoided. Using these techniques, one is able to investigate the interplay between band alignment, charge accumulation at surfaces and the polarization orientation in Schottky-like structures involving ferroelectric substrates, taking into account various sources of charge accumulation at interfaces, involving also the continuity of metal films [1,2].

By combining the abilities of ultraclean surface synthesis with the high resolution and photon tunability offered by the SuperESCA beamline, the group managed to synthesize graphene single layers on atomically clean lead zirconate titanate, to control *in situ* the polarization of the substrate by a dedicated setup and to investigate the transport properties of graphene and its resistance hysteresis browsing, by ruling out any possible effects of contamination [3]. The picture emerging was that the hysteresis browsing was in the opposite sense than expected, due to a combined share of charge accumulated between the graphene layer and the first two layers of the ferroelectric thin film. Interestingly, such interface charge accumulation phenomena are evidenced also in photocatalytic systems with internal fields, a novel area since about one decade [4]. In the above Ref. it was shown that interface charge transfer promotes titania as a degenerated semiconductor, with beneficial effects on charge transport across the photocatalyst, yielding a very elevated efficiency of water splitting.

As mentioned in the group leader's CV, one of the areas where the group had noticeable results during the last year was that of catalytic processes at ferroelectric surfaces. Ref. [5] presented such an extended study by high resolution XPS, AFM and desorption followed-up in real time of CO uptake by $\text{Pb}(\text{Zr,Ti})\text{O}_3(001)$ (PZT) surfaces decorated with negatively charged Au nanoparticles. Of the data available in literature, this system showed one of the largest CO uptakes, with reversible adsorption and desorption of CO. Therefore, the Au/PZT system can be used as a tunable catalyst for subsequent reactions involving CO (e. g. methanol synthesis).

Another area where the group was specialized was to setup other strategies for fixing molecules under a two-dimensional cover (e. g. a graphene) to improve their residence time for subsequent reaction. Such a 'two-dimensional nanoreactor' was demonstrated by our studies with CO fixation between graphene and $\text{Pt}(001)\text{-hex}$ [6]. The interest to use this substrate is that it is the least reacting with graphene, therefore the best suited to trap molecules under the graphene layer.

The studies mentioned above have obvious applications in industry, mainly involving various catalytic and photocatalytic processes (the studies with molecular fixation on ferroelectric substrates or in 2D nanoreactors, together with photocatalysts with internal junctions), but also memcomputing devices or ultrafast field effect transistors with graphene channels (the case of graphene in-plane conduction on ferroelectric substrates). Another achievement with applicative potential was the easy and reproducible synthesis of $\text{Ag}(111)$ on $\text{Si}(111)$, well characterized by XPS, STM and LEED [7]. This research was triggered by a demand from external users to provide them with $\text{Ag}(111)$ substrates. *Fundamental research.* The group is probably the single one in this area of Europe dealing with experimental band structure determination by ARPES, combined with density functional theory DFT. In Ref. [8] the electron-phonon interaction was evidenced as one of the leading mechanisms controlling the metal-insulator transition in Ce-doped CaMnO_3 , while in Ref. [9] it was shown how the carrier mobility at the interface between a ferroelectric, BaTiO_3 (BTO) or PZT, and the half-metal $(\text{La,Sr})\text{MnO}_3$ can be tuned by the polarization orientation. In Ref. [10] an interplay was demonstrated between the ferromagnetism of Ni overlayers with the ferroelectricity of substrate BTO, thus allowing the control of the magnetism of the ferromagnetic layers through the polarization of the substrate. Note also that the group was leading the research yielding for the first time the three-dimensional polarization-sensitive band structure of PZT, a study published in *Advanced Science* [11].

The group leader concentrated during the last four years also on fundamental aspects of ferroicity (ferroelectricity and ferromagnetism), and on the interplay between these two kind of ordering. As opposed to ferromagnetism, ferroelectricity lacked until recently a microscopic model, the best fundamental understanding was that of the Berry phase approach connecting the polarization to the phase of the Wannier electron wavefunctions obtained by DFT when the structure is progressively distorted. It is known that single domain ferroelectric thin films present a huge

‘depolarization field’, oriented opposite to the polarization of the material, which would destroy the ferroelectric polarization of the material. Thick materials form domains where, according to Kittel’s theory (which was also recently revised and extended by the group leader [12,13]), the depolarization field decreases exponentially towards the bulk, but this model is not valid for single domain thin films. Thus, one has to accept that in these materials, charges are generated and accumulated towards the surfaces or interfaces of the films, with the surface charge density numerically equal to the polarization, such as to compensate the depolarization field. Experimental investigations by X-ray photoelectron spectroscopy of the surface band bending in ferroelectric thin films confirmed this hypothesis. In Ref. [14], instead of regarding charge accumulation at surfaces or interfaces of a ferroelectric thin film as *a consequence* of the establishment of the ferroelectric state, it was proposed as *its origin*. The interaction of a dipole in the material with charges accumulated at surfaces or interfaces may be regarded as a stabilization energy for the ferroelectric state. Starting with the microscopic energy from the above hypothesis, one may apply statistical mechanics and derive the equations of state, more particularly the P – E curves at different temperatures, yielding correctly ferroelectric and paraelectric states. By integrating EdP , one may recover stabilization free energies, which are derived on a microscopic basis and not just on general considerations, as in Landau-Ginsburg-Devonshire model. All parameters of the free energy have then well defined meanings; at the same time, the coercive fields, remnant polarization and their dependence on temperature may be calculated starting with microscopic parameters and yield reasonable values. A non-constant permittivity could be used in the stabilization energy of the ferroelectric phase, and it can be identified self-consistently with the function resulting after applying the statistics based on the microscopic model [15]. This model is able to predict self-consistently the equation of state of a ferroelectric, and in particular the linear decrease of the coercive field with temperature. Microscopic parameters may be expressed directly from experimental quantities.

The next contribution presents a new and more reliable theory of band ferromagnetism, as compared with the venerable Stoner theory. The Stoner criterion connects the one-electron density of states (DOS) $g(\varepsilon)$ evaluated at the Fermi level ε_F with the Hubbard repulsion parameter when two electrons with opposite spins are placed on the same atomic site U , such that $g(\varepsilon_F)U > 1$. It was acknowledged very early that the Stoner theory is unable to predict in a convenient way Curie temperatures of metals, the result being one to two orders of magnitude higher than the experimental values. As a consequence, the basic model of ferromagnetism found nowadays in textbooks is based on localized electrons and their exchange interaction, which is a forced generalization of the Heitler-London model for the hydrogen molecule. In this case, the Curie temperature is connected to the value of the exchange interaction. This model predicts also the magnetic hysteresis, but it can be shown that the resulting coercive fields are several orders of magnitude larger than the corresponding

experimental values in metals. Domain wall migration can be shown to partially solve this issue [12,13], but, nevertheless, it can be shown that the extrapolation of the exchange interaction from the hydrogen molecule to a crystal composed by many electron atoms is simply not appropriate. The band theory was reconsidered starting from a simple observation that the one-electron band energy which has to be taken into account should not be just the kinetic energy, but the total energy, taking into account the shifts of the bottoms of the conduction band for majority or minority spin electrons [16]. A new criterion is derived such that $(dg/d\varepsilon)(\varepsilon_F) \int_{(\varepsilon < \varepsilon_F)} g(\varepsilon) d\varepsilon < g^2(\varepsilon_F)$, where there is no need to introduce the Hubbard parameter. Ferromagnetism is solely dictated by the shape of the DOS. It can be shown that this new theory: (i) predicts the most stable crystal structures along all 3d elements; (ii) predicts correctly why some metals in some crystal structures exhibit ferromagnetism and others not; (iii) predicts correct Curie temperatures; (iv) explains the low coercive fields of metals; (v) predicts that for very large temperatures (5000–7000 K for Fe) the crystal (if it survives) features again a ‘re-entrant’ ferromagnetism. The latter finding proposes the origin of the geomagnetic field as stemming in the ferromagnetism of the Earth’s inner solid core [17]. This implies that during the geomagnetic field reversal, the Earth’s magnetic field is simply rotated without any decrease in magnitude, therefore the planet’s surface will still be screened from the cosmic radiation. No catastrophe related to the vanishing of the geomagnetic field is expected to occur.

In the area of photoelectron spectromicroscopy from ferroelectric surfaces, a multi-D software package was developed, allowing one to manage ‘big data’-like spectromicroscopy data cubes and perform curve fitting at each point of the sample, allowing one to attribute correctly the nature of the components in XPS [18] and the confirmation of an older method (from 2017, see the CV of the group leader) using LEED to derive the surface potential of ferroelectrics by low energy electron microscopy (LEEM) and photoemission electron microscopy (PEEM) performed at Bessy, Berlin.

Recent results are related to the observation of spin asymmetry in the first two surface layers of Pt(001)-*hex* [20], explained using the criterion for ferromagnetism described above, and in the O 2p valence states of SrTiO₃(001), explained by indirect exchange mediated by extended in-gap states due to the generation of defects in the crystal [21]. One PhD thesis supervised by the group’s leader made relevant theoretical contributions in the field of transport through graphene dots in presence of light with various polarizations (including elliptically polarized light) and magnetic field [22–25], revealing interesting control possibilities, and in the field of Floquet topological insulators [26].

The group is actively collaborating with several synchrotron radiation centers: Elettra Trieste (Italy); Soleil Saint Aubin (France); Bessy Berlin (Germany), SLS Zürich (Switzerland). The group from NIMP was recently contacted by Bessy to participate as a founder member to a new international laboratory called GELEM (German-Eastern-European-Laboratory for Energy Materials Research).

8. References

8.1. References to the above application (common papers of the group members), with Journal Impact Factors (JIF) and Article Influence Scores (AIS) from the publication year.

* denotes the corresponding author

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8.2. All group's References from the last 5 years – with Journal Impact Factors (JIF) and Article Influence Scores (AIS) from the publication year.

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12. *Pulsed laser deposited V₂O₃ thin-films on graphene/aluminum foil for micro-battery applications*, T. Tite, C. Ungureanu, M. Buga, I. Stavarache, E. Matei, C.C. Negrila, L. Trupina, A. Spinu-Zaulet,

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13. *Carbon-based heterostructure from multi-photo-active nanobuilding blocks SrTiO₃@NiFe₂O₄@Fe₀@Ni₀@CNTs with derived nanoreaction metallic clusters for enhanced solar light-driven photo-degradation of harmful antibiotics*, A.I. Borhan, A.I. Ghemes, M.A. Husanu, D.G. Popescu, C.N. Borca, T. Huthwelker, I. Radu, A.C. Dirtu, D. Dirtu, G. Bulai, N. Lupu, M.N. Palamaru, A.R. Iordan, D. Gherca, **Applied Surface Science** **622**, 156987:1-156987:17 (2023). JIF = 6.7, AIS = 0.867.

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16. *Boron and nitrogen co-doped carbon-based nanomaterials/nickel oxide/hydroxide hybrids for sunlight induced photocatalytic water cleaning*, P.G. Lebiere, R. Ivan, A.P. del Pino, C. Logofatu, C. Negrila, E. Gyorgy, **Colloids and Surfaces A-Physicochemical and Engineering Aspects** **676**(A), 132159:1-132159:14 (2023). JIF = 5.2, AIS = 0.600.

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18. *Antibacterial activity of PVA hydrogels embedding oxide nanostructures sensitized by noble metals and ruthenium dye*, D. Pelinescu, M. Anastasescu, V. Bratan, V.A. Maraloiu, C. Negrila, D. Mitrea, J. Calderon-Moreno, S. Preda, I.C. Gifu, A. Stan, R. Ionescu, I. Stoica, C. Anastasescu, M. Zaharescu, I. Balint, **Gels** **9**(8), 650:1-650:22 (2023). JIF = 4.6, AIS = 0.626.

19. *Co- and Ni-doped TiO₂ nanoparticles supported on zeolite Y with photocatalytic properties*, G. Petcu, F. Papa, I. Atkinson, A. Baran, N.G. Apostol, S. Petrescu, L. Richaudeau, J.L. Blin, V. Parvulescu, **Nanomaterials** **13**(15), 2200:1-2200:19 (2023). JIF = 5.3, AIS = 0.712.

20. *Silver nanoparticles decorated ZnO-CuO core-shell nanowire arrays with low water adhesion and high antibacterial activity*, A. Costas, N. Preda, I. Zgura, A. Kuncser, N. Apostol, C. Curutiu, I. Enculescu, **Scientific Reports** **13**(1), 10698:1-10698:15 (2023). JIF = 4.6, AIS = 1.132.

21. *From non-stoichiometric CTSe to single phase and stoichiometric CZTSe films by annealing under Sn plus Se atmosphere*, M.Y. Zaki, F. Sava, I.D. Simandan, A.T. Buruiana, A.E. Bocirnea, I.

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22. Structural and electrical properties of novel Cr/Fe mixed transition-metal phosphates, Z. Mighri, K. Souiwa, A.M. Rostas, R.E. Patru, A.E. Bocirnea, N. Iacob, V. Kuncser, O. El Khouja, L.N. Leonat, M. Hidouri, H. Nasri, A.C. Galca, **Inorganic Chemistry** **62**(22), 8530-8542 (2023). JIF = 4.6, AIS = 0.750.
23. Liquid phase oxidation of alkenes and glycerol with molecular oxygen over mixed-ligand copper(II) complexes grafted on GO as catalysts, C. Rizescu, M. El Fergani, D.I. Eftemie, B. Cojocaru, D. Popescu, M. Andruh, V.I. Parvulescu, **Applied Catalysis A-General** **663**, 119302:1-119302:9 (2023). JIF = 5.5, AIS = 0.859.
24. *Floquet topological insulators with spin-orbit coupling*, A. Pena, C. Radu, **Physical Review B** (accepted, 2024). AIS = 0.971, JIF = 3.7.

9. Projects

9.1. Projects lead by the candidate (CMT) during the last 5 years

a. 75PCCDI/2018 (PN-III-P1-1.2-PCCDI-2017-0152), “Technologic paradigms in the synthesis and characterization of variable dimensionality systems”

Funding: RON 1,538,374 (2018); 1,625,907 (2019); 1,825,498 (2020); 297,721 (2021); total RON 5,287,500 and RON 3,749,126 from 2019 to 2021 (about € 750,000). 99 team members.

(<https://infim.ro/project/vardimtech/>)

b. The Core Program of the National Institute of Materials Physics, Project #2 “New developments in the area of functional materials for high technology applications (electronics, optoelectronics, sensors)”, PN23080202, funding RON 13,538,157 in 2023 (ca. € 2,700,000), 112 team members.

c. PN-III-P4-ID-PCCF2016-0047: *Control of electronic properties in heterostructures based on ferroelectric perovskites: from theory to applications* (CEPROFER), Team 1 Project leader: RON 400,000 (2018); 600,000 (2019); 600,000 (2020); 400,000 (2021); total RON 2,000,000 and RON 1,600,000 from 2019 to 2021 (about € 320,000), 13 team members.

(<https://infim.ro/en/project/control-of-electronic-properties-in-ferroelectric-perovskite-heterostructures-from-theory-to-applications/>)

Total amount: ca. € 4,070.000

9.2. Projects lead by other group members:

a. Electronic double layer high mobility Mott transistors, PN-III-P4-ID-PCE-2020-2540, Project leader Marius A. Huşanu, 2020–2023, RON 1,200,000 (ca € 240,000), 6 team members.

b. Integrated Rashba-type platform for data storage and bit manipulation, PN-III-P1-1.1-TE-2021-0136/TE-2021-1053, Project leader Dana G. Popescu, 2022–2024, RON 450,000 (ca € 90,000), 5 team members. (<https://infim.ro/en/project/integrated-rashba-type-platform-for-data-storage-and-bit-manipulation/>)

c. Molecular adsorption and reactions under two-dimensional shells, PN-III-P1-1.1-TE-2019-0916, Project leader Nicoleta G. Apostol, 2021–2022, RON 450,000 (ca € 90,000), 5 team members.

[\(https://infim.ro/en/project/molecular-adsorption-and-reactions-under-two-dimensional-shells/\)](https://infim.ro/en/project/molecular-adsorption-and-reactions-under-two-dimensional-shells/)

d. Investigation by photoelectron spectro-microscopy of the interplay between surface chemistry and polarization landscape of ferroelectric surfaces, PN-III-P1-1.1-PD-2019-0763, Project leader Laura E. Abramiuc, 2020–2022, RON 250,000 (ca € 50,000), 2 team members.

[\(https://infim.ro/en/project/investigation-by-photoelectron-spectro-microscopy-of-the-interplay-between-surface-chemistry-and-polarization-landscape-of-ferroelectric-surfaces/\)](https://infim.ro/en/project/investigation-by-photoelectron-spectro-microscopy-of-the-interplay-between-surface-chemistry-and-polarization-landscape-of-ferroelectric-surfaces/)

10. Patents

10.1. Patent applications of the group leader (published in the Romanian Bulletin of Intellectual Property B.O.P.I.)

a. *Sistem de selecție nanoparticule în funcție de dimensiuni și sarcină, separat, folosind un filtru electric și magnetic funcționând în vid împreună cu o secțiune de frânare într-o zonă cu gaz rarefiat, funcționând în regim continuu / System for nanoparticle selection as function of their size and charge, separately, by using a magnetic and electric filter operating in vacuum together with a braking section in a rarefied gas environment, operating in continuous mode*, C. M. Teodorescu, CBI OSIM a2019 00706/04.11.2019. B.O.P.I. No. 5/2021, p. H01J (# 135010).

b. *Sistem de analiză de timp de zbor în gaz rarefiat, cu determinarea separată a dimensiunilor și sarcinii nanoparticulelor și aerosolilor / System for time-of-flight analysis in rarefied gas environment, with separate determination of dimensions and charges of nanoparticles and aerosols*, C. M. Teodorescu, CBI OSIM a2019 00705/04.11.2019. B.O.P.I. No. 5/2021, p. H01J (# 135011).

10.2 Patents granted during the last 5 years to other group members

a. *Procedeu de pasivare a suprafeței de n-GaSb(100) / Passivation procedure of the surface n-GaSb(100)*, R. Ghita, C. Logofatu, C. C. Negrila, F. Frumosu, D. Predoi, OSIM Patent granted No. 132453 / 28.08.2020.

b. *Procedeu de realizare a unei structuri fotoactive / Procedure for realization of a photoactive structure*, R. Ghita, C. Logofatu, C. C. Negrila, M. D. Mihai, D. Predoi, M. Stoicu, OSIM Patent granted No. 133228 / 28.02.2020.

c. *Structură de superlentilă electrooptică pentru imagistica cu rezoluție sub limita de difracție / Structure of an electro-optical lens for imaging below the diffraction limit*, C. Cotirlan-Simioniuc, S. A. Manea, C. Logofatu, OSIM Patent No. 131292 / 26.02.2021.

d. *Ochelari cu metasuprafețe plasmonice / Glasses with plasmonic metasurfaces*, C. Cotirlan-Simioniuc, OSIM Patent No. 132835 / 30.06.2022.

e. *Dispozitiv optoelectronic cu metasuprafață configurabilă electric pentru controlul polarizării luminii / Optoelectronic device with electrically configurable metasurface for control of the light polarization*, C. Cotîrlan-Simioniuc, A. Rizea, D. V. Ursu, OSIM awarding decision No. 44/82 from 30.05.2022, RO 132167 B1 published in BOPI No. 10/2022.

Feb. 09. 2023,



Cristian-Mihail TEODORESCU

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1. Compliance to criteria of the “Romanian Research Gala”

Overview of publications for the last 5 years (publication date: Jan. 31, 2019 to Jan. 31, 2024)

#	Journal	Ref. (see below)	Publi- cation year	Author count (n _a)	AIS	AIS/n _a	Quar- tile	Main author*	Citation count	Self- citations excluded	Citation count in Q1 journals
1	Catal. Today	143	2019	9	0.837	0.093	Q1	no	60	60	34
2	Appl. Surf. Sci.	144	2019	4	0.867	0.217	Q1	CA	4	4	0
3	Phys.Stat.Sol.–RRL	145	2019	5	0.588	0.118	Q2	no	8	6	3
4	Appl. Surf. Sci.	146	2020	5	0.867	0.173	Q1	no	15	14	7
5	RSC Adv.	147	2020	8	0.57	0.071	Q2	CA	4	2	0
6	ChemCatChem	148	2020	7	0.893	0.128	Q2	no	12	12	10
7	Catal. Today	149	2021	5	0.837	0.167	Q1	CA	3	3	1
8	Catal. Today	150	2021	7	0.837	0.120	Q1	CA	4	1	1
9	Phys.Chem.Chem.Phys.	151	2021	1	0.681	0.681	Q2	SA	10	3	4
10	Res. Phys.	152	2021	1	0.654	0.654	Q2	SA	5	0	0
11	Catal. Today	153	2022	10	0.837	0.084	Q1	no	14	14	10
12	Phys.Chem.Chem.Phys.	154	2022	1	0.681	0.681	Q2	SA	4	0	2
13	Phys.Earth Planet.Inter.	155	2022	2	0.95	0.475	Q2	CA, FA	0	0	0
14	Res. Phys.	156	2022	5	0.654	0.131	Q2	CA	1	0	1
15	Commun. Phys.	157	2022	13	2.254	0.173	Q1	no	1	1	0
16	Catalysts	158	2022	9	0.592	0.066	Q2	no	1	1	0
17	Adv. Sci.	159	2023	14	3.548	0.253	Q1	no	2	2	2
18	Res. Phys.	160	2023	1	0.654	0.654	Q2	SA	3	2	0
19	Res. Phys.	161	2023	1	0.654	0.654	Q2	SA	0	0	0
20	Nanoscale	162	2023	11	1.258	0.114	Q1	no	0	0	0
Total						5.707	9(Q1)	11	151	125	75

* CA = Corresponding Author (unique); FA = First author (unique); SA = single author (i. e. SA and CA included)

- 9 (> 7) papers published in Q1 journals according to the UEFISCDI ranking over the Article Influence Score (<https://uefiscdi.gov.ro/scientometrie-reviste>)
- 11 (> 6) papers published as main author in Q1 and Q2 journals according to the previously mentioned ranking
- Sum of the Article Influence score of all publications from the last 5 years, weighted by the author count

$$\sum_{j=1}^{20} \frac{AIS_j}{n_a^{(j)}} = 5.707 > 5$$

- “Section Editor-In-Chief” at Physics (Basel), <https://www.mdpi.com/journal/physics/editors>
- R&D Projects lead during the last 5 years:

a. 75PCCDI/2018 (PN-III-P1-1.2-PCCDI-2017-0152), “Technologic paradigms in the synthesis and characterization of variable dimensionality systems”

Funding: RON 1,538,374 (2018); 1,625,907 (2019); 1,825,498 (2020); 297,721 (2021); total RON 5,287,500 and RON 3,749,126 from 2019 to 2021 (about € 750,000). 99 team members.

(<https://infim.ro/project/vardimtech/>)

b. The Core Program of the National Institute of Materials Physics, Project #2 “New developments in the area of functional materials for high technology applications (electronics, optoelectronics, sensors)”, PN23080202, funding RON 13,538,157 in 2023 (ca. € 2,700,000), 112 team members.

c. PN-III-P4-ID-PCCF2016-0047: *Control of electronic properties in heterostructures based on ferroelectric perovskites: from theory to applications* (CEPROFER), Team 1 Project leader: RON 400,000 (2018); 600,000 (2019); 600,000 (2020); 400,000 (2021); total RON 2,000,000 and RON 1,600,000 from 2019 to 2021 (about € 320,000), 13 team members. (<https://infim.ro/en/project/control-of-electronic-properties-in-ferroelectric-perovskite-heterostructures-from-theory-to-applications/>)

Total amount: ca. € 4,070.000

2. Biography

Cristian M. Teodorescu (CMT) distinguished himself the first time at the age of 17, when he was still in the last year of the “Gheorghe Lazăr” high-school in Bucharest (mathematics-physics module, Baccalaureate achieved with the maximal mark 10/10), by qualification at the 15th International Physics Olympiad, Sweden (1984), where he won a Bronze Medal (<https://ipho-unofficial.org/timeline/1984/individual>). After this, he was admitted with the maximal mark (10/10) at the University of Bucharest (Romania), Department of Applied Physics. Six years later, after one year military service (artillery) and five years spent at the University, he earned an Engineering degree with the final mark 9.88/10 (third in the 1990 promotion of 110 scholars). The Dissertation title was *Geometric effects and measurement methods of galvanomagnetic effects on circular samples*, advisor Dr. Bogdan Logofătu, presented also at the CAS’90 International Semiconductor Conference, Sinaia, 1990. This was CMT’s first publication, presenting original results both from the theoretical point of view (conformal transformation method), numeric computational and experimental validation.

After his studies, CMT was immediately hired in the Institute of Physics and Technology of Materials, Bucharest (the actual National Institute of Materials Physics, NIMP), in the group of Structure and Thin Films, founded by Prof. Radu Grigorovici and lead at that time by Dr. Andrei Devenyi and Dr. Rodica Mănăilă. Before starting to work in the institute, CMT obtained a two month summer fellowship at DESY, Hamburg, where he became familiar with synchrotron radiation. (Although the contest for this fellowship consisted in problems of nuclear and particle physics.) His whole career afterwards was more or less connected to synchrotron radiation research.

In 1991, CMT was selected for a PhD grant offered by the French Government to study at the University Paris-Sud, *Laboratoire de Spectroscopie Atomique et Ionique*. He earned the PhD degree in 1995 with a thesis entitled: *Study of evolution of inner-shell excitations from free atoms to solids. X-ray photoabsorption of metal and insulating clusters*, advisor Dr. Jean-Marc Esteve, with 6 papers resulting from this work (J. Phys. B 1993 [2] and 1997 [12], Nucl. Instrum. Meth. Phys. Res. A 1994 [4], J. Electron Spectrosc. Relat. Phenom. 1999 [22] and 2000 [25], Phys. Rev. B 2001 [29], first author for all these papers). The main PhD work was to set up and demonstrate installations for trapping clusters in rare gas matrices, combined with mass spectroscopy. CMT set up both installations, learning during these four years the basics of synchrotron radiation based X-ray absorption spectroscopy (XAS), ultrahigh vacuum and mass spectroscopy. Though, the first two papers cited above were rather theoretical, pointing on the precise determination of XAS thresholds and the proposal of a ‘quasi-continuous region’ in XAS extending from the first unresolvable Rydberg line to the series limit [2], and the proposal of an analytic approximation of the Voigt profile, which is still widely

used nowadays in XAS and X-ray photoelectron spectroscopy (XPS) [4]. In Refs. [25,29] CMT proposed for the first time that the XANES structures in the spectra of alkali halides near the K-edges of cations have to be interpreted as having a discrete nature, by comparing the spectra of solids, vapors and clusters. CMT also continued the relation with his former group from Romania by performing Extended X-ray Absorption Fine Structure (EXAFS) and X-ray absorption near-edge structure (XANES) whenever some beamtime was available at the French synchrotron radiation facility *Laboratoire pour l'Utilisation du Rayonnement Électromagnétique* (LURE), which resulted in several publications on catalytic systems (Langmuir 1995 [7], Appl. Surf. Sci. 1999 [19]).

In 1995, six month before the defense of his PhD thesis, CMT was selected for a post-doc position at LURE, in the French-Spanish collaboration dedicated to surface science and angle-resolved photoelectron spectroscopy. During almost two years, CMT worked in this group, becoming a specialist in XPS, angle-resolved photoemission (ARPES), together with other surface science methods, such as low energy electron diffraction (LEED), X-ray photoelectron diffraction (XPD), setting up various devices for sample preparation and manipulation for molecular beam epitaxy (MBE). The work consisted mainly in assistance to external users 24/24 and 7/7, but CMT lead also his own research project consisting in the synthesis and characterization of body centered cubic (bcc) cobalt on GaAs, especially pointing on the role of Sb as a surfactant to improve the crystallinity and enhance the magnetic properties of bcc Co (Surf. Rev. Lett. 1998 [16], J. Electron Spectrosc. Relat. Phenom. 1999 [23], Appl. Surf. Sci. 2004 [44], Phys. Rev. Lett. 2005 [45]). He was involved more generally in many experiments related to the growth of magnetic metals on semiconductors, e. g. Fe/Si(111) with evidence of substitution of Si by Fe in the first atomic layers (Phys. Rev. B 1997 [11], Surf. Sci. 1997 [13], Appl. Surf. Sci. 1998 [17]) or experimental band structure of single crystal superconductors (EPL 2000 [26]).

In 1996, CMT moved for two years at the University of Osnabrück, Germany, to lead a subgroup performing synchrotron radiation based experiments on free molecules and clusters (5 employees). The techniques utilized were XAS, XPS and time-resolved techniques such as time-of-flight mass spectroscopy, partial ion yield XAS, photoelectron-photoion coincidences (PEPICO), triple coincidences (PEPIPICO) allowing one to quantify the kinetic parameters of fragmentation following inner-shell excitation, and zero kinetic energy electron spectroscopy (ZEKE). Experiments were performed at the synchrotron radiation facilities Bessy I (Berlin) and Hasylab (Hamburg). The most relevant results were obtained on sulfur aggregates (J. Chem. Phys. 1998 [15], J. Electron Spectrosc. Relat. Phenom. 1999 [21]), in particular the PEPIPICO patterns were for the first time interpreted correctly and also the fragmentation pathways together with XAS allowed one to discriminate between several structures proposed theoretically for some sulfur moieties. Noticeable research was achieved for the setup of a miniature electron energy analyzer (Rev. Sci. Instrum. 1998 [14]), nowadays commercialized (<https://rbdinstruments.com/products/microcma.html>) and by analyzing XAS and conduction properties of inner shell excited rare gas matrices (Phys. Rev. B 1999 [20]).

In 1999, CMT returned in France, back to LURE where he was firstly hired as an associated CNRS researcher, the appointed as Research Engineer (2000), a tenured position for the management of one of the most demanded beamlines of LURE, SU23, for experiments combining MBE with XPS and with X-ray magnetic circular dichroism (XMCD). CMT renewed the acquisition software of the beamline (monochromator and various detection setups, including control of the applied magnetic field) and managed several interconnecting complex setups, an MBE chamber, a XPS chamber and three setups for performing XMCD at applied magnetic fields up to 7 T and lowest temperatures in the range of 1 K. Obviously, managing these setups required gaining further experience in cryogenics, together with gaining new abilities in MBE, especially in reflection high energy electron diffraction (RHEED). The main part of the work was assistance to external users (Eur. Phys. J. B 2000 [25], J. Appl. Phys. 2001 [31], Surf. Sci. 2001 [32], J. Magn. Magn. Mater. 2002 [34], Phys. Rev. B 2002 [36], Phys. Rev. B 2003 [40]); at the same time, CMT's scientific subject was to continue with the growth and characterization (XPS, XAS, XMCD, LEED, RHEED) of magnetic metals on III-V semiconductors, for both spintronics applications and for the synthesis of diluted magnetic semiconductors (Appl. Surf. Sci. 2000 [28], Surf. Sci. 2001 [33], Eur. Phys. J. B 2002 [35], Appl. Surf. Sci. 2003 [41], J. Alloys Compds. 2004 [42], Surf. Sci. 2006 [50]). For Fe/InAs(001), CMT evidenced the enhanced Fe magnetism and proposed a charge transfer mechanism from Fe to the substrate to explain the enhancement by a factor of three of the orbital magnetism. Another own research was related to magnetism of two-dimensional systems, where according to the Mermin-Wagner theorem there should be no ferromagnetism at nonzero absolute temperature. But CMT demonstrated that in the case of Ni grown on Cu(001) there exists a Ni XMCD signal at ultralow temperature and the magnetization decreases linearly with the temperature, as expected from a Bloch-like law for 2D systems; the explanation of the occurrence of this magnetism relies on the finite size of the magnetic islands, which impose a highest wavelength admissible for the spin waves, or a

lowest possible wavevector, preventing the divergence of the integral Bose-Einstein distribution for the 2D case (Surf. Sci. 2007 [52]). Within the collaborations where he was involved, the soundest results were the synthesis of magnetic hexagonal close packed chromium (Phys. Rev. Lett. 2000 [27], Phys. Rev. B 2002 [37]) and the observation of surface magnetic ordering of manganese in the $c(2 \times 2)$ superstructure grown on Cu(001) (Phys. Rev. B 2001 [30]).

Despite his tenured position, CMT decided in 2001 to come back in NIMP for six months in 2001, then accepted a one year post-doc at the British synchrotron radiation facility Daresbury, again in a group performing XMCD and surface science, at Daresbury and ESRF Grenoble. Here the main result was the synthesis of magnetic vanadium on Cu(001) (Phys. Rev. B 2003 [38]). During this time, CMT participated to the setup and the demonstration of a new detector for X-ray fluorescence (J. Synchr. Radiat. 2003 [39]). By end 2002, CMT returned definitely in NIMP as Senior Scientist III. He became Senior Scientist II in 2005 and Senior Scientist I in 2009.

Up to 2007, in Romanian R&D system there were still hard times. The equipment was out-of-date and the funds were scarce. The former Structure and Thin Films group, with over 30 personnel in 1990, had by that time only three scientists and one technician. CMT managed to win 4 R&D collaborative projects in 2004, one still dealing with spintronics in metal-semiconductor systems, one dealing with TiO_2 -based photocatalysts, one with the setup of a cluster source and one with the setup of time-of-flight experiments (one may recognize several areas in which CMT was involved abroad). Progressively, the situation started to improve; a new scientist was hired for X-ray diffraction, CMT contributed to the setup of an interfaced XR diffractometer, CMT also developed the first turbomolecular pumping based deposition chamber from NIMP and was appointed as operator to the only XPS machine operating by that time in Romania. The group was then able to synthesize thin films by vacuum evaporation and characterize them by XPS and XRD, with the possibility to perform also EXAFS and XANES at DESY, Hamburg. Such mix of techniques was rare in 2004–2006. CMT developed several collaborations with other valid groups across the country, in particular with the National Institute for Lasers, Plasma and Radiation Physics (Măgurele), the Faculty of Physics from the University “Alexandru Ioan Cuza” (Iași), and with the National Institute for Isotopic and Molecular Technologies (Cluj-Napoca). Despite the experimental constraints and the monster bureaucracy, CMT’s group managed to obtain valid and well cited results especially on photocatalytic systems (Surf. Sci. 2006 [51], Surf. Sci. 2007 [53,55], Thin Solid Films 2007 [56], Mater. Chem. Phys. 2008 [58], Top. Catal. 2009 [61], Thin Solid Films 2009 [65], J. Mater. Sci. 2009 [63], Thin Solid Films 2011 [81]) and on core-shell magnetic systems (Surf. Sci. 2007 [55], J. Appl. Phys. 2012 [87]). Maybe CMT’s personal most important achievement from these studies was the evidence of different line widths in the Ti 2p XPS doublet owing to the considerable decrease of the $2p_{1/2}$ core hole lifetime due to the opening of Coster-Kronig decay channels, and the fact that introducing different inelastic background coefficients for different components used in XPS data simulation one can discriminate between surface and bulk origin of these coefficient (the inelastic background associated to surface atoms should vanish). CMT continued his own research on diluted magnetic semiconductors (J. Exper. Nanosci. 2010 [68], Phys. Stat. Solidi A 2010 [69]).

In 2008, CMT won as Project director an infrastructure project “Euro-Regional Centre for Studies of Advanced Materials, Surfaces and Interfaces” (CEUREMAVSU, 2009–2011), about € 11 M, which boosted definitely the R&D infrastructure in NIMP. The newly funded Laboratory of Surfaces and Interfaces was equipped (also with help from other projects, most of them led by CMT) with up-to-date installations, including two clusters with MBE, angle-resolved photoemission and scanning tunneling microscopy (STM) with atomic resolution, a setup for low energy and photoemission electron microscopy (LEEM-PEEM), and a laboratory EXAFS installation. Later, during another infrastructure project “Research, Innovation and Technology Center for New Materials” (RITeCc, 2013–2014, about € 9 M) where CMT was deputy director, a new setup for XPS on limited areas combined with *in situ* treatment at high temperatures and pressures was added to the Laboratory. The MBE machines were constantly upgraded, and in 2013 one of the clusters, which includes MBE, spin-resolved ARPES and STM was delocalized on a synchrotron radiation beamline at Elettra, Trieste, being renamed there as CoSMoS (combined spectroscopy and microscopy on surfaces). The last updates to the R&D equipment of the Surfaces and Interfaces laboratory are from 2023 and consist in a upgrade of one STM setup to AFM based techniques (also with atomic resolution) and the installation and commissioning of a magneto-optical Kerr effect (MOKE) microscope.

At the same time, in 2008 CMT was one of the rare winners of a PCCF (complex project of fundamental research) “Surface and interface science: physics, chemistry, biology, applications” with about € 2 M funds and 9 partner institutions. This constitutes the birth date of real surface science experiments in Romania. “The first atomically clean cm^2 from Romania”, a Si(001) $(2 \times 1) - (1 \times 2)$ sample with contamination below 1 % of a monolayer, was synthesized in May 2009. Other relevant funding include the

participation of CMT as team leader in other PCCF projects, a ANR-ANCS (French-Romanian € 300 k) project with CEA Saclay, a PCCDI (extended partnership, with 5 partner institutions, € 1.2 M), the responsibility of one of the three Core Projects of NIMP. Last but not least, CMT leads from 2014 the “National Interest Installation” (IOSIN) whose name is nowadays “System of complex installations for XPS/ESCA and research using synchrotron radiation”. The IOSIN funding rose progressively from about € 40 k in 2015 to € 400 k in 2023, and one hopes for a funding by about € 1.5 M from IOSIN in 2024. This rise is a sign of a good reputation of the Laboratory within the interested R&D community. With all this funding, with the help of the Core Program of NIMP where surfaces and interfaces are consistently represented, and with the projects won by other group members, the Laboratory of Surfaces and Interfaces created by CMT grew progressively at 21 personnel nowadays.

CMT’s scientific output, especially during the last 15 years (from the start of the CEUREMAVSU and of the first PCCF projects) showed, obviously, a staggering increase. Of the > 100 papers co-authored by CMT during this period, many are collaborations with various users of the infrastructure, especially in the field of catalysis, where a long term collaboration was set up with the Faculty of Chemistry, University of Bucharest. But during this period CMT was main (i. e. single corresponding) author for 48 papers, the ones with the highest impact factors being J. Mater. Chem. A 2014, Nanoscale 2017, Phys. Rev. Appl. 2018, Catal. Today 2021 ($\times 2$), all of them published with no other prestigious or influential co-author from outside Romania. A selection of the most important achievements is given in the following paragraphs, and for the last 5 years is detailed in the Application document.

Validation of XPS to quantify band bending at surfaces and interfaces. Applications in standard and area selected XPS. High resolution and well calibrated XPS spectra may be used to analyze band bending at surfaces and interfaces and in particular to detect the out-of-plane polarization orientation in ferroelectrics (Appl. Surf. Sci. 2013 [99], Thin Solid Films 2013 [100], Mater. Sci. Eng. 2013 [103], J. Mater. Sci. 2014 [109], Appl. Surf. Sci. 2015 [117], Surf. Sci. 2016 [120], Appl. Surf. Sci. 2018 [138]). This method was extended by CMT to photoelectron spectromicroscopy, providing an almost non-invasive method to detect the domain structure in ferroelectric materials by assessment of the contrast in binding energies of core levels (Phys. Chem. Chem. Phys. 2015 [113], Appl. Surf. Sci. 2015 [116], Nanoscale 2017 [130], Res. Phys. 2022 [156]). In particular, for photoelectron spectromicroscopy, CMT developed a software package to analyze 3D and 4D data (hyper)cubes, which was provided free of charge to the community of two synchrotron radiation beamlines specialized on sub-micron area selected spectromicroscopic photoemission experiments Spectromicroscopy (Elettra) and Antares (Soleil). Another important achievement is using the above technique combined with XPS compositional analysis to evidence self-doping of ferroelectric thin films, necessary to produce enough charge carrier for the compensation of the depolarization field (Sci. Rep. 2015 [118]) and to propose a model connecting the polarization orientation of a (atomically clean) ferroelectric thin film as function on the characteristics of the interface formed with the substrate (whether it is insulating, n- or p-doped semiconductor or metal, and also as function on the difference between workfunctions of the substrate and of the ferroelectric, Phys. Rev. Appl. 2018 [139]).

Studies of adsorbates on ferroelectric surfaces, in order to reveal their (photo)catalytic properties. Starting with the evidence of preferential adsorption of contaminants on areas with defined out-of-plane polarization (J. Mater. Chem. A 2014 [112]), CMT’s group succeeded to achieve atomically clean ferroelectric surfaces and then to perform controlled adsorptions on them (Sci. Rep. 2016 [124]), then to extend these studies in the case of coupling noble metal nanoparticles (which became negatively charged on ferroelectric surfaces with outwards polarization) with ferroelectric surfaces (Catal. Today 2021 [150]). CO is adsorbed in both molecular and dissociated form, and upon the sample heating up to the loss of the substrate polarization, the molecules are desorbed, by uptaking also oxygen from the substrate. Using Au negatively charged nanoparticles, the amount of CO adsorbed increases noticeably.

Studies of interfaces formed by graphene on ferroelectric thin films, in view of the explanation of memristor effects for memcomputing applications. The resistance hysteresis expected for such a system stems in the charge accumulation in graphene, driving it towards being p- or n-polarized, as function of the polarization orientation of the substrate ferroelectric. Nonetheless, most experiments from around 2010 evidenced a “anti-hysteretic” behavior, i. e. the hysteresis is browsed in the opposite sense with respect to the expectations. Explanations pointed on the controversial role of adsorbates between the ferroelectric and the graphene, since all experiments to date were performed in air. CMT’s group performed these experiments in ultrahigh vacuum on atomically clean ferroelectrics and well characterized graphene (RSC Adv. 2016 [121]) and finally combined high resolution XPS allowing one to derive the sample composition and polarization orientation with XANES allowing one to evidence the sp^2 hybridization of graphene and its orientation, and with *in situ* electrical transport experiments using a newly dedicated setup, finally evidencing the “anti-

hysteretic" behavior also in this case and proposing a model where charge at surface was located both in graphene and in the first layers of the ferroelectric, to explain this behavior (RSC Adv. 2020 [147]).

Validation of the LEED method to detect the polarization orientation in ferroelectrics. This work was a joint theoretical and experimental work and the unexpected side result occurred when combining the observations from XPS and LEED, with the latter explained by a consistent potential energy of the surface seen from outside (several eV), while the band bending inside the sample due to the ferroelectric polarization was of at most 1 eV. Putting together these results, it followed that the dielectric constant near a ferroelectric surface, in the depleted region, decreases considerably with respect to its bulk value (Phys. Rev. B 2017 [136]). This is in line with other experiments performed in collaboration by CMT with his French collaborators, by using photoelectron diffraction to detect a reduced surface rumpling of the first layers of a ferroelectrics from the surface (Phys. Rev. B 2013 [102]).

Continuation of the study of interfaces formed by magnetic metals and semiconductors, by combining LEED with spot profile analysis with XPS and XANES (J. Mater. Sci. 2012 [83,90], Appl. Surf. Sci. 2013 [95]). Maybe the most important result was the correct attribution of Sm^0 , Sm^{2+} and Sm^{3+} binding energies in Sm 3d XPS spectra and the evidence that the spin-orbit splitting is sensitive to the ionization state [90,95]. *Continuation of studies on diluted magnetic semiconductors,* in particular by successful insertion of Mn substitutionally in Ge(001) by a very simple method (evaporation on the heated substrate), the phenomenon being evidenced by LEED (the same pattern before and after a consistent Mn deposition), EXAFS and high resolution transmission electron microscopy (Materials 2014 [107]).

Insertion of CO between graphene and metal substrates. To date, only one paper was published (Catal. Today 2021 [151]), but there are a wealth of data taken and analyzed in collaboration with the team of Elettra Trieste. *Synthesis of high quality Ag(111) films by growth on Si(111)*, although there is no lattice matching between the two materials (Appl. Surf. Sci. 2019 [144]). *Evidence of spin asymmetry* in surface Pt layers from Pt(001) (submitted to Res. Phys. [163]) and in $\text{SrTiO}_3(001)$ (submitted to Phys. Rev. Res. [164]). These activities are detailed in the Application.

During the last years, CMT concentrated also on the *theoretical basics of ferroic ordering*. He proposed a microscopic model for ferroelectricity (Phys. Chem. Chem. Phys. 2021 [151] and 2022 [154]) by considering the charge accumulated at ferroelectric surfaces or interfaces not as an effect of the establishment of the ferroelectricity, but as the origin of it. Also, CMT revised the Stoner model for ferromagnetism in metals, with surprising results in modelling metal ferromagnets (Res. Phys. 2021 [152]) and prediction of high temperature re-entrant ferromagnetism as a possible origin of the geomagnetic field (Phys. Earth Planet. Inter. 2022 [155]). During the last year, CMT modelled 1D and 2D ferromagnetic domains, including the occurrence of hysteresis and the validity of Kittel's scaling law for the size of domains (Res. Phys. 2023 [160,162]). These theoretical developments are explained in more details in the Application.

In 2015, CMT earned the Habilitation degree from the Faculty of Physics, University of Bucharest and become officially PhD advisor. To date, 5 PhD students graduated under his supervision (4 of them with "excellent" grade, one with "very good") and he is still supervising another 6 PhD students. CMT is teaching Molecular Beam Epitaxy, X-ray Photoelectron Spectroscopy and X-ray Absorption Spectroscopy at the Doctoral School of Physics, University of Bucharest and at the Masters degree of the Faculty of Physics. He also taught such topics during three summer schools. He is teaching XPS, MBE, XAS also at the lectures organized in NIMP for Research Assistants, and from 2021 on he is also teaching three topics in theoretical physics: Electronic Structure of Solids, Semiconductors and Semiconducting Heterostructures and Transport Phenomena in Solids.

CMT participated in > 50 international conferences as invited speaker. He is the owner of one granted patent for a cluster source using adiabatic expansion and based on a novel type of directly resistive heating (Patent # 129723 from Nov. 29, 2016).

In 2018 CMT was elected President of the Scientific Council of NIMP, and re-elected in 2022 (the first re-election for this position in NIMP history). He was awarded in 2015 for results obtained in 2013 with the "Radu Grigorovici" Prize of the Romanian Academy, and in 2018 by the Excellence Award of the Ad Astra Association for researchers with over 7 years of experience in Physical and Chemical Sciences.

He is fluent in French and English and has a fair practice of the German language.

A survey of the main mastered techniques is outlined below:

- Photoelectron spectroscopy (PES): X-ray photoelectron spectroscopy (XPS) or electronic structure for chemical analysis (ESCA), core-level and valence-band PES, photoelectron diffraction (PED), Fermi surface mapping, angle-resolved PES, angle-resolved ultraviolet photoelectron spectroscopy (ARUPS), spin-resolved PES.

- Surface science techniques: low energy electron diffraction (LEED), reflection high energy electron diffraction (RHEED), Auger electron spectroscopy, secondary ion mass spectroscopy (SIMS), sample preparations in UHV, molecular beam epitaxy (MBE).
- Photoelectron spectroscopy, low energy electron microscopy (LEEM), photoelectron microscopy (PEEM), NanoESCA.
- X-ray absorption: extended X-ray absorption fine structure (EXAFS), X-ray absorption near-edge structure (XANES), near-edge absorption fine structure (NEXAFS), X-ray absorption spectroscopy (XAS), X-ray fluorescence.
- Scanning tunneling microscopy / spectroscopy (STM/STS), atomic force microscopy (AFM), all of them with atomic resolution.
- Coincidence spectroscopy: photoelectron-photoion-photoion coincidences (PEPIPICO), zero electron kinetic energy (ZEKE) spectroscopy, threshold electron spectroscopy.
- Magnetism: magneto-optical Kerr effect (MOKE), including MOKE microscopy, vibrating sample magnetometry (VSM), superconducting quantum interference device (SQUID), X-ray magnetic (circular, linear) dichroism (XMCD, XMLD).
- X-ray diffraction.
- Development of various devices apparatuses for UHV, surface science, low temperatures, cluster production and analysis.
- Proficient in Igor Pro software, including image and movie analysis.

Current fields of interest :

- Ferroelectric thin films; molecular reactions on ferroelectric surfaces; catalytic and photocatalytic properties of ferroelectric surfaces.
- Band bending at free ferroelectric surfaces and at Schottky contacts.
- Diluted magnetic semiconductors.
- Magnetic metal / semiconductor heterostructures.
- Multiferroic heterostructures.
- Interfaces between graphene and insulators or ferroelectrics.
- Photocatalysts for air and water decontamination.
- Nanoparticles with biological applications (core-shell systems, iron oxide nanoparticles).
- Theoretical aspects of ferroic (ferroelectric, ferromagnetic, multiferroic) ordering.

CMT is also a recognized science fiction writer, with 3 books published (2008, 2010 and 2014), one book in press, several national literary awards, founder and President of the Romanian Society for Science Fiction and Fantasy (SRSFF).

3. Publications

3.1. Papers:

(* = corresponding author)

Papers and projects relevant for the last 5 years (Jan. 31, 109 to Jan. 31, 2025) outlined in [blue](#) color.

1. *Possible multiple scattering effects on the EXAFS phase shifts in metallic manganese*, D. Macovei, [C.M. Teodorescu](#), **Rev. Roum. Physique** **36**, 945–951 (1991).
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4. Projects

Project	Position, amount (RON)	Amount, EUR	Period:
Grant of the Romanian Academy No. 317 / 2001-2002: <i>Structure, electronic properties, reactivity and magnetism of thin films of transition metals deposited by epitaxy on semiconductor substrates</i>	Project Director, 60 mil. ROL	2 152	2001-2002
CNCSIS Grant No. 1493 / 2002-2003: <i>Metal-semiconductor interfaces and ferromagnetic semiconductors</i>	Project Director, 110 mil. ROL	3 150	2002-2004
Matnantech No. 262(409) / 2004: <i>Source of nanoparticles produced by adiabatic expansion, size selected by a Wien filter</i>	Project Director, 1 750 mil. ROL (NIMP: 1 249,5 mil ROL)	44 122 (31503)	2004-2006
CERES No. 4-40 / 2004: <i>Materials and structures for spintronics based on associating magnetic metals with semiconductors</i>	Project Director, 1 300 mil. ROL (NIMP: 1 014 mil. ROL)	32 776 (25565)	2004-2006
CERES No. 4-67 / 2004: <i>Studies of doping effects on photocatalytic properties of TiO₂</i>	Project Director, 1 100 mil. ROL (NIMP: 550 mil. ROL)	27 734 (13867)	2004-2006
CERES No. 4-100 / 2004: <i>Studies of cluster condensation dynamics in plasma environment by time-of-flight spectrometry</i>	Project Director, 1 400 mil. ROL (NIMP: 700 mil. ROL)	35 297 (17649)	2004-2006
Matnantech No. 263(409) / 2004: <i>Nanostructures of manganite perovskites for applications as microwave attenuators controlled by magnetic field</i> (Project Director Dr. Ovidiu Pana, INCDTIM Cluj-Napoca)	NIMP Principal Investigator, 350 mil. ROL	8 824	2004-2006
CERES No. 4-93 / 2004: <i>Magnetic micro and nanocomposites on the type Mn perovskite – diamagnetic materials</i> (Project Director Dr. Ovidiu Pana, INCDTIM Cluj-Napoca)	NIMP Principal Investigator, 240 mil. ROL	6 051	2004-2006
CEEX No. CEx05-D11-32/2005: <i>Magnetism of interacting clusters: fundamental processes and applications</i>	Project Director, 1 500 000 RON (NIMP: 600 000 RON)	407 930 (163 172)	2005-2008
CEEX-RELANSIN No. 69/2005: <i>Microsystems with nanometer sized magnetic multilayers with giant magnetoresistance (GMR) and spin-dependent tunneling (TMR) for spintronics</i> (Project Director Dr. Jenica Neamtu, INCDIE ICPE-CA Bucuresti)	NIMP Principal Investigator, 150 000 RON	40 793	2005-2008
CEEX No. CEx06-D11-9/2006: <i>Development and optimization of new plasma sources for surface</i>	NIMP Principal Investigator,	26 614	2006-2008

<i>diagnostics by ionic ablation: studies and applications</i> (Project Director Dr. Agavni Surmeian, INFLPR Magurele)	90 000 RON		
CEEX-RELANSIN No. 229/2006: <i>Development of new plasma sources for efficient processing of surfaces of metallic materials</i> (Project Director Dr. Constantin Diplasu, INFLPR Magurele)	NIMP Principal Investigator, 52 000 RON	15 377	2006-2008
CEEX-Matnantech No. 59/2006: <i>Magnetic nanoparticles with core-shell structure covered with noble metals and conducting polymers – synthesis, characterization and applications</i> (Project Director Dr. Ovidiu Pana, INCDTIM Cluj-Napoca)	NIMP Principal Investigator, 150 000 RON	44 356	2006-2008
PN2-Partnerships No. 71-063: <i>Materials with induced magnetization, controlled by external parameters</i> (MAMAINCOPAE)	Project Director, 2 000 000 RON (NIMP: 900 000 RON)	553 986 (249 294)	2007-2010
PN2- Partnerships No. 71-119: <i>Ordered configurations of ferromagnetic and superparamagnetic nanoparticles</i> (Project Director Dr. Ovidiu Pana, INCDTIM Cluj-Napoca)	NIMP Principal Investigator, 300 000 RON	83 098	2007-2010
PN2-Capacities No. 73 CP/I/2007: <i>Development of molecular beam epitaxy techniques and of in situ characterization of surfaces and interfaces in ultrahigh vacuum (UHV)</i>	Project Director. 2 000 000 RON	553 986	2007-2009
PN2- Partnerships No. 12-134/2008: <i>Semiconductor nanodevices for applications in nanoelectronics and nanomedicine</i> (Project Director Dr. Jenica Neamtu, INCDIE ICPE-CA Bucuresti)	NIMP Principal Investigator, 500 000 RON	12 546	2008-2011
Contract PN2-Parteneriate No. 72-165/2008: <i>Transparent oxide semiconductor nanostructures with properties controlled by doping for applications in optoelectronics, spintronics and piezotronics</i> (Project Director Dr. Jenica Neamtu, INCDIE ICPE-CA Bucuresti)	NIMP Principal Investigator, 500 000 RON	12 546	2008-2011
POS-CCE SMIS 2665/2009: Euro-Regional Center for Studies of Advanced Materials, Surfaces and Interfaces (CEUREMAVSU)	Project Director, 43 004 595 RON	10 170 898	2009-2011
PCCE ID_76/2010: Surface and interface science: physics, chemistry, biology, applications	Project Director, 7 000 000 RON (NIMP: 1 750 000 RON)	1 633 682 (408 420)	2010-2013
IFA-CEA cooperation project No. C1-08/2010: <i>Ferroelectric and diluted magnetic semiconductor based multiferroic heterostructures for energy applications</i> (MULTIFERRODMS)	Project Director, 600 000 RON	140 030	2010-2013
PCCE PN-II-ID-PCCE-2011-2-0006, <i>Interface effects in charge transport in ferroelectric / multiferroic heterostructures</i> (Project Director Dr. Lucian Pintilie, INCDFM)	NIMP – T2 team Principal Investigator 1 250 000 RON	282 250	2012-2015
PN2- Partnerships No. 152/2012: <i>Evaporation cells, operating at high temperatures, high stability</i>	Project Director, 3 000 000 RON	677 400 (372 570)	2012-2015

<i>and low cost, for molecular beam epitaxy (HITEVACE)</i>	<i>(NIMP: 1 650 000 RON)</i>		
PN2- Partnerships No. 128/2012: <i>Hyperthermic magnetic nanoparticle ablation of liver and pancreatic tumors (NANO-ABLATION)</i>	NIMP Principal Investigator, 300 000 RON	67 740	2012-2015
ANR Blanc International (RO-F) 2013: <i>Chemical switching of surface ferroelectric topology (CHEM-SWITCH)</i>	Project Director, 250 000 EUR	250 000	2013-2015
R&D Project, <i>Positron related experiments. Experiments with spin-polarized positrons</i> , Contract no. 36/24.03.201 with ELI-NP – Institutul Național de Cercetare-Dezvoltare pentru Fizică și Inginerie Nucleară “Horia Hulubei”	Project Director, 64 200 EUR	64 200	2015
POS-CCE SMIS 49185 <i>Center for Research, Innovation and New Technologies (RITecC)</i>	Deputy Director, 42 984 228 RON	9 674 944	2014-2015
ELI-RO Project No. 18-ELI <i>Surface Science with Positrons: Optimization of solid Ne Moderators and First PAES Experiments (SuSciPo)</i>	Project Director, 1 200 400 RON	278 818	2016-2019
POC - G: <i>Smart multifunctional materials for high technology applications (MATI2IT)</i>	Deputy Director, 15 950 000 RON	3 544 444	2016-2021
POC - E: <i>Nanostructured electrochemical biosensors for medical diagnosis and screening of compounds with pharmaceutical properties: development, surface characterization and applications (NANOBIOSURF)</i>	Deputy Director, 9 000 000 RON	2 000 000	2016-2020
PCCDI PN-III-P1-1.2-PCCDI- 2017-0152 <i>Technological paradigms in the synthesis and characterization of systems with variable dimensionality (VARDIMTECH)</i>	Project Director, 5 287 500 RON <i>(NIMP 2 463 500 RON)</i>	1 134 657 (528 648)	2018-2020
PNIII-1.2PDI-PFC-C1-2018 ID_339: <i>Institutional Development for Excellence in Research in Advanced Materials (EXMAV)</i>	Deputy Director, 6 900 000 RON	1 483 871	2018-2020
PN-III-P4-ID-PCCF2016-0047: <i>Control of electronic properties in heterostructures based on ferroelectric perovskites: from theory to applications (CEPROFER)</i>	Team 1 Principal Investigator, 2 000 000 RON	430 107	2018-2022
Core Program of the National Institute of Materials Physics, Project #2 “New developments in the area of functional materials for high technology applications (electronics, optoelectronics, sensors)”, PN23080202	Project Director, 13,538,157 RON (2023)	2 730 794	2023-2026

Signature:



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I took my PhD in Nonlinear Optics in December 2011 then I decided to extend my expertise going towards surface science and electron spectroscopies. After a Swiss Excellence Grant at the Swiss Light Source of Paul Scherrer Institut in 2015-2016, I am now Researcher I@NIMP in Magurele. My main expertise is material design by molecular beam epitaxy and pulsed laser deposition, their surface and interface characterization by means of conventional X-ray and synchrotron radiation electron spectroscopies, in combination with first principles calculations. My focus presently lies in particular on: (i) the interplay of charge, spin, orbital and lattice degree of freedom in oxides, aiming to bridge the gap between fundamental knowledge and device fabrication; (ii) systems with strong electronic correlations (2DEGs at oxide and nitride interfaces revealed in k-dependent photoemission - ARPES) and (iii) cross-coupling of different ferroic phases at the interface of functional materials.

During 2015-2016 I received an **Excellence grant** from the Swiss Federal Government to conduct my research *on multiferroic systems and correlated oxides heterostructures* at the Swiss Light Source synchrotron facility of Paul Scherrer Institut by using soft X-ray photoemission at ADRESS beamline, which delivers the highest photon flux worldwide (<https://www.psi.ch/en/sls/adress/endstations#sx-arpes-endstation>) – critical to overcome the dramatic drop of photoionisation cross section in the soft X-ray regime. Accessing such infrastructure gave me the unique opportunity to access the **k**-resolved electronic structure of various buried interfaces which cannot be accessed by other experimental techniques.

During 2020-2023 I have been the **PI of the PCE project** “*Electronic double layer high mobility Mott transistors*” - PN-III-P4-ID-PCE-2020-2540 (PCE96/2021) funded by Romanian UEFISCDI which explores the interplay between induced correlations in Mott insulator and the enhancement of the mobility in devices with two dimensional gases at their interfaces.

Between 2016-2022 I obtained 8 grants allowing me to conduct our experiments at synchrotron facilities across Europe, performing X-ray photoelectron spectroscopy (XPS), spectromicroscopy, photoemission microscopy (PEEM), hard X-ray photoemission (HAXPES), soft X-ray angle resolved photoelectron spectroscopy (SX-ARPE), X-ray absorption spectroscopy (XAS) measurements. Currently, as experienced synchrotron user, I am among the founding members of the Romanian Synchrotron User Organisation which, among other objectives, aims to represent the interests of the still small Romanian community of users at synchrotrons and free electron lasers – FELS; to elaborate strategies for trans-national access at large facilities; encourages the contacts between users in different countries, channeling the growth of expertise in the field.

Some of my most important scientific results, obtained as a member of the Surface&Interface group of Dr. Habil CS1. Cristian Mihail Teodorescu include:

- Delivering the worldwide first k -resolved electronic band structure of prototypical ferroelectric $\text{PbZr}_x\text{Ti}_{1-x}\text{O}_3$. Our results published recently (*Popescu et al. *Adv. Sci.* **10**, 2205476 (2023), IF=15.1; (Q1)) **give the worldwide first experimental, ferroelectric-dependent band structure of PbZrTiO_3 - PZT**, which is probably the best-known ferroelectric material. Such fundamental information was missing due to the insulating character of PZT and due to its 3D character, which introduces significant broadening in the k_z direction of the reciprocal space – precluding any experimental study in UV angle resolved photoelectron spectroscopy (ARPES). By employing soft X-ray ARPES performed at the Swiss Light Source synchrotron, which extends the probing depth towards the bulk, we recorded with sharp resolution in the k_z momentum the band structure of PZT as a function of its ferroelectric (FE) polarization state (P^+/P^-). By using thin films instead of bulk-like systems grown epitaxially, we additionally enforce self-doping which prevents the charging effects, thus **overcoming the previous limitations** to record the experimental band structure in ARPES. Most important, we *identify the mechanisms*, which stabilize the well-defined FE state and extend these observations to the entire class of FE oxides. This results summarize **a direction which opens new perspectives** on understanding the connection between functionality and electronic structure of perovskite oxides, in particular *giving new insights* on how to engineer topologic systems such as magnetic skyrmions or effects triggered by the strong spin – orbit coupling in oxides and their signature in photoemission.

- Elucidate and formulate a general framework of the interplay between transport, electronic structure and the coupling with elementary excitations in the crystalline solid

Studies involving large, interdisciplinary teams were conducted, combining complex investigations performed at synchrotron radiation facilities with preparation and structural characterization performed at NIMP.

Our results **elucidate for the first time** the mechanisms which accompany and trigger the metal to insulator transition in correlated oxides. One example is the Ce-doped CaMnO_3 , which undoped is a Mott insulator due to the strong Coulomb repulsion. However, upon n -doping it with Ce atoms, it transitions from the insulating to the metallic state when the gradual evolution of its electronic structure can be experimentally recorded. In *Husanu et al. *Commun. Phys.* **3**, 62 (2020)(IF=5.5; (Q1)), by identifying the gradual increase of the electron-phonon coupling while approaching the insulating phase, we undoubtedly *established the critical relevance of the polaronic coupling in the localization of the electrons*. In the insulating phase, the strong electron-phonon coupling keep the electrons trapped within the lattice, thus defining large polarons. Upon increasing the Ce doping, the electron density n increases and the screening of the electron-phonon interaction is stronger. Such predicted effect was identified in a series of **pioneering experiments** started in 2015 (**Phys. Rev. B* **92**, 235442 (2015) **Q1**, IF=3.72, *Phys. Rev. Materials* **4**, 034402 (2020)-IF 4). They continued at Swiss Light Source, at the ADDRESS beamline, where **the worldwide first k -resolved electronic structure of the buried LSMO interface was experimentally obtained** as a function of the FE state of the top layer and of the magnitude of FE polarization (*Husanu et al. *Commun. Phys.* **5**, 209 (2022) IF=5.5; (Q1)). Then, the charge modulation at the interface triggered by the FE state, by better screening the polaronic interaction in electron accumulation state or weaker screening the electron-phonon coupling in the hole accumulation state, transits LSMO between the weak to intermediate electron-phonon coupling regime and back.

This effect is general to any other interface with FEs and illustrates **a new way of controlling the electronic structure of interfaces** using ferroelectricity state as a knob.

- Worldwide first results on the electronic structure of buried interfaces.

Separating the electronic properties of the interface from that of the bulk is *notoriously difficult*. One of the few ways of accessing it is to inspect the buried interface in photoemission through a capping layer. This however requires high photon flux, available only at large facilities such as synchrotrons or free electron lasers. Together with teams from high ranked universities and research institutes across Europe and USA, we **conducted pioneering experiments** in lab and at large experimental facilities on 2D electron gases stabilized at SrTiO₃/LaAlO₃ with papers published in high profile journals (*ACS Nano* **12**(8), 7927 (2018), *Phys. Rev. Mater.* **3**, 106001 (2019), *ACS Nano* **16**(4), 6437 (2022)) SrTiO₃/Al₂O₃ (*ACS Nano* **15**(3), 4347 (2021)), GaN/AlGaN (*Nature Commun.* **9**, 2635 (2018)) or LaAlO₃/NdNiO₃ (*Nano Lett.* **19**(11), 8311 (2019)).

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Patents:

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Bucuresti
30.01.2024

Dr. CS I Marius-Adrian Husanu



Capitole de carte:

1. *Compensation and screening of ferroelectricity in perovskite oxides*, D.G. Popescu, M. Husanu, **Perovskites Ceramics. Recent Advances and Emerging Applications**, Elsevier Series in Advanced Ceramic Materials, Editors: J.L. Clabel H. and V.A.G. Rivera, 125-154 (2023)
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Nicoleta G. Apostol (b. 1985; other name: Gheorghe) earned her PhD degree in Chemistry at the Institute of Physical Chemistry of the Romanian Academy in 2013, is hired since 2009 in the National Institute of Materials Physics (NIMP) Măgurele, in the group of Surface and Interface Science. Between March 2014 and March 2015 she obtained a Post-Doctoral position at Elettra - Sincrotrone Trieste in Italy, at the SuperESCA beamline (Dr. Silvano Lizzit).

She earned the "Radu Grigorovici" Prize of the Romanian Academy for 2012, awarded for the group of works "Surface and interface phenomena highlighted by electron spectroscopies XPS/Auger and other characterization techniques of surfaces and interfaces", date of award 19th December 2014, is one of the winners of the L'Oréal - UNESCO National scholarship "For Women in Science", section Physical Sciences, 9th edition, 2018, and she earned the **1st prize at the "Rada Mihalcea" awards for young researchers in science and engineering, in August 2019**. Currently, she is employed as Senior Scientist II, author or co-author for 84 papers published in ISI quoted journals and 7 book chapters, 30 oral presentations or invited to national/international conferences, project manager for 3 national projects: a Post-Doctoral Project and 2 Young Research Team projects.

From all the above, in the last 5 years, she published 20 papers in ISI quoted journals, 1 book chapter and was project manager for 1 Young Research Team project (~ 85.000 Eur) "Molecular adsorption and reactions under two-dimensional shells" (acronym: CHEM2DSHELL), 11.01.2021-31.12.2022. And was also involved in many projects for the popularization of science (H2020-MSCA-NIGHT-2020: nr. 954638/2020, HORIZON-MSCA-2022-CITIZENS-01). The main goal of Young Research Team project pertained to the study of carbon monoxide (CO) intercalation and reactions involving CO (insertion, oxidation and desorption) with the aim to synthesize hydrogen or alkanes (Fischer-Tropsch reaction) at the graphene (Gr)/Pt(001) surface, by way of high resolution XPS, NEXAFS, LEED, STM and TPD methods, using synchrotron radiation. This study will provide fundamental insight and the possibility to determine insertion sites and reaction pathways together with relevant parameters such as adsorption energy, energy barrier for reaction, and turnover frequency for these processes. Moreover, it could constitute a significant step in the technological advance towards using ultrathin carbon layers deposited on atomically clean Pt monocrystal at industrial scale, for applications involving CO depletion and/or conversion.

Between 2019-2023, she was a member of the evaluation committee of the Rada Mihalcea competition for Young Researchers in Science and Engineering, is co-responsible within the IOSIN – Special Systems and Objectives of National Interest –programme and is one of the persons responsible for CoSMoS (detached installation at the SuperESCA beamline, from the Elettra Synchrotron, in Trieste, Italy) and co-responsible for XPS spatial resolution in INCDFM. She was recently elected as the leader of the NIMP employees' Union. The published works have accumulated about 1300 citations (self-citation excluded) and a Hirsch index of 23. These are elements defining a solid scientific reputation at international level and the ability to extract the maximum information from X-ray Photoelectron Spectroscopy.

Research ID: I-9399-2016

Brainmap UEF – ID: U-1700-039K-3342

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Publication list (the publications from the last 5 years are evidenced with blue color)

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CS II Dr. Dana-Georgeta Popescu

(<https://www.scopus.com/authid/detail.uri?authorId=49961978000>)

Age: 38, Nationality: Romanian, Gender: Female, Contact: ,

I received my PhD degree in 2014 at “**Politehnica**” **University of Bucharest**. In 2010 I joined National Institute of Materials Physics (NIMP) in the Surface&Interfaces Science group. Here I build my expertise and autonomy in the field of semiconductor surfaces, their interface with magnetic metals and on multiferroics. I elaborated the experimental protocol to fabricate a 2D photonic crystal device with additional vertical confinement of radiation. Performed under my initiative, the approach of converging materials science with spectroscopic investigation to create photonic functionality such as waveguides and resonant cavities was at the moment a complete novelty and opened a new research direction in NIMP (**Patent * A/00668 – 2022**). Spending three months at the Institut Rayonnement Matiere de Saclay(@CEA France, I performed research in the laboratory led by Dr. N. Barrett, which was an excellent opportunity to enlarge my experience in the field of electron spectroscopy techniques, especially applied to complex ferroelectric and multiferroic oxide surfaces and interfaces (**Patent * A/00715 2019**). These findings were awarded with the „**Radu Grigorovici**” **prize of Romanian Academy** in 2017.

Moreover, in conjunction with the papers ***Phys. Stat. Solidi – RRL 13(1900077 (2019))** ***Appl. Surf. Sci. 502 (144101 (2020))** and ***Phys. Rev. Mat. 4, 34402 (2020)**, derived from my **TE-2014-4-1117 project** , the puzzling behavior of the oxygen vacancies migration as a function of the polarization state of the FE BaTiO₃ has been established when gradually depositing metals ad-layers on top of BTO. It was found that depending on the nature of the metal top layer, either ferroelectricity pointing upwards or downwards can be stabilized and that the adsorption is selective depending on the termination domain.

My research involved conducting experiments at large experimental Synchrotron facilities such as Elettra (Italy), Swiss Light Source (Switzerland), Solaris (Poland) and at Catalan Institute of Nanoscience and Nanotechnology (Barcelona) (**Comm. Phys. 5, 209 (2022)**). There, I performed *pioneering experiments*, which for example gave the *worldwide first* experimental picture of the surface band bending of single crystal ferroelectric materials at submicron resolution.

Recently, in *Adv. Sci.* **10**, 2205476 (2023), we extended the results reported earlier in *Phys. Stat. Solidi – RRL* **13**(1900077 (2019)), **Appl. Surf. Sci.* **502** (144101 (2020)) and **Phys. Rev. Mat.* **4**, 34402 (2020), **IF 4**, **Patent A/00715-2019** – awarded in 2022 with Excellence diploma and Gold Medal at Pro Invent, **Best Poster Award** (SCES Conference 2021, Brasil) derived from my **TE 150/2015** and **TE50/2022** (*1st place in Engineering Domain ~99p*) projects. We gave the first experimental band structure of a ferroelectric material and clearly revealed the signature in the electronic structure of the oxygen or cation vacancies stabilizing the well-defined ferroelectric state. My leader talents helped in combining the engineering expertise with fundamental research, with excellent results in electronics and materials science (*Phys. Stat. Sol. – RRL* **13** (2019), *Appl. Surf. Sci.* **502** (2020) and *Phys. Rev. Mat.* **4** (2020) and *a patent* (**A 2019 00715**). The team coagulated in the previous TE project, evolved exactly as we assumed in the ethical guidelines, in the previous proposal, pursuing their own, independent scientific route (Dr. Liviu Tanase - Fritz Haber Institute in Berlin, Dr. Cristina Bucur – postdoctoral fellow at NIMP).

My new TE project was funded in 2022 *ranking first in the Engineering Section* (**TE 50/2022** – “Integrated Rashba-type platform for data storage and bit manipulation” - <https://infim.ro/en/project/integrated-rashba-type-platform-for-data-storage-and-bit-manipulation/>). The objective of this project is to provide an alternative solution to random access memories through the development of an integrated platform based on Rashba-type effects, enabling efficient data storage and bit manipulation. The utilization of Rashba-coupled metal/semiconductor systems and Rashba-type ferroelectrics (such as GeTe) grown on Ge(111) and Si(111) substrates, which exhibit significant Rashba effects and efficient spin-to-charge conversion, has enhanced expertise and visibility in this innovative research direction (**patent A 2023 00775**).

Despite the *4-years maternity* leave I managed young research team collaborative project, published papers in journals with high impact in the field (*Phys. Rev. Appl.* **10** (2018) – **Q1**, **IF 4.62**, top 17%, *Appl. Surf. Sci.* **502**, 144101 (2020), *Phys. Rev. Mat.* **4**, 34402 (2020), *Physica Status Solidi – RRL* **13**, 1900077 (2019)).

From the beginning of my research career, I was involved in scientific events like “*Scoala Altfel – School from other perspectives*”, “*Researchers’ Night*”, “*Summer School*”, and other

scientific events organized by the Romania Ministry of Research, attracting kids and young researchers to learn more and make science popular. I was also one of the speakers at Romanian UNESCO center, focused on *women in science, entrepreneurship and leadership*. I contributed to “research for everyone” writing articles/giving interviews or filming for different events (<https://physicscommunity.nature.com/posts/ferroelectricity-modulates-polaronic-coupling-at-multiferroic-interfaces>). I also have in recent view to habilitate for supervising PhD students and already started a **spin-off** at NIMP focusing on producing custom smart materials. I designed and integrated in the old cluster (XPS, STM, MBE) from NIMP a new MBE chamber special for chalcogenide materials and for the moment I am **Review Editor** for Frontiers in Chemistry Journal and **Guest Editor** for Materials Journal since 2021.

Summarizing, my main **original** achievements are capitalized in **31 articles** (9 publications since 2019) – **18 as main/corresponding author**, **3 patents**, **3 book chapters** and **47 international conferences** (6 invited, **20 oral presentation** – 13 since 2019), **2 young team research projects**, **3 grants projects** (L’Oréal-UNESCO „For women in science”; POSDRU grant 2010-2013 Contract no. 4/28; POSDRU/107/1.5/S/76909) and the membership in the other **10 projects**, **2 patents**, **2 scholarships**. The scientific record has more than 224 citations (without self-citation), and **H-index Scopus = 11**. From the total number of published articles after the defending my PhD Theses, **65% of the published one are in Q1** and **24% are in Q2**.

Note: * means **main authorship** of the papers.

Articles

1. C. Rizescu, M. El Fergani, D.I. Eftemie, B. Cojocaru, D. Popescu, M. Andruh, V.I. Parvulescu, *Liquid phase oxidation of alkenes and glycerol with molecular oxygen over mixed-ligand*, **Applied Catalysis A, General** **663**, 119302 (2023)
(<https://www.sciencedirect.com/science/article/pii/S0926860X2300282X?via%3Dihub>)
(Q2; IF=5.5; AIS=0.859; Citations: 0).
2. A.I. Borhan, A.I. Ghemes, M.A. Husanu, **D.G. Popescu**, C.N. Borca, T. Huthwelker, I. Radu, A.C. Dirtu, D. Dirtu, G. Bulai, N. Lupu, M.N. Palamaru, A.R. Iordan, D. Gherca, Carbon-based heterostructure from multi-photo-active nanobuilding blocks

SrTiO₃@NiFe₂O₄@FeO@NiO@CNTs with derived nanoreaction metallic clusters for enhanced solar light-driven photodegradation of harmful antibiotics, **Appl. Surf. Sci.** 622, 156987 (2023).

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4. **D.G. Popescu**, M.A. Husanu, P. C. Constantinou, L.D. Filip, L. Trupina, C.I. Bucur, I. Pasuk, C. Chirila, L.M. Hrib, V. Stancu, L. Pintilie, T. Schmitt, C. M. Teodorescu, V.N. Strocov, Experimental band structure of Pb(Zr,Ti)O₃: Mechanism of ferroelectric stabilization, **Advanced Science** 10, 2205476 (2023).

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5. A. Rendón-Patiño, A. Primo, B. Cojocaru, S.G. Ion, **D.G. Popescu**, V. Parvulescu, H. García, Nanometric-Thick Metal-Free h-Boron Nitride/Graphene Films as Base Catalyst for the Synthesis of Benzoxazoles **ChemCatChem** 14, e202200356 (2022)

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(Q2; IF=4.5; AIS= 0.893; Citations: 2 / 2 (without self-citations)).

6. M.A. Husanu, **D.G. Popescu**, F. Bisti, L.M. Hrib, L.D. Filip, I. Pasuk, R. Negrea, M.C. Istrate, L. Lev, T. Schmitt, L. Pintilie, A. Mishchenko, C.M. Teodorescu, V.N. Strocov Ferroelectricity modulates polaronic coupling at multiferroic interfaces, **Communications Physics** 5, 209 (2022).

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 9. **D.G. Popescu***, M. Husanu, C. Chirila, L. Pintilie, C. Teodorescu, *Impact on ferroelectricity and band alignment of gradually grown Au on BaTiO₃*, **Physica Status Solidi – RRL** **13**, 1900077 (2019)
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 15. **D.G. Popescu**, M.A. Husanu, L. Trupina, L. Hrib, L. Pintilie, A. Barinov, S. Lizzit, P. Lacovig,

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 17. **D.G. Popescu**, M.A. Husanu, *Epitaxial growth of Au on Ge(001) surface: photoelectron spectroscopy measurements and first-principles calculations*, **Thin Solid Films** **552**, 241–249 (2014);
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 20. G.A. Lungu, N.G. Apostol, L.E. Stoflea, R.M. Costescu, **D.G. Popescu**, C.M. Teodorescu, *Room temperature ferromagnetic, anisotropic, germanium rich FeGe(001) alloys*, **Materials** **6**, 612–625 (2013);
 21. **D.G. Popescu***, *Two dimensional photonic crystals with different symmetries for waveguides and resonant cavities applications*, **U.P.B. Sci. Bull., A Series** **75**, 237–252 (2013);
 22. **D.G. Popescu***, P. Sterian, *Photonic Crystal Fibre Mode Characterization with Multipole Method*, **U.P.B. Sci. Bull., A Series** **75**, 205–215 (2013);
 23. **D.G. Popescu***, P. Sterian, *Analysis of even and odd modes of a two-dimensional photonic crystal at Si/SiO₂/Cu interface*, **J. Optoelect. Adv. Mater.** **15**, 610–614 (2013);
 24. R.M. Costescu, N.G. Gheorghe, M.A. Husanu, G.A. Lungu, D. Macovei, I. Pintilie, **D.G. Popescu**, C.M. Teodorescu, *Epitaxial ferromagnetic samarium and samarium silicide synthesized on Si(001)*, **J. Mater. Sci.** **47**, 7225 (2012);
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 28. **D.G. Popescu***, P. Sterian, *FDTD analysis of photonic crystals with square symmetry and defects*, **AWERProcedia Information Technology and Computer Science** **2**, 364-369 (2012);
 29. R.M. Costescu, G.A. Lungu, G. Socol, N.G. Gheorghe, D. Macovei, C.C. Negrila, C. Logofatu, M.A. Husanu, **D.G. Popescu**, C.A. Tache, C.M. Teodorescu, *Atomic structure and magnetism of PLD deposited TiO₂: Fe*, **Dig. J. Nanomater. Biostr.** **7**, 73-78 (2012);
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 31. **D.G. Popescu***, P. Sterian, *FDTD analysis of photonic crystals with square and hexagonal symmetry*, **Journal of Advanced Research in Physics** **2**, 021105 (2011);
 32. **D.G. Popescu**, Development of some methods and techniques of analysis and characterization of devices with photonic crystals (PhD Thesis)
 33. N.G. Gheorghe, M.A. Huşanu, G.A. Lungu, D. Macovei, V. Kuncser, R.M. Costescu, **D. Popescu**, C.M. Teodorescu, *Growth and characterization of ultrathin Fe magnetic layers deposited on atomically clean Si(001) by molecular beam epitaxy*, Editura Academiei Române, Bucureşti, România, 2012 (**book chapter**)
 34. Compensation and screening of ferroelectricity in perovskite oxides, D.G. Popescu, M. Husanu, Perovskites: Ceramics, Editors: J.L. Clabel H. and *V.A.G. Rivera, deadline 30 November 2020 (**book chapter**)
(<https://www.sciencedirect.com/science/article/abs/pii/B9780323905862000012?via%3Dihub>)
 35. Polaronic effects in perovskite oxides, M. Husanu, D.G. Popescu, Perovskites: Ceramics, Editors: J.L. Clabel H. and *V.A.G. Rivera, deadline 30 November 2020 (**book chapter**)
(<https://www.sciencedirect.com/science/article/abs/pii/B9780323905862000073?via%3Dihub>)

Patents

1. **D.G. Popescu**, M.A. Husanu, Preparation method of Ni thin films, **A/00715 2019**
2. **D.G. Popescu**, M.A. Husanu, 2D Photonic Crystal in Ge Matrix, **A/00668 – 2022**
3. M.A. Husanu, **D.G. Popescu**, C. Chirila, C. Besleaga-Stan, Oxide field-effect transistor operated by an electronic double layer and design, **A 2023 00775**

Projects

1. TE 150/2015 – **project leader** (125000 Euro)
2. Grant: Programul L'Oréal-UNESCO „Pentru femeile din știință” (9500 Euro)
3. TE50/2022 - **project leader** (90000 Euro)

Prizes and awards

- 25.11.2023-27.11.2023 – Excellence diploma and Gold Medal at Pro Invent, XX Edition, Cluj-Napoca, Romania, Preparation method of Ni thin films
- 14.09.2023-16.09.2023 – Gold Medal at InventCor, 4th Edition, Deva, Romania, Preparation method of Ni thin films
- 26.10.2022-28.10.2022 – Excellence diploma and Gold Medal at Pro Invent, XX Edition, Cluj-Napoca, Romania, 2D Photonic Crystal in Ge matrix
- 27.09.2021-02.10.2021 – Best poster award at the International Conference on Strongly Correlated Electron Systems <https://scs2020.org/program-2/> (SCES) 2021
- 14.12.2017 - Academy Award ('Radu Grigorovici' Prize) - "Photoelectron spectroscopy and ab-initio calculations applied to the study of surfaces and interfaces";
- 12.11.2015 - 18.11.2015, TRENDOXIDE2015: New trends in correlated oxides and interfaces – International School & Workshop, Brescia, Italy- Scholarship;

- 01.06.2012 – 30.12.2012: Human resources inspector certification - POSDRU/97/6.3/S/64240 „ProFeminAntrep – Promoting equal opportunities in entrepreneurship” - Scholarship;
- 06.02.2012 - 17.02.2012: Winter College on Optics: Advances in Nano-Optics and Plasmonics, Trieste, Italy - Scholarship;
- 01.10.2010 – 30.09.2013: POSDRU/107/1.5/S/76909 Capitalization of the Human Capital through Doctoral Scholarships (ValueDoc);

A handwritten signature in blue ink, consisting of a stylized star or cross shape with a vertical line extending upwards from the center.

Dr. Ruxandra M. Costescu earned her PhD in Materials Science and Engineering at University of Illinois Urbana-Champaign, USA in 2006, with the dissertation „Thermal transport on the nanometer scale and the effect of microstructure and interface resistance”. As a research assistant in the group of Electronic Materials and Thin Films led by Prof. David Cahill at University of Illinois, she reported for the first time in *Science*, as first author, the existence of an ultra-low thermal conductivity of metal-metal oxide multilayers (W/Al₂O₃). Between 2004 and 2008 Ruxandra Costescu occupied a post-doctoral position in the Molecular Beam Epitaxy (MBE) group coordinated by Dr. Oliver G. Schmidt first at Max-Planck-Institut für Festkörperforschung in Stuttgart, Germany, and then at Institute for Integrative Nanosciences within Leibniz Institute for Solid State and Materials Research in Dresden, Germany. Since early 2010, she has been part of the group of Surface and Interface Science led by Dr. Cristian Teodorescu at the National Institute for Materials Physics, Romania (NIMP), specializing in X-ray Photoelectron Spectroscopy (XPS). In 2010 she was given the „IN HOC SIGNO VINCES” award (in Math and Natural Sciences) from the Romanian National Council of Scientific Research in Higher Education (CNCSIS) and the Award for Best Young Researcher in 2010 from the State Department of Education, the Romanian Research and Design Patronage and the Romanian Academy. Between 2010 and 2012, with the help of a CNCSIS reintegration grant for young researchers, Dr. Costescu purchased and implemented a new MBE chamber, currently used as part of a Complex Surface Science System at NIMP (included in the Special Systems and Objectives of National Interest “IOSIN” program), for which she is one of the responsible persons. She also administers another IOSIN instrument at NIMP (an XPS system with spatial resolution). Since 2018, she has been the NIMP coordinator for European Commission “Horizon 2020” science popularization projects in partnership with a consortium including other research institutes and universities both in Magurele and nationally, as well as the coordinator of science education activities/outreach at NIMP.

Dr. Costescu has published a total of 31 papers in ISI-listed journals, with close to 1000 citations and a Hirsch index of 11, and has an accepted patent (and another one recently registered).

Publication list (chronological; #24-31 published in the last 5 years):

1. *Thermal conductivity and sound velocities of hydrogen-silsesquioxane low-k dielectrics*, Costescu R.M., Bullen A.J., Matamis G., O'Hara K.E., and Cahill D.G., **Phys. Rev. B** 65 (9), 094205 (2002).
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5. *Atomic structure and magnetic properties of cobalt doped ZnO thin films prepared by the sol-gel method*, J. Neamtu, G. Georgescu, T. Malaeru, N.G. Gheorghe, R. M. Costescu, I. Jitaru, J. Ferre, D. Macovei, C.M. Teodorescu, **Digest J. Nanomater. Biostr.** 5, 873-885 (2010).
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7. *Enhanced contamination of Si(001) when analyzed by AES with respect to XPS*, N.G. Gheorghe, G.A. Lungu, R.M. Costescu, D.G. Popescu, C.M. Teodorescu, **Optoelect. Adv. Mater. - Rapid Commun.** 6 (2), 508-513 (2011).
8. *Significantly different contamination of atomically clean Si(001) when investigated by XPS and AES*, N.G. Gheorghe, G.A. Lungu, R.M. Costescu, C.M. Teodorescu, **phys. stat. sol. (b)** 248 (8), 1919-1924 (2011).
9. *Illumination-dependent HF Etching of ALAs Sacrificial Layers for the Formation of "Rolled Up" Nanotubes from Strained InGaAs/GaAs Films*, R. M. Costescu, Physics Conference TIM-10, **AIP Conf. Proc.** 1387, 179-185 (2011).
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11. *Successful Cleaning and Study of Contamination of Si(001) in Ultrahigh Vacuum*, N. G. Gheorghe, G. A. Lungu, M. A. Husanu, R. M. Costescu, Physics Conference TIM-10, **AIP Conf. Proc.** 1387, 218-225 (2011).
12. *Reactivity, magnetism and local atomic structure in ferromagnetic Fe layers deposited on Si(001)*, N.G. Gheorghe, M.A. Husanu, G.A. Lungu, R.M. Costescu, D. Macovei, D.G. Popescu, C.M. Teodorescu, **Dig. J. Nanomater. Biostr.** 7, 373-384 (2012).
13. *Atomic structure and magnetism of PLD deposited TiO_2 : Fe*, R.M. Costescu, G.A. Lungu, G. Socol, N.G. Gheorghe, D. Macovei, C.C. Negriila, C. Logofatu, M.A. Husanu, D.G. Popescu, C.A. Tache, C.M. Teodorescu, **Dig. J. Nanomater. Biostr.** 7 (1), 73-78 (2012).
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20. *Structural and magnetic properties of Ni nanofilms on Ge(001) by molecular beam epitaxy*, Amelia Elena Bocirnea, Ruxandra Maria Costescu, Iuliana Pasuk, George Adrian Lungu, Cristian Mihail Teodorescu, **Appl. Surf. Sci.** **424**, 337-344 (2017).
21. *Band bending at magnetic Ni/Ge(001) interface investigated by X-ray photoelectron spectroscopy*, Amelia Elena Bocirnea, Liviu Cristian Tanase, Ruxandra Maria Costescu, Nicoleta Georgiana Apostol, George Adrian Lungu, Cristian Mihail Teodorescu, **Appl. Surf. Sci.** **424**, 269-274 (2017).
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30. *Photocatalytic and Antibacterial Properties of Doped TiO_2 Nanopowders Synthesized by Sol-Gel Method*, Silviu Preda, Jeanina Pandeale-Cușu, Simona Viorica Petrescu, Elena Mădălina Ciobanu, Gabriela Petcu, Daniela C. Culiță, Nicoleta G. Apostol, Ruxandra M. Costescu, Iuliana Raut, Mariana Constantin, Luminița Predoană, **Gels** **8**, 673 (2022). **IF=4.6 (Q1)**, **AIS= 0.626**, **4 citations without self-citation (5 with self-citation)**
31. *Copper-/Zinc-Doped TiO_2 Nanopowders Synthesized by Microwave-Assisted Sol-Gel Method*, Predoana, Luminita, Petcu, Gabriela, Preda, Silviu, Pandeale-Cusu, Jeanina, Petrescu, Simona Viorica, Baran, Adriana, Apostol, Nicoleta G., Costescu, Ruxandra M., Surdu, Vasile-Adrian, Vasile, Bogdan Stefan, Ianculescu, Adelina C., **Gels** **9**, 267 (2023). **IF=4.6 (Q1)**, **AIS= 0.626**, **1 citation without self-citation**



Curriculum Vitae Negrila Constantin Catalin

Career resume

I am a graduate of the University of Bucharest, Faculty of Physics - Electronic Physics department, graduation 2001. The thesis was in the field of Electronic Physics with the title "Study of the absorption of electromagnetic waves in the plasma of an annular discharge" - Scientific Supervisor Prof. Dr. Nicolae Gherbanovschi . The training activity in the field of physics continued with the graduation of Master's studies, Electronic Physics department, in 2003 with a dissertation thesis entitled "Study of the phenomenon of photoluminescence in semiconductor materials", Scientific Supervisor Dr. Mihai Dinca. In 2010, I presented my doctoral thesis - "Semiconductor structures with junctions for devices for electromagnetic radiation detection", Scientific Supervisor Dr. Toni Botila. The professional training included the following stages: starting on November 1, 2001, I joined the National Research and Development Institute for Materials Physics as a Junior Research Assistant in the Laboratory of Advanced Materials for Special Applications, in 2002 I passed the Research Assistant exam, in 2003 the Scientific Researcher exam and in 2009 I took the certification contest as Scientific Researcher grade III. Since 2020 I became Scientific Researcher grade II.

In the last 5 years the Research Activity was focused on several directions specific to the Physics of Materials, these being detailed as follows.

➤ **Physics and technology of semiconductor materials.** In the framework of several projects carried out within NIMP-Bucharest, I have performed studies on semiconductor materials such as Si, GaAs, GaP, CdTe, GaSb, activities in obtaining structures and active devices with applications in electronics and optoelectronics. The interest for compound semiconductors of type III-V was maintained throughout the research activity and represented the foundation for more than 5 research projects in which I was involved. Within them, I participated in the processes of obtaining semiconductor structures, in the preparation of semiconductor surfaces and in the measurements by electron spectroscopies, in the electrical and optoelectronic characterization of devices. I have carried out experimental studies on the Schottky metal/GaAs-Semi-insulator contact, on AuGe/GaAs(SI), InGe/GaAs(SI), AuGeNi/GaSb, InGeNi/GaSb ohmic contacts, or on Pd-Ge alloy ohmic contacts. These studies followed the process of defining some structures sensitive to electromagnetic radiation and the creation of experimental devices performed by PVD

techniques. The original experimental results obtained were the subject of several scientific works. We undertook studies on semiconductor structures modified with self-assembled layers (SAM) from the class of metal sulfides and thiols, regarding the passivation of semiconductor surfaces, bringing new experimental results in the case of GaAs, GaSb and Si semiconductors. The passivation method using aromatic thiols leads to obtaining a semiconductor (Si) surface with a reduced surface density of states, in which the aromatic thiols form a uniform and adherent self-assembled layer (SAM) thin film. The use of aromatic thiols to passivate silicon is the first attempt of this kind known in the specialized literature. The obtained results are the subject of two published patents: "Procedure of passivation of semiconductor surfaces from III-V compounds and obtaining a sensitive structure of the $\text{GaCl}_3\text{-Sb}_2\text{S}_3/\text{GaSb}$ type" (Ghita R, Frumosu F, Logofatu C, Predoi D, Negrila C. C., Trupina L, OSIM Patent RO131881, 29.03.2019), and "n-GaSb(100) Surface Passivation Process", (R. Ghita, C. Logofatu, C.C. Negrila, F. Frumosu, D. Predoi, OSIM Patent No. 132453, 28.08.2020). Obtaining of semiconductor devices is described by the patent "Procedeu de realizare a unei structuri fotoactive" (R. Ghita, C. Logofatu, C.C. Negrila, M.D. Mihai, D. Predoi, M. Stoicu, Brevet OSIM Nr. 133228, 28.02.2020). Lately I have focused on obtaining high k dielectric/GaAs and high k dielectric/GaSb interfaces, using HfO_2 and ZrO_2 and implementing the oxide-MBE technique. The results are about to be published.

➤ **Analysis and characterization of surfaces through electron spectroscopy and STM (Scanning Tunneling Microscopy) techniques.**

From the beginning of my research activity, I participated in the implementation of the XPS (X-Ray Photoelectron Spectroscopy) technique by putting into operation a VG Esca II Mk3 type installation, at that time being the only laboratory in the country that had such a technique. This has obtained the status of Installation of National Interest since 2004 by HG 786/2014. Later we implemented the Multimethod System for Surface Analysis – SPECS, a modern spectrometer, equipped with XPS, AES, UPS, STM and later also with the MBE technique. Since 2023 I am responsible for XPS testing method accredited by RENAR in accordance with SR EN ISO / CEI 17025:2005, accreditation certificate LI 1281/03.11.2023.

More than 75% of the works published in co-authorship include results obtained through surface characterization techniques. During the last 5 years, I have performed surface measurements, especially through the XPS technique, on various classes of materials: catalysts, photocatalysts, semiconductors, metals and alloys, ceramics, oxides, graphene materials, polymers, biomaterials, glasses, other organic materials. More than 50 works have been published since 2019. We

designed a method for the reduction of graphene oxide using vacuum electron bombardment, we implemented REELS type measurements and improved the ARXPS technique for semiconductor interface characterization.

➤ **The management of research topics.** In the last 5 years I was involved in the implementation of some topics and research stages within the PCCDI and Core Programs, all related to the study and realization of III-V semiconductor and Si devices. Specific to my field of expertise, I am an editorial board member of the *Materials* journal and a reviewer for the *Surfaces and Interfaces* journal. I am also involved with the training of groups of young students and master's students in the field of surface science through collaborations with the Solid Physics Department of the Faculty of Physics of the University of Bucharest.

The Research Identifiers:

<https://www.webofscience.com/wos/author/record/B-9285-2012>

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UEF-ID Brainmap Code : U-1700-039K-8673

Dae

30.01.2024

Dr. Constantin-Catalin Negrila

List of Publications

Negrila Constantin-Catalin

PhD Thesis

1. **“Structuri semiconductoare cu joncțiuni pentru dispozitive de detecție a radiației electromagnetice”, Negrila Constantin-Catalin**, Faculty of Physics, University of Bucharest, 2010.

Books, Chapters

2. **Sinteza și cristalizarea unor materiale avansate – semiconductori și aliaje**, Mihail Florin Lăzărescu, Constantin Logofătu, Adrian Ștefan Manea, **Cătălin Constantin Negrilă**, Electra, 2008, ISBN 978-606-507-011-0
3. **Surface Modification of III-V Compounds Substrates for Processing Technology**, Ghita R.V.; Logofatu C.; **Negrila C.C.**, Trupina L., Cotirlan-Simioniuc C., Capitol in cartea: *Nanoscaled Films and Layers*, Editor Laszlo Nanai INTECH, London, UK, 2017, ISBN 978-953-51-3143-4, p. 115-146
4. **Characteristics of Metals Thin Film Deposition on III-V Semiconductor Compounds**, Rodica V. Ghita, **Constantin-Catalin Negrila**, Constantin Logofatu, Daniela Predoi, Capitol in cartea: *Advances in Microelectronics: Reviews*, Volume 2, Editor Sergey Y. Yurish, International Frequency Sensor Association Publishing, 2019, ISBN: 978-84-09-08160-8

Articles

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