Şcoala Doctorală de Fizică
Facultatea de Fizică
Universitatea din Bucureşti

Teme de cercetare propuse pentru admiterea la studii universitare de doctorat
sesiunea septembrie 2024

Direcţia: **Biofizică experimentală și computațională, Fizică medicală**

1) **Protonation-coupled dynamics of membrane transporters** (prof.univ.dr. Ana-Nicoleta BONDAR)
Membrane transporters are nano-machineries that facilitate the transfer of ions or larger solutes across membranes that surround cells and cell compartments. A common aspect of membrane transport is coupling to protonation change, whereby one or more protein groups change protonation state, which alters the local network of non-bonded protein and water interactions, and subsequently associates with changes in protein conformational dynamics. That is, the protonation-coupled dynamics of a membrane transporter involves changes in the electronic structure of the group that protonates/ deprotonates, and coupled changes in a water-mediated interaction network –which can rapidly adjust to the altered protonation state– and slower time-scale changes in the global protein dynamics. We study these fundamental processes using quantum mechanics, combined quantum mechanical/ molecular mechanical (QM/MM) simulations, classical mechanics, and statistical mechanics; we access large scale supercomputing to perform our work.
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2. Bondar A-N (2022). Mechanisms of long-distance allosteric couplings in proton-binding membrane transporters. Advances in Protein Chemistry and Structural Biology 128, 199-239 (available upon request, please contact nbondar@fizica.unibuc.ro).

2) **Quantum chemical and molecular mechanical studies for the development of force-field parameters of drugs and cofactors** (prof.univ.dr. Ana-Nicoleta BONDAR)
Molecular transporter and receptor proteins, and proteins that function as enzymes, often bind ligands with specific chemical structures. Description of the molecular recognition processes, and of the response elicited by the binding of the ligand, are essential for basic science and pharmacology, and can guide the rational development of drugs to cure human disease. As these recognition processes involve dynamic non-bonded interactions, often mediated by water molecules, computational approaches are required to derive the atomic-level description of the ligand-bound biosystem. In order to perform reliable computations of ligand-bound proteins, accurate force-field parameters are required for all components of the computation system – and, oftentimes, ligands are non-standard molecules that require force-field parameters to be derived based on quantum and classical mechanical computations. We are particularly interested in drug molecules for cancer treatment. For computations we access large-scale supercomputing time.
References

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2. MacKerrel AD Jr. Empirical force fields: Overview and parameter optimization. https://comp.chem.umn.edu/Chem8021/EmpiricalForceFields.pdf

3) **Development of graph-based algorithms for backbone hydrogen-bonding in membrane receptors** (prof.univ.dr. Ana-Nicoleta BONDAR)
Membrane receptors mediate communication between cells (or cell compartments) and their environment. In order to do that, receptors must relay signals across distances of ~3-4nm. Signal relay is typically based on orchestrated rearrangements within networks of non-bonded interactions between protein groups, protein-bound water and, in some receptors, ligands with specific biological function. We have developed highly efficient graph-based algorithms to analyze networks of hydrogen bonds in membrane receptors. We are interested in methodological developments that would allow us to include into the graph computation specific backbone groups. The research planned involves computations with classical mechanics, and graphs. For computations we access large-scale supercomputing time.
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https://bpspubs.onlinelibrary.wiley.com/doi/full/10.1111/bph.16387

4) **Reaction mechanisms of a lipid-modulated intra-membrane proteases** (prof.univ.dr. Ana-Nicoleta BONDAR)
Proteases are enzymes (proteins) that catalyze the cleavage, at specific sites, of covalent bonds between amino acid residues of the polypeptide chain of another protein called the substrate. Their action is essential for cell physiology and disease. Because the proteolysis reaction catalyzed by proteases requires water, proteases that sit in membranes (intra-membrane proteases) must ensure that water molecules can access the catalytic active site; moreover, intriguing experimental data suggest that the lipid membrane environment can influence significantly the activity of the enzyme. We work on intramembrane proteases from the rhomboid family. The project aims to characterize the general mechanism by which intra-membrane proteases cleave substrates in physiological lipid membrane environments. We will use classical mechanical and combined quantum mechanical/molecular mechanical computations, and access large-scale supercomputing time.
References
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5) **Utilizarea tehnicilor de inteligenţă artificială pentru localizarea zonelor epileptogene la pacienţii cu epilepsie farmacorezistentă** (prof.univ.dr. Andrei BARBORICĂ)
Descriere: Învățarea profundă oferă o soluție alternativa clasificarii manuale a biomarkerilor intracranieni ai epileptogenicitatii, cum ar fi descărcările inter-ictale şi oscilaţiile de înaltă frecvenţă. Distribuţia spaţială 3D a acestor biomarkeri este un indicator important al zonelor epileptogene a căror rezecţie poate duce la reducerea sau suprimarea crizelor pacienţilor suferind de epilepsie

farmacorezistentă. Tema îşi propune extinderea utilizării tehnicilor de învățare profundă la o analiză multi-modală ce agregă informaţiile reprezentate de biomarkerii tradiţionali cu cele privind semiologia crizelor epileptice sau cu datele referitoare la conectivitate.

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4. Alim-Marvasti A, Pérez-García F, Dahele K, Romagnoli G, Diehl B, Sparks R, Ourselin S, Clarkson MJ, Duncan JS. Machine Learning for Localizing Epileptogenic-Zone in the Temporal Lobe: Quantifying the Value of Multimodal Clinical-Semiology and Imaging Concordance. Front Digit Health. 2021 Feb 10;3:559103. doi: 10.3389/fdgth.2021.559103. PMID: 34713078; PMCID: PMC8521800.

Direcţia: **Fizica atmosferei şi a pământului – Surse regenerabile de energie**

1) **Procesele fizice care duc la apariția furtunilor severe și influența încălzirii globale asupra acestora**
(C.Ş.I dr. Bogdan ANTONESCU)

Furtunile severe, caracterizate prin grindină mare, vânturi puternice, fulgere, tornade și precipitații extreme, reprezintă fenomene meteorologice deosebit de periculoase. Înțelegerea proceselor interne ale acestor furtuni este crucială pentru anticiparea și gestionarea efectelor acestora, în special în contextul încălzirii globale. Această cercetare își propune să investigheze procesele interne din cadrul furtunilor severe și să analizeze modul în care schimbările climatice influențează frecvența, intensitatea și impactul acestor fenomene.

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3. Taszarek, M., Allen, J. T., Púcik, T., Hoogewind, K. A., and Brooks, H. E. (2020b), Severe Convective Storms across Europe and the United States. Part II: ERA5 Environments Associated with Lightning, Large Hail, Severe Wind, and Tornadoes, Journal of Climate, 33, 10263–10286, https://doi.org/10.1175/JCLI-D-20-0346.1
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5. Wapler, K. (2017), The life-cycle of hailstorms: Lightning, radar reflectivity and rotation characteristics, Atmospheric Research, 193, 60–72. https://doi.org/10.1016/j.atmosres.2017.04.009

2) **Contribuții la înțelegerea aportului, transformării și a variabilității spațio-temporale a negrului de fum în sistemele acvatice** (C.Ş.I dr. Bogdan ANTONESCU)
Negrul de fum este un reziduu organic provenit din arderea incompletă a materiei organice, transportat atât în sol, cât și în mediul acvatic. Râurile transportă aproximativ 34% din negrul de fum produs anual de incendiile de vegetație, jumătate fiind sub formă dizolvată, cu mecanisme diferite de transport și transformare în apă. Există numeroase necunoscute privind rolul negrului de fum dizolvat în procesele biogeochimice, inclusiv interacțiunea cu materia organică naturală și impactul factorilor antropici asupra transportului acestuia.
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4. Wagner S., Jaffe R., Stubbins A., (2018), Dissolved black carbon in aquatic systems, Limnology and Oceanography Letters, 3(3), 168-185. https://doi.org/10.1002/lol2.10076

3) **Procesele fizice ale furtunilor convective cu vânt intens și impactul acestora asupra aviației și altor domenii critice** (C.Ş.I dr. Bogdan ANTONESCU)
Această cercetare doctorală își propune să investigheze procesele fizice care stau la baza formării și dezvoltării furtunilor convective cu vânt intens și să analizeze impactul acestor fenomene asupra siguranței aviației, precum și asupra altor domenii critice, cum ar fi infrastructura, transporturile și energia. Furtunile convective, caracterizate prin vânturi puternice, reprezintă o amenințare semnificativă nu doar pentru zborurile comerciale și de agrement, dar și pentru stabilitatea și funcționalitatea altor sectoare esențiale.
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3. Romanic, D., M. Taszarek, and H. Brooks (2022): Convective environments leading to microburst, macroburst and downburst events across the United States, Weather and Climate Extremes, 37, 100474.
https://doi.org/10.1016/j.wace.2022.100474

4) **Evaluari multi-hazard pentru cutremure și fenomene meteorologice extreme în contextul schimbărilor climatice** (C.Ş.I dr. Bogdan ANTONESCU)
Obiectivul general al tezei de doctorat este de a analiza și cuantifica efectele combinate ale hazardurilor seismice și ale schimbarilor climatice asupra infrastructurii și comunităților din diferite zone ale României. Utilizând o abordare multi-hazard, lucrarea dezvoltă un cadru conceptual și metodologic pentru evaluarea hazardurilor integrate, combinând analiza expunerii la cutremure și fenomene meteorologice extreme si estimarea posibilului impact asupra populatiei.

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5) **Investigarea impactului la scară globală al Circulaţiei Meridianale din Atlantic, o componentă critică centrală a sistemului climatic** (prof.univ.dr. Mihai DIMA)
Descriere: Circulaţia Meridianală din Atlantic este o componentă climatică critică, care poate genera variaţii climatice cvasi-globale, ireversibile. Potenţialul impact al acesteia a fost investigat preponderent prin simulări realizate cu Modele de Circulaţie Generală a Atmosferei şi Oceanului. Impactul climatic al acesteia va fi investigat pe bază de date observaţionale, cu accent pe influenţa Circulaţiei Meridianale din Atlantic asupra Europei, a Americii de Nord, a Pacificului Tropical şi a Atlanticului de Sud, precum şi asupra altor componente climatice critice.
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6) **Investigarea impactului aerosolilor asupra norilor, cu ajutorul tehnicilor "remote-sensing" şi a modelelor** (prof.univ.dr. Mihai DIMA)
Descriere: În cadrul programului doctoral va fi realizată o investigare sinergică a impactului aerosolilor asupra norilor, integrând metode de măsurare de tip "remote sensing" (realizate de la suprafaţa Pământului şi din sateliţi) cu analize bazate pe modele. Extinderea înţelegerii proceselor de interacţiune

dintre aerosoli şi nori poate contribui la îmbunătăţirea proiecţiilor climatice realizate cu modele de circulaţie generală.

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7) **Analiză comparativă a intensităţii turbulenţei atmosferice pe bază de date obţinute prin metode diferite** (prof.univ.dr. Mihai DIMA)

Descriere: Hazardurile legate de aviaţie sunt reprezentate de obiecte, condiţii, evenimente şi circumstanţe care au potenţialul de a genera incidente sau accidente. Turbulenţa atmosferică este cel mai periculos şi cel mai dificil de gestionat hazard, fiind cauza dominantă a accidentelor aviatice. În cadrul programului doctoral investigaţiile vor fi focalizate pe calcularea vitezei de disipare a vârtejurilor (Eddy dissipation rate - EDR) de-a lungul traiectoriei de zbor a unui avion de dimensiuni medii. Va fi dezvoltat un algoritm de calcul a acestor traiectorii. Va fi dezvoltat un algoritm de calcul al EDR de-a lungul acestor traiectorii, iar valorile obţinute vor fi comparate cu cele derivate din modelele de predicţie numerică.

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8) **Predicţia climatică extinsă multi-anuală -decenală în climat tranzient: cercetări şi dezvoltări pentru Europa şi România utilizând modele complexe Earth System Models (ESM)** (C.Ş.I dr. Mihaela CAIAN)
Descriere: Scopul este de a implementa şi exploata, pentru prima data în România, un sistem climatic regional (rezoluţie fină) pentru predicţii multi-anuale. Se va utiliza modelarea climatică regională cuplată cu modele climatice globale ale centrelor de predicţii decenale. Rezultatele vor include aspecte de cercetare fundamentală (e.g. dinamica spaţială a zonelor de risc climatic (cauze, mecanisme), incertitudini, interacţiunea dintre variabilitatea internă şi forţată) dar vor urmări şi diseminarea largă a acestor rezultate noi la nivelul factorilor de interes.
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9) **Explorarea potenţialului modelelor de inteligenţă artificială (AI) pentru prognoza vremii şi a climatului** (C.Ş.I dr. Mihaela CAIAN)
Descriere: Utilizând metode AI, date şi rezultate teoretice se urmăreşte:
i) îmbunătăţirea prognozelor atmosferice prin: regionalizare (rezoluţii foarte fine); extinderea bazelor de date (acolo unde nu există măsurători sau seriile de timp nu sunt complete), utilizarea de ansamble mari (rulări rapide) pentru estimarea mai precisă a incertitudinii;
ii) contribuţii la creşterea gradului de explicare a scorului AI utilizând metode bazate pe operatori de identificare de structuri coerente în datele de intrare-ieşire pentru explicarea abilităţilor AI în predicţia climatică.
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2. Amir Ali, 2024. Explainable AI: Examining Challenges and Opportunities in Developing Explainable AI Systems for Transparent Decision-Making. Journal of Artificial Intelligence Research , Vol.4 No 1 (2024)

10) **Explorarea potenţialului modelelor de inteligenţă artificială (AI) în scopul adaptării şi diminuării impactului la schimbările climatice în sectoare cheie de activitate** (C.Ş.I dr. Mihaela CAIAN)
Descriere: Utilizarea metodelor AI pentru prognoza impactului condiţiilor de vreme în timp real şi în scenarii climatice, asupra diferitelor aspecte sectoriale importante: agricultura (monitorizarea şi prognoza culturillor, optimizarea scenariilor de management), poluare şi sănătate (monitorizarea şi prognoza calităţii aerului, scenarii optime de reducere); utilizarea optimă a acoperirii terenurilor pentru maximizarea captării CO_2.

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11) **Understanding the climate change interaction with air pollution and human health in Madagascar** (C.Ş.I dr. Mihaela CAIAN)
Description: We propose this study to focus on climate change – air pollution -human health over Madagascar region. The main aim is to advance the scientific knowledge linking climate change and air pollution over the region to health related risks. This work will allow identification of key features of these events, understand the climate mechanisms behind events of extreme impact, and propose, derive and validate methods to predict in advance climate context for the occurrence of these risk conditions. The analysis will investigate both the current climate and future climate conditions, in the support of climate-impact national services for adaptation measures and impact mitigation (e.g. identify future hot -spot regions of impact, changes in intensity, frequency).
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12) **MXene-based nanomaterials for redox flow batteries and sodium-ion (Na-Ion) batteries** (prof.univ.dr. Ioan STAMATIN)
Context: Redox flow batteries (RFB) and sodium-ion batteries have limited capacity and life cycle due to anode capacity to store intercalation ions and charge storage. Materials used in intercalations are GIC, hard carbon with mesoporous structures and some of the oxides based titanium, alloys based silicon (Si-Sn ex). Main drawback: (ex LiC 6) low ion concentration intercalated in anode, respective low storage energy in redox batteries. Materials known until now are hard interleaved or have ionic-covalent strength that damper Na- reversibility.
Challenges. MXene, 2D layered structures made of Metal-Metal-carbon- Terminal organic functions, have large capacity to collect and insert in their interlayers Na ions ($Ti_3C_2T_x$ has shown reversible sodium storage capacities ranging from 100 to 400 mAh/g and, V_2CT_x has demonstrated capacities between 150 and 350 mAh/g.)
Project: MXene and MBene are screening related to the storage capacity and designed appropriate Na-ion batteries to evaluate their performances with reference cathode Prussian white
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13) **Technological innovations to sense and mitigate new and emerging contaminants in surface and subsurface waters** (prof.univ.dr. Ioan STAMATIN)

Challenge: With all the technological advances in recent years, the two impending challenges to human existence are climate change and scarcity of clean water. The two “grand” challenges contrast each other in that, while the former would affect society, the latter would affect every individual for their basic existence. The concern is growing over novel and previously undetected contaminants that are increasingly found in water sources, their potential health impacts, and the challenges in monitoring and managing these contaminants which are chemical, biological, radioactive materials, disinfectant byproducts, and a category termed as “emerging contaminants” consisting of returned pharmaceuticals, personal care products, macro/nano plastics and forever chemicals [1-4]. The health implications of these new and emerging contaminants are being investigated by the scientific community; however, initial findings show the presence of higher levels of estrogen and viral vectors in water and decreased oxygen concentrations. While more research is necessary to understand the scope of such contaminants on human health, it is obvious that sensing, identification, and mitigation of contaminants using novel materials is extremely important.

Aim and Scope of the project: Several characterization methods are commercially available to sense/detect conventional contaminants, however more research is needed to sense/detect nano plastics in water, returned pharmaceuticals, Toxic Industrial Chemicals and Materials (TICs/TIMs), Chemical Warfare Agents (CWAs), and Novel and emerging Non-Traditional Agents (NTAs). The project aims to study the use of nanomaterials-based sensors to study such contaminants, Additionally, nanomaterials-based membranes, used in conjunction with 3D printed scaffolds can be used for capturing such contaminants from aquatic sources. Nano-photocatalysis is a powerful tool to degrade higher-order carbons into biodegradable products and will be used to mitigate plastics, herbicides, pesticides, and pharmaceuticals present in drinking water. This project provides the means for the identification of key knowledge gaps, technologies to mitigate environmental pollution, and recommendations for policies to limit its emission.

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14) **Micro/Nano plastics – detection and mitigation** (prof.univ.dr. Ioan STAMATIN)

Challenge: The diversity of polymers and the versatility of their properties have transformed our everyday lives. While their widespread use, including for disposable aspects was anticipated, some of

the recent reports associated with the extent of environmental pollution created by nano/microplastics were not articulated. The presence of microplastics in treated tap and bottled water has raised serious questions and concerns about the impact that microplastics in drinking water have on human health and aquatic well-being [1-3]. Due to ingestion and other pathways, the ecological risks posed by micro and nano plastics as vectors for chemical contaminants and their accumulation through trophic transfer are very serious and of utmost importance. Very little data exists on the toxicokinetic effects of micro/nano plastics on human health [4]. Aquatic life or aquatic ecosystems are already affected by a multitude of environmental stressors, and now microplastics and nanoplastics may represent a significant additional risk to food security [4].

Aim and scope of the project: This project aims to study various aspects of nano/microplastics in the environment to better assess risks posed to human health to develop appropriate mitigation and management strategies. Since the use of plastics is essential to our lifestyle, it is crucial to reap the benefits of plastics while keeping pollution to a minimum. The project aims to sense/detect the quantity of micro/nanoplastics in our surrounding aquatic environment and use a combination of methods for nanoplastics removal. While macro/microplastics can be separated using typical filtration, nano plastics escape from such treatment. The knowledge gap has significantly increased since the use of plastics has exponentially increased and the research to mitigate resulting pollution has not kept up with the pace. Hence, this project aims to study various methods to sense/detect the size of micro/nanoplastic and find appropriate removal technologies such as membrane separation, and photocatalysis. These methods will serve as practical/effective measures along with the traditional procedures (filtration, coagulation, centrifugation, flocculation, and gravity settling). It is critical to identify specific methods that offer clear advantages and to refine national and international standards and associated product labeling along with ways to use, reuse, recycle, and even upcycle, to indicate appropriate usage and appropriate disposal methods. This project provides the means for the identification of key knowledge gaps, technologies to mitigate environmental pollution, and recommendations for policies to limit its emission.

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15) **Composites based nanomaterials high resistance against fire with maximum comfort and zero emissions** (prof.univ.dr. Ioan STAMATIN)

Context: Buildings with zero emissions, high thermal comfort, and sustainability require , nanocomposites, renewable energies, efficient water and waste management systems, for robust protection against fire and natural disasters. The implementation of IoT and AI technologies aims to optimize building performance and resource efficiency.

Key Components: 1) Nanomaterials and Nanocomposites (for enhanced insulation, strength, and durability, thermal management, 2) Renewable Energies: (solar panels, wind turbines, and other renewable energy sources to achieve zero-emission energy supply; storage solutions using advanced nanomaterials to ensure a stable and reliable energy supply 3) Water and Waste Management: (nanofiltration systems for efficient water purification and recycling, 4) Fire and Disaster Protection (fire-resistant nanomaterials to enhance building safety, nanocomposites to withstand extreme weather conditions and seismic activity, 5) IoT and AI Integration: Employ IoT sensors to monitor and manage building systems in real-time.

Implementation Plan: Research and Development: Conduct R&D on suitable nanomaterials and nanocomposites for building applications, Develop prototypes and test their performance under various conditions.
Expected Outcomes: Achieve zero-emission buildings with high thermal comfort; Enhance the sustainability and resilience of buildings; Optimize resource efficiency through IoT and AI technologies; Set new standards for green building practices and contribute to environmental conservation.
Supplementary support: training in AI and IOT, during the first year- teaching and experimental set to get high level abilities.
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16) **CO_2-electroreductions and conversion in by-products** (prof.univ.dr. Ioan STAMATIN)
Context: Capture and sequestration have limited impact on the CO_2 concentration. Storage in mines and geological deposits rise other negative effects on the local/ regional communities. The opportunity to convert CO_2 in new green products useful for society such as new fuels or chemicals from simple organics (formic, acetic, carboxylic acids) to complex molecules is a challenge
Aim and scope. New device based on advanced electrocatalysts enable to convert CO_2 in appropriate ions which in turn interact with H_2, N_2, urea, other ions leading to new products.
Device concept- three cells. Electrocatalysts design & physico-chemical methods using AI- in silico advanced software and combination from advanced physico-chemical methods.
Infrastructure: The First experimental model already developed and new compounds obtained (carboxylic acids)
Objective- new electrocatalysts & ion exchange membranes to increase the conversion yields. To design and construct an electrochemical cell capable of reducing carbon dioxide (CO_2) to ethanol (C_2H_5OH) using copper as a catalyst. The project aims to explore the feasibility and efficiency of this electrochemical method for converting CO_2 into a valuable chemical product, ethanol. Metal (such as copper)-MXene composite for CO_2 reduction is an innovative approach that leverages the strengths of both materials to enhance catalytic performance. Here's a detailed proposal based on current research findings
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Supplementary support: training in AI and IOT, during the first year- teaching and experimental set to get high level abilities.

Direcţia: **Fizică atomică, fizică nucleară, fizica particulelor elementare, astrofizică şi aplicaţii**

1) **Evaluarea unor parametrii de producere și dezintegrare ale proceselor cromodinamice și electroslabe ce apar în ciocniri proton-proton la √s ≥13 TeV** (prof.univ.dr. Alexandru JIPA)

Tema propusă pentru teza de doctorat are în vedere realizarea unui studiu care să folosească date din baza HEPdata (High Energy Physics Database), precum și date simulate în vederea analizării unor procese fizice care să implice atât probleme specifice Cromodinamicii cuantice, cât și unificării interacțiilor electromagnetică și slabă (interacția electroslabă).

Pentru determinări experimentale se vor folosi date obținute cu sistemul de detectori LHCb (Large Hadron Collider beauty) de la CERN Geneva pentru ciocniri proton-proton la √s ≥13 TeV. Fasciculele de protoni vor fi accelerate folosind sistemul de acceleratori LHC (Large Hadron Collider). O direcție de studiu de interes este producerea unor stări a materiei nucleare bogate în cuarci de diferite tipuri, care se pot combina și da naștere la diferite tipuri de particule. O direcție de studiu alternativă este investigarea producerii de bosoni intermediari de tip Z^0, în conexiune cu producerea de jeturi sau hadroni specifici, precum kaonul neutru cu timp de viață scurt (K^0s) sau hiperonul Λ^0, ca posibili constituenți ai jeturilor. Analiza datelor se va face cu pachetele de programe specifice Colaborării LHCb. Analizarea diferențelor dintre valorile măsurate ale unor mărimi, valori incluse în HEPdata, simulări și rezultate noi va permite verificarea limitelor de detecție și acuratețea pachetelor de programe folosite în analiză, inclusiv prin compararea predicțiilor diferitelor tipuri de generatori cu datele experimentale. Se va putea avea în vedere, acolo unde este cazul, modificări și îmbunătățiri ale modelelor folosite în codurile de simulare, pentru diferite condiții de generare, respectiv, măsurare. Printre acestea se numără codurile PYTHIA, HERWIG și SHERPA. Unele din extensiile lor se vor putea folosi Datele Monte Carlo vor fi generate cu aceste generatoare, iar unele extensii ale lor – de exemplu, POWHEG BOX, PHOTOS – pot fi folosite în analize complexe. Studiile care se vor întreprinde au ca scop selectarea unui semnal ffizic de încredere pentru procele fizice menționate. Analiza datelor obținute în experimentul LHCb ar putea permite dezvoltarea și optimizarea unui sistem de declanșare a unor subsisteme de detectori care să permită selectarea de încredere a unor candidați pentru procesele fizice investigate. Se vor estima eficacități de reconstrucție și alți parametrii de interes ai detectorilor implicați în măsurare. Pentru creșterea încrederii în smnalele selectate, în analiza datelor, experimentale și simulate, se va avea în vedere metode de luare în considerare a fondului de radiații, cu luarea în considerare a proprietăților specifice ale detectorilor folosiți. Tema va fi realizată în colaborare cu un grup de fizicieni de la IFIN-HH.

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2) **Corelații azimutale în diverse sisteme de ciocnire utilizând Detectorul ALICE** (prof.univ.dr. Alexandru JIPA)

Cromodinamica cuantică, teoria interacțiilor tari ce descrie procesele de interacție ale partonilor (cuarci și gluoni), prezice tranziția de fază a materiei nucleare la plasma de cuarci și gluoni, fază a materie nucleare în care partonii nu mai sunt confinați in interiorul hadronilor. Ciocnirile nucleare la energii relativiste oferă posibilitatea de a produce și a studia proprietățile plasmei de cuarci și gluoni. Studiile au evidențiat faptul că plasma de cuarci și gluoni prezintă un comportament colectiv puternic, ca un lichid aproape perfect. Un comportament colectiv similar a fost observat în ciocniri proton-proton (pp) și proton-plumb (p-Pb). Un astfel de comportament nu era așteptat în sisteme de mărime redusă, din cauza dimensiunii transversale mici a regiunii de suprapunere a sistemelor care se ciocnesc, având în vedere dimensiunea protonului. Procesele și fenomenele fizice care stau la baza acestor observații în sistemele de mărime redusă nu sunt încă foarte bine cunoscute, ceea ce face ca ele să fie larg dezbătută. Aceste dezbateri sunt legate de faptul că diferite modele care încorporează diverse mecanisme de ciocnire (modele microscopice bazate pe cuarci și gluoni și modele macroscopice bazate pe formarea plasmei de cuarci și gluoni) explică calitativ măsurările.

Tema propusă, „Corelații azimutale în diverse sisteme de ciocnire utilizând detectorul ALICE” va aborda problema originii colectivității în sistemele de mărime redusă prin intermediul corelațiilor azimutale. Corelațiile dintre două sau mai multe particule identificate, dar și neidentificate, vor fi măsurate în ciocniri pp, p-Pb și O-O, datele experimentale folosite fiind obținute cu Detectorul ALICE. Rezultatele obținute cu acest sistem complex de detectori vor fi comparate cu predicțiile unor modele. Măsurările propuse vor oferi informații decisive pentru a diferenția între cele două căi de descriere ale materiei nucleare formate în sisteme de mărime redusă.

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3) **Investigarea evoluției Universului prin experimente terestre** (prof.univ.dr. Alexandru JIPA)

Evoluția Universului nostru este descrisă în prezent de diferite scenarii cosmologice care au la bază observații și măsurări. Acestea au fost făcute atât în experimente efectuate pe sateliți, dar și în

experimente terestre. Teza de doctorat își propune considerarea rezultatelor experimentale obținute în experimente terestre, cu luarea în considerare a conexiunilor cu ipotezele unor scenarii cosmologice, cu deosebire cu cele ale „Exploziei primordiale" („Big Bang"). De-a lungul anilor au fost luate în considerare diverse surse de particule, cu evoluții specifice, în încercarea de a explica procese și fenomene fizice complexe care sunt implicate în această evoluție. Deoarece nu există posibilitatea de a controla parametrii inițiali ai unui fascicul de radiații cosmice (intensitate, energie, natura sistemului nuclear incident ș.a.) care poate produce o reacție nucleară de interes, în ultimele decenii s-a acordat o atenție deosebită folosirii unor ioni grei, cu energii din ce în ce mai mari și intensități semnificative, în sisteme de acceleratori de diferite tipuri. Experimentele desfășurate în cei peste 50 de ani de experimente terestre cu ioni grei relativiști și ultrarelativiști, la sisteme de acceleratori, au permis obținerea de informații științifice valoroase pentru descrierea acestei evoluții a Universului. De asemenea, sisteme de acceleratori noi și experimente asociate, sunt în pregătire în câteva mari laboratoare internaționale, ceea ce va permite obținerea de noi informații, în experimente dedicate. De aceea, în această teză de doctorat se vor aborda probleme specifice domeniului, folosind rezultate experimentale existente, simulări pentru experimente viitoare, cu propunerea unor metode noi de abordare. Se vor avea în vedere condiții specifice, procese termodinamice asociate, astfel încât să se poată încerca descrierea evoluției Universului pe baza unor ecuații de stare specifice materiei nucleare extrem de dense și fierbinte folosind parametrii de încredere. O atenție deosebită se va acorda tentativei de descriere, pe baza rezultatelor unor experimente terestre, a evoluției Universului, incluzând formarea unor tipuri de stele, cum ar fi stelele neutronice. Câteva experimente, cum ar fi CBM și HADES, de la FAIR-GSI, dar și altele, vor putea oferi curând rezultate experimentale de încredere care vor putea ajuta la realizarea obiectivelor tezei de doctorat.

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4) **Contributions to the development of a Low Background Liquid Argon detector at kTons-Scale**
(prof.univ.dr. Ionel LAZANU)

DUNE is a large international project to design, construct and operate a multi-kton scale liquid argon detector for neutrino physics, neutrino astrophysics and a search for physics beyond the Standard Model. The detector will be built deep underground at the SURF facility (Sanford Underground Research Facility, South Dakota, USA), but presently the prototypes of these detectors are in use at CERN. We find that it is possible to increase sensitivity to low energy physics with careful controls over radiopurity of the materials which will be used and including supplementary shielding materials. These idea proposals were accepted in the US strategy for the next decade. If in the active zone of the detector you will use argon obtained from underground extractions compared to the usual argon separated from the

atmospheric air, then the radioactive background only from the presence of the 39Ar isotope will decrease by a factor of about 1400.

New materials used for shielding will be investigated in detail, as well as innovative solutions for achieving protection, including through active methods. The realization of a detector (as a result of a large international collaboration) will pave the way for studies of the interactions of solar and supernova neutrinos, with energies below the current detection limits, the search for new phenomena and particles predicted by different phenomenological models developed above the Standard Model. This PhD project is a mixing between experimental and computational physics and offers an opportunity for a student to apply the knowledge of particle and astroparticle physics to direct applications. The candidate should have a good knowledge of particle physics at low and high energies and experience in programming skills and to be an advanced user in simulation using MC codes (FLUKA, Geant, MCNP).

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5) **Scintillation and ionisation properties of liquified and solid rare gases with applications for neutrino and dark matter experiments** (prof.univ.dr. Ionel LAZANU)

The atoms of the rare gases get excited or ionized by the incident particle, which might be a charged particle exciting the atoms directly, or an electrically neutral particle interacting via nuclear recoil. The energy deposited in the rare gas is converted into scintillation light, originating from the de-excitation and recombination of the atoms or generate ionization as effect of ionizations of electronic shells of atoms. In the particular case of argon, emission spectrum presents the first, second and third continuum, as well as the classical left turning point.

The explanation of the scintillation process is done considering the following process: in the case of two gas atoms, considering the potential curve, while for the ground state the potential is always repellent, in the case of an excited system a bound state (excimer) may form. Due to the Franck-Condon principle transitions happen vertically. Therefore, the transition energy is dependent on the internuclear distance. Not only excited atoms lead to an emission of light, but also ionized ones. Here, the scintillation processes are rather complex and are or must be modelled.

The PhD student will investigate potential experimental signatures that could be used to detect neutrinos, stable supermassive particles or other exotic exploiting the peculiarities of the scintillations and ionizations in Ar or Xe as Time Projection Chambers or other technologies.

This PhD project is a mixing between phenomenological and experimental physics. It is expected as the candidate should have a good knowledge of particle physics at low and high energies, but also atomic and the molecule physics. Programming skills and to be an user in simulation using MC codes are also expected.

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6) **Atomic and Nuclear Methods in Forensics Science** (prof.univ.dr. Octavian DULIU)
Nuclear Forensics: One of the main outcomes of forensic sciences focused on enhancing national nuclear security capabilities of the states, emphasizing that more work has to be done in order to prevent the unauthorized possession of nuclear materials or radioactive sources by non-state actors. Nuclear forensics is a new, multidisciplinary domain that was developed in the last decades, and like classical forensics, nuclear forensics seeks to link people, places, things, and events. But in the case of nuclear forensics, this means to identify the nuclear of radioactive material's origin, age and process history, the location where the material was produced, the possible pathway by which the material traveled.
Signature Analysis and Forensics Interpretation: In the case of present proposal, nuclear forensics investigations leading to identifying a nuclear or radioactive material found outside the regulatory control, often referred as "fingerprint analysis". Such complex qualitative and quantitative analysis results in obtaining information regarding the geometry, mass, activity, chemical form, isotopic composition and isotopic ratios, major element composition and trace elements, microstructure, morphology, crystallinity, markings, traces of the tools used, etc.
Purpose of Research: With the research activities plan of Nuclear Forensics Laboratory of Romania (NFL-Ro), such as Center of Excellent focused on resilience studies, characterization of various types of samples for development of nuclear forensics and safeguards libraries. CMX-8 which is inter-comparison exercises. Environmental monitoring for the FCN-ICNM site. Characterizing nuclear & radioactive materials in IFIN-HH safeguard deposit.
Analytical Methods To Be Used: i) High Resolution Gamma-ray Spectrometry, ii) X-rays Fluorescence, iii) X-ray Diffraction (XRD), iv) Inductively Coupled Plasma Mass Spectrometry (ICP-MS), v) Energy Dispersive X-ray spectrometry (EDX), vi) Scanning Electron and Optical Microscopy (SEM, OM), vii) Particle Induced X-ray Emission (PIXE) and Particle Induced Gamma-ray Emission (PIGE), viii) Muon Induced X-ray Emission (MIXE)
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7) **Atomic and Nuclear Methods in Geological Formations** (prof.univ.dr. Octavian DULIU)
Geological Formations: The study of geological formations is fundamental to understanding Earth's history, structure, and dynamic processes. Geological formations contain valuable information about the Earth's past environments, climate changes, and tectonic activities, which are crucial for natural resource exploration, environmental management, and hazard assessment. The advent of advanced atomic and nuclear methods has revolutionized the field of geology, providing precise and detailed insights into the composition, age, and evolution of geological materials.
Atomic and Nuclear Methods: Atomic and nuclear methods have become indispensable tools in geological research, enabling scientists to unravel the intricate details of Earth's geological formations.

These methods, grounded in the principles of atomic physics and nuclear science, provide unique insights that are unattainable through conventional geological techniques. These techniques have made significant contributions: Geochronology, Geochemical Analysis, Resource Exploration, Environmental Monitoring.
Key Techniques: Radiometric Dating, X-Ray Fluorescence (XRF),High Resolution Gamma-ray Spectrometry, Muon Flux Detection
Purpose of Research: The purpose of this PhD research is to investigate and enhance the application of atomic and nuclear methods in the study of geological formations. By leveraging techniques such as radiometric dating, high-resolution gamma spectrometry, X-ray fluorescence, and muon flux detection. The research is expected to produce advancements in the methodological toolkit available for geological studies, leading to a deeper and more precise understanding of Earth's history, resources, and environmental conditions.
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8) **Study of deuteron-induced reactions at low energies (<60 MeV)** (C.Ş.I dr. Marilena AVRIGEANU)
Extensive efforts in producing accurate cross sections for deuteron induced reactions are of fusion relevance as they are used the design and commissioning of the IFMISDONES and similar deuteron beam facilities. The modelling approach used (with explicit contributions from direct and break up reaction channels) gives improved agreement with available experimental data compared to current evaluations. High fidelity calculations of this nature are required to accurately predict deuteron induced activation cross sections. It is very worthwhile that detailed results and discussion are written for each reaction channel. Even for channels for which there is insufficient experimental data to derive spectroscopic coefficients for a particular channel, for which there is a lack of experimental data to compare, or for which there are some differences from experimental data, such details given would help to resolve problems as they arise in future activation analyses

The doctoral thesis will focus on a) consistent evaluation of deuteron interaction at low energy [1]; b) study of deuteron-induced reactions at the SPIRAL2/IFMIF accelerators [2]; c) deuteron 'breakup' description [3,4].

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9) **Study of alfa particles' emission at low energies (<50 MeV)** (C.Ş.I dr. Vlad AVRIGEANU)

The proposed work deals with the experimental data of (n,alpha) reactions and their theoretical explanation and modelling. Besides prevalent contribution of mechanisms based on optical potential and Hauser-Feshbach approach, the given reaction cross-section below ~10 MeV contains significant contribution of what is interpreted as the effect of isoscalar giant quadrupole resonance (ISGQR) in the compound nuclei. Such interpretation is further supported by the data on various other target nuclei (which appear in applied fusion research), where the ISGQR contribution is less pronounced. Finally, a correlation of the total estimated ISGQR (n,alpha) strength in terms of EWSR fraction, and (N-Z)/A will be concerned. The research results, of good quality, will describe a novel effect of alpha-decay of ISGQR in medium-mass nuclei, and take care also of error analysis

The doctoral thesis will focus on a) consistent evaluation of alfa particle emission in nucleon-induced reactions [1]; b) study of alfa particle-induced reactions for nuclear fusion (ITER/IFMIF) [2]; c) description of alfa emission for nuclear fusion [3,4].

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Direcţia: **Fizica stării condensate**

1) **Nanostructuri multistrat de carbon-titan cu proprietăţi îmbunătăţite: Obţinere şi caracterizare** (prof.univ.dr. Victor CIUPINĂ)

Descriere: Structurile multistrat de carbon-titan prezintă un interes tot mai mare în ultima vreme, în special datorită proprietăților mecanice, electrice și optice determinate de faza de carbură de titan (TiC) și faza de titan (Ti) . Astfel de structuri pot avea multiple aplicaţii datorită posibilităţii de modificare a coeficientului de frecare, şi a durităţii, precum şi datorită fezabilităţii trecerii de la caracterul semiconductor la caracterul metalic şi implicit schimbarea semnului coeficientului de variaţie a rezistenţei electrice cu temperatura. Scopul pe care îl urmărim constă în obţinerea de structuri multistrat de C-Ti cu anumite proprietăţi determinate de conţinutul de Ti_xC_y şi Ti, folosind metoda Arcului Thermionic în Vid (TVA) şi caracterizarea acestor structuri. Se va urmări punerea în evidenţă a fazelor Ti_xC_y prin măsurători de difracţie cu raze X (GIXRD), tehnici de microscopie electronică (TEM, HRTEM, STEM), precum şi prin măsurători ale coeficientului de frecare, ale durităţii şi modulului de elasticitate prin nanoindentaţie şi proprietăţi electrice prin măsurători de conductivitate electrică. Pentru a obţine filmele subţiri multistrat de Ti-C pe substraturi de siliciu prin metoda TVA se va folosi un dispozitiv constând din două sisteme anod-catod independente (surse de plasmă) plasate în interiorul camerei de depunere.

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2) **Studiul unor noi compuşi organici binari şi ternari pentru aplicaţii în dispozitive electronice şi optoelectronice** (prof.univ.dr. Ştefan ANTOHE)
În ultima perioadă s-au făcut progrese foarte mari atât în ceea ce priveşte eficienţa de conversie (depăşind uneori 20% [1]) dar şi în privinţa stabilităţii celulelor solare organice (OSC), aparţinând generaţiei a III-a de celule solare, iar dacă ne referim la structurile bazate pe Perovskiţi (PSC) acestea au depăşit eficienţa de 25% [2]. Ţinând seama de expertiza grupului de cercetare şi de infrastructura de la Centrul de Cercetare Dezvoltare pentru Materiale şi Dispozitive Electronice şi Optoelectronice (MDEO)[3-5], obiectivul general al temei propuse va fi testarea unor noi compuşi ternari de tipul ,,two in one": doi donori cu un acceptor ne-fulerenic (D1, D2, A) sau un donor cu doi acceptori ne-fulerenici (D, A1, A2) în structuri de celulă fotovoltaică cu un singur strat absorbant.
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3) **Prepararea şi caracterizarea unor filme subţiri din compuşi semiconductori A2-B6 fără cadmiu pentru aplicaţii în dispozitive electronice şi optoelectronice** (prof.univ.dr. Ştefan ANTOHE)
Ţinând seama de expertiza grupului de cercetare şi de infrastructura de la Centrul de Cercetare Dezvoltare pentru Materiale şi Dispozitive Electronice şi Optoelectronice (MDEO), [1-5] obiectivul general al temei propuse va fi prepararea şi caracterizarea unor filme subţiri din compuşi A2-B6 fără cadmiu, şi testarea lor în aplicaţii de fotodetecţie în domeniul UV-Vis, şi în aplicaţii spaţiale.
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4) **Theoretical and experimental investigations on the absorption and desorption process of hydrogen isotopes in semiconductor and metallic alloy structures** (prof.univ.dr. George-Alexandru NEMNEŞ)
The development of technologies and the identification of sources for producing non-polluting energy are major areas of interest. In addition to energy sources like photovoltaic, hydroelectric, wind, geothermal, and biomass, nuclear energy provides good long-term stability, reducing dependence on coal, oil, and natural gas. Unlike fission, thermonuclear fusion offers the advantage of a cheap and abundantly available fuel, creating the potential for an almost inexhaustible energy source with low costs.

Among the major projects in thermonuclear fusion is ITER (International Thermonuclear Experimental Reactor), a Tokamak toroidal system that achieves magnetic confinement of the plasma. A key concern is the composition and structure of the elements exposed to plasma (plasma-facing components), which require several properties: high thermal conductivity to manage heat flux, radiation resistance, high melting point and low hydrogen retention. Until 2023, the main candidates were beryllium (Be) and tungsten (W). Recent studies have shown that boron (B) is also a material of interest due to its chemical stability, high hardness and high melting point.

In the doctoral thesis, the student will address both theoretical and experimental aspects regarding the absorption and desorption of hydrogen isotopes in semiconductor layers (e.g., boron layers) and/or in metal alloys. The diffusion of atomic species will be investigated using both ab initio methods within density functional theory (DFT) and molecular dynamics methods with classical force fields. The study will determine the activation energies in the diffusion process and examine defect production, the appearance of chemical bonds stemming from diffusing species, surface adsorption processes, and the influence of the film's microstructure. Experimentally, thin layers of boron and/or metal alloys with hydrogen and/or deuterium insertion will be analyzed. Morphological (SEM, AFM) and structural (XRD) characterizations will be performed. The desorption of hydrogen isotopes can be analyzed using the Thermal Desorption Spectroscopy (TDS) technique in order to determine the activation energies.

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5) **Applications of machine learning techniques for the prediction of material properties and device modeling** (prof.univ.dr. George-Alexandru NEMNEŞ)

Machine learning techniques (ML) have seen an impetuous development in recent years, being used on a large scale for the exploration of electronic, mechanical, magnetic, optical, etc. properties in extended classes of materials, for which an exhaustive high-throughput computing approach is not feasible. In essence, to train the ML models, a database is built that contains the structure/composition of the materials/nanostructures and the corresponding physico-chemical properties, these being calculated (e.g. by ab initio methods) or obtained experimentally.

In the doctoral thesis, the student will develop ML applications for the prediction of material properties in a class of systems such as vitreous materials, high-entropy metal alloys, materials for photovoltaic technology, etc. A first step consists in identifying the features that are found in close correlation with the properties of the targeted materials. To determine them for the training set, density functional theory (DFT) calculations shall be employed, using specialized software packages such as SIESTA, Quantum Espresso, etc. Both supervised learning techniques, especially artificial neural networks, and unsupervised ML techniques, such as clustering algorithms, will be considered. Libraries such as TensorFlow, SciKit-learn, etc. will be used for their implementation.

Also, generative techniques such as image translation will be used for modeling electronic devices and inverse design. Thus, starting from the targeted properties, it is possible to identify the structure of the device and the composition of the materials necessary to achieve its functionality.

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6) **Dezvoltarea filmelor subţiri nanostructurate prin metode electrochimice, cu aplicaţii în domeniul dispozitivelor electronice şi optoelectronice** (prof.univ.dr. Vlad-Andrei ANTOHE)

Conversia directă a energiei solare în energie electrică prin efect fotovoltaic reprezintă o alternativă viabilă pentru noi surse de energie. Există în permanență o preocupare intensă pentru creșterea eficienței de conversie a celulelor solare de diferite generații în paralel cu scăderea prețului lor. O opțiune în acest sens este de a exploata avantajele nanotehnologiilor moderne ce pot aduce un plus de performanță sau funcționalități noi dispozitivelor electronice și optoelectronice. Astfel, o platformă experimentală modulară de implementare a unor procese electrochimice a fost dezvoltată în ultimii ani, în cadrul Centrului de Cercetare-Dezvoltare pentru Materiale și Dispozitive Electronice & Optoelectronice (MDEO), aparținând Facultății de Fizică a Universității din București. Această configurație experimentală și-a demonstrat deja utilitatea la sinteza electrochimică a unor filme subțiri de Telurură de Cadmiu (CdTe), dar și la creșterea unor matrici ordonate de nanofire sau nanotuburi orientate vertical în raport cu substratul vizând diverse aplicații [1,2].

În aceste circumstanțe, obiectivul general al acestei teme de doctorat se bazează pe implementarea unor procese electrochimice de preparare a unor filme subțiri nanostructurate, cu aplicații în realizarea unor dispozitive optoelectronice, cum ar fi celule solare sau foto-detectori. Se va

avea în vedere cu precădere optimizarea proceselor de sinteză electrochimică a unor compuși A2-B6 fără Cadmiu (Cd) pentru care Centrul MDEO dispune de expertiza și infrastructura necesară [3-5].

Ținând așadar seama de expertiza dezvoltată în ultimii ani la centrul MDEO, de experiența grupului de cercetare, dar și de infrastructura de cercetare existentă, premizele îndeplinirii cu succes a obiectivelor de cercetare propuse prin această temă doctorală sunt asigurate.

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7) **Development of novel three-dimensional networks of interconnected nanowires for energy-harvesting devices** (prof.univ.dr. Vlad-Andrei ANTOHE; PhD Partnership Agreement, UB – UCLouvain)
Recent developments of three-dimensional (3D) networks of interconnected nanowires triggered new prospects from the practical point of view, mainly because these crossed nanowires (CNWs) combined with polymeric membranes form nanocomposite films, with special electrical, thermal and mechanical properties. As demonstrated so far, the applicative range of these CNWs can vary from gas sensing scenarios [1], to electrodes for micro-batteries and micro-supercapacitors [2-4], as well as more recently to thermoelectric devices [5].

In relation to the latter, this PhD Research Program is based on the fabrication and characterization of such CNWs made-up of pure bismuth (Bi) and its alloys. These flexible thermoelectric nanocomposites can be used in specific applications to harness the thermal energy of the hot surfaces or even of the human body, for subsequent conversion into electricity to power-up lightweight and portable electronic appliances, as well as wearable or implantable medical equipment.

The entire framework program will be carried out in a PhD partnership agreement established between University of Bucharest (UB, Romania) and Catholic University of Louvain (UCLouvain, Belgium), both institutions possessing a very good scientific expertise and research infrastructure. The long-lasting cooperation as well as the skills developed in the two institutions over the last years complement each other perfectly to allow the implementation of a PhD Program in this interesting and actual research topic, as well as in a modern experimental environment.

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8) **Caracterizarea structurală a filmelor subţiri epitaxiale depuse prin ablaţie laser pulsată**
(C.Ş.I dr. Valentin CRĂCIUN)
Tema de doctorat cuprinde i) Depunerea prin ablaţie laser pulsată de filme monocristaline de nitrură de titan şi oxid de ruthenium pentru aplicaţii în reacţii de descompunere a apei şi ii) Studiul structurii cristaline a filmelor depuse pentru eficientizarea procesului de descompunere a apei.

În funcţie de parametrii ablaţiei laser (temperatura substratului, fluenţa laser şi atmosfera gazoasă utilizată) şi a orientării cristaline a substratului folosit, filmele subţiri depuse prin ablaţie laser pot fi policristaline, texturate sau epitaxiale. Pentru a înţelege orientarea cristalină a filmelor în raport cu cea a substratului, calitatea lor cristalină şi eventualele tensiuni mecanici generate datorită diferenţelor dintre parametrii reţelei cristaline a filmului şi cei ai substratului, investigaţii avansate de difracţie de raze X, omega-rocking curve, scanare phi, sau achiziţionarea de figuri polare sunt necesare. Pe baza înţelegerii relaţiei dintre film şi substrat se poate optimiza structura lor cristalină şi îmbunătăţi proprietăţile fizico-chimice.
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9) **Study of the interaction of ultrashort (fs) laser pulses with matter** (C.Ş.I dr. Valentin CRĂCIUN)
The thesis will be focused on a) Fabrication of materials with ultralow density for enhancement of the coupling of ultra-high laser pulses with matter and b) Studies of the laser damage threshold of optical components due to the interaction of fs laser pulses with matter.

Regarding a), of importance is the target optimization for ultra-high power fs-laser irradiation. The use of near critical density (NCD) targets is a promising route to enhance laser-driven proton acceleration, due to efficient conversion of the laser energy into hot electrons. This includes NCD in foam or other type of controlled low-density layer deposited on a foil in which laser self-focusing and efficient energy coupling to electrons enhances sheath acceleration. Also, ultrathin foils expanding to NCD enables relativistic transparency-enhanced acceleration mechanisms to occur.

We propose to carry out experiments with engineered multilayer micron-size targets and with ultrathin nanometer size foils. The multilayer targets consist of a low-density foam deposited on a substrate or a double or triple layer structure with controlled density gradient (few mg/µm) across its thickness. Common to both approaches, the role of density gradient will be investigated for the first time via controlled expansion by variation of the thickness of the foil and the use of a second prepulse beam. The optimum target expansion conditions for enhancing proton acceleration in both approaches

involving NCD targets will be identified, and the scaling of the proton maximum energy with the laser pulse intensity will be measured

Regarding b), a key part of the laser installations in ELI-NP is the optical beam transport system, which uses many high-quality, high-price mirrors. The most important parameters of these mirrors are their reflection coefficient and the laser induced damage threshold (LIDT) value. W developed the most sensitive LIDT measurement setup so far based on the Langmuir probe and compensation charge monitoring, which offers the additional benefits of being both in situ and real time monitoring techniques. It was also shown in an article published in Dec. 2023 [4] that the determination of the endurance limit of a mirror employing these two techniques could be performed using less than 10 laser pulses. The presentation of these results at the international conference Laser Damage, San Diego, Sept. 2023 won the Arthur Guenther Best Poster Award. We are now are in a privileged position to have the best tools, team, and expertise to analyze the role of mirror coatings physical and chemical properties on their LIDT value and better understand the physics of subthreshold laser irradiation. We will implement these diagnostic tools on the ELI-NP laser system to ensure an in situ and real time monitoring of the correct functioning of the mirrors, with significant cost benefits.

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4. Exploring fs-laser irradiation damage subthreshold behavior of dielectric mirrors via electrical measurements, Petrisor Gabriel Bleotu, Radu Udrea, Alice Dumitru, Olivier Uteza, Maria-Diana Mihai, Dan Gh Matei, Daniel Ursescu, Stefan Irimiciuc, Valentin Craciun, High Power Laser Science and Engineering, Vol 12, e15, 2023.

10) **Efecte magnetice și tranziții de spin asociate adsorbțiilor moleculare** (C.Ş.I dr. Cristian-Mihail TEODORESCU)

Unul din procesele fundamentale care guvernează proprietățile catalitice ale metalelor de tranziție pentru procese care implică oxizi de carbon este procesul de retro-donare, propus de Blyholder [1,2]. Acest proces presupune că, în cursul formării legăturii metal-carbonil, electroni din ultima stare ocupată (HOMO) a moleculei (stare π, orbital de legătură) sunt donați metalului, care, în schimb, "retro-donează" electroni moleculei pe ultima stare neocupată a moleculei (LUMO, stare π^*, orbital de antilegătură). În consecință, legătura dintre carbon și oxigen slăbește, iar molecula se poate disocia ușor sau poate fi implicată în diferite reacții (hidrogenare, oxidare).

În general, substraturile metalice fiind metale cu păturile d aproape complet ocupate, efecte magnetice sau de asimetrie de spin nu au fost luate în considerare până în prezent. Cu toate acestea, există raportări privind inducerea de momente magnetice nete nenule în metale sub influența unor câmpuri electrice [3] sau la adsorbții moleculare [4]. Recent, s-a evidențiat și apariția asimetriei de spin pentru stratul de suprafață al Pt(001) cu reconstrucție hexagonală [5], îmbogățit în electroni [6]. Aceste procese pot fi emulate simplu luându-se în calcul modelul Stoner [7] sau un model mai nou al feromagnetismului de bandă [8]. În consecință, adsorbțiile moleculare pe suprafețe de metale nobile, dacă sunt însoțite de un transfer net de electroni între molecule și straturile metalice de suprafață, sunt susceptibile să inducă tranziții magnetice în substratul metalic. Acesta este un prim aspect care merită investigat.

Un al doilea aspect care va fi analizat se referă la tranziții de spin ale moleculelor adsorbite. La adsorbția de CO pe o suprafață de Pt(001), procesele de retro-donare de tip Blyholder cel mai probabil conduc la alinierea energetică a orbitalilor HOMO (π) și LUMO (π^*). În aceste condiții, presupunând că molecula dispune în continuare de doi electroni pe stările energetice cele mai ridicate, aceștia ar trebui să aibă spinul paralel, fiind amplasați pe șase stări energetice degenerate, conform regulii lui Hund. Cu alte cuvinte, efectul de retro-donare însoțit de alinierea orbitalilor HOMO–LUMO ar trebui să fie însoțit de o tranziție a spinului total al electronilor din moleculă din starea $S_{total} = 0$ în starea $S_{total} = 1$. Acest tip de tranziții ar putea explica și formarea de clusteri bidimensionali la adsorbția de CO pe Pt(001) [9]. Schimbări vizibile ale structurii atomice sunt puse în evidență prin creșterea densității de molecule adsorbite [10].

Metodologia de lucru va folosi facilitățile de știința suprafețelor și interfețelor existente în INCDFM și la facilitatea de radiație de sincrotron Elettra din Trieste (combined spectroscopy and microscopy on surfaces, CoSMoS). Substraturile metalice vor fi preparate până la dispariția completă a oricăror contaminanți de pe suprafață, ceea ce se va pune în evidență prin spectroscopie de fotoelectroni (XPS) de înaltă rezoluție folosind radiația de sincrotron. Structura atomică a substratului se va analiza prin difracție de electroni lenți (LEED) și prin microscopie de baleiaj cu efect tunel (STM). Asimetria de spin se va detecta prin spectroscopie de fotoelectroni din banda de valență cu rezoluție unghiulară și de spin (SARPES). Odată substraturile caracterizate, se va proceda la adsorbții moleculare. Se vor varia dozele de molecule adsorbite, temperatura de adsorbție și natura acestor molecule (CO, CO2, alcooli, acizi grași, esteri, aldehide). După adsorbție, se vor caracteriza din nou substraturile prin XPS de înaltă rezoluție, LEED, STM și SARPES. Procesele de desorbție vor fi monitorizate prin XPS ultrarapid combinate cu analiza moleculelor desorbite prin spectrometrie de masă.

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11) **Obţinerea şi caracterizarea particulelor viromimetice** (C.Ş.I dr. Cristian-Mihail TEODORESCU)
Investigarea cineticii şi termodinamicii de autoasamblare de particule viromimetice (VLP) pornind de la obţinerea de nanoparticule de aur de dimensiune controlată, funcţionalizarea acestora cu diverşi liganzi ce permit formarea de legături covalente cu proteine capsidă. Se vor efectua experimente de reacție de autoasamblare dirijată de NP pentru a obține energia liberă de asamblare în funcție de raza șablonului sferic al NP. Pentru experimente, se va pune la punct producția și caracterizarea VLP-urilor cu nucleu de NP de Au, inclusiv sinteza de NP anorganice funcționalizate cu rază controlată, a CP-urilor virale (care vor fi exprimate prin recombinare în E. coli) și coasamblarea in vitro a NP-CP. Rapoartele molare ale CP în stare asamblată și liberă vor fi măsurate spectroscopic, la echilibru, în funcție de raza NP de Au, profitând de semnăturile spectroscopice diferite ale fluorescenței CP intrinseci între starea CP asamblată și cea liberă.

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12) **Electrozi şi sisteme de electrozi flexibili pentru aplicaţii wearables** (C.Ş.I dr. Cristian-Mihail TEODORESCU)

Dezvoltarea şi caracterizarea de noi tipuri de electrod şi sisteme de electrozi flexibili utilizând tehnici de electrofilare şi filare centrifugală cu control ridicat al parametrilor de proces, noi metode de funcţionalizare a acestora cu biomolecule (proteine, acizi nucleici) sau molecule biomimetice pentru obţinerea de biosenzori. Integrarea acestora cu sisteme (micro)fluidice polimerice poroase (hârtie, filme subţiri de PDMS, replicarea matricilor poroase) paternate 3D pentru obţinerea de sisteme de tip lateral- şi vertical- flow cu aplicaţii în domeniul dispozitivelor purtabile şi portabile, pentru detecţia de biomarker-i de anomalii medicale.

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13) **Dynamic non-collinear magnetic nanostructures and associated magneto-functionalities** (C.Ş.I dr. Victor KUNCSER)

The prediction, formation, investigation and manipulation of non-collinear spin structures in new magnetic systems will be considered. Following theoretical and computational studies providing a full set of material specific parameters and associated magnetic configurations, the most interesting systems will be chosen for the experimental investigation. The selected systems will be prepared by different processing routes and finally extensively analysed with respect to morpho-structural aspects in relation to their magneto-functionalities. New methodologies and concepts for Hall devices for the indirect probing of formation and specific dynamics of the non-collinear magnetic structures at nano-scale, including different types of skyrmions, will be proposed. Except of initial studies on the well known metallic multilayers based on ultrathin ferromagnetic/havy metal stacks, the topic will mainly involve the preparation and complex investigation of ferrimagnetic (FI) rare earth (RE)- transition metal (TM) amorphous thin films asymmetrically coupled to heavy metal (HM) films. Various thicknesses and compositions of the FI films of type Gd-Fe-Co (Gd is an isotropic RE) and Tb-Fe-Co (Tb is an anisotropic RE) will be considered, in order to tune the Dzyaloshinkii-Moriya interaction (DMi) at the FI/HM interfaces and to cross the compensation/composition points in FI films. A complete morpho-structural, magnetic, magneto-optic and electron transport investigation will be performed at various temperatures with a focus on ferrimagnetic spintronics related aspects.

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14) **Developing a new generation of magnetoresistive and magnetoplasmonic elements** (C.Ş.I dr. Victor KUNCSER)

Magnetoresistive and magnetoplasmonic systems can be either in multilayer or in granular thin film configuration, each one with specific magneto-functionalities. Starting from the processing simplicity of the granular thin films, the topic proposes the development of a new generation of giant magnetoresitive and magnetoplasmonic nanogranular thin films elements, by inducing the organization of magnetic clusters (e.g. Fe or Co) in a highly conductive matrix susceptible to support surface plasmons (e.g. Au). Our previous results pointed to the possibility to induce organization of the Fe clusters (from lamellar to filiform) with different nm-sized inter-cluster distances, leading to different types of magnetic order. The overall magnetic configuration of the system, the magnetisation reversal and the associated spin dependent scattering and magnetoplasmonic mechanisms can be therefore tailored by an extensive range of parameters (size and density of magnetic clusters, intra- and inter-lamellar distances, etc). Different processing routes of the Fe-Au nanogranular films will be considered as well as their complex morpho-structural magnetic, magnetoresistive and magneto-plasmonic characterization. The final scope is to optimize such Fe-Au nanogranular thin films with organization of magnetic clusters with respect to either a magnetoresistive or a magnetoplasmonic response.

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15) **Nontrivial magnetic textures in cylindrical magnetic structures and associated spintronic effects** (C.Ş.I dr. Victor KUNCSER)

Arrays of complex cylindrical nanostructures with tuned geometrical, compositional and magnetic anisotropy parameters will be firstly designed by micromagnetic modeling and then grown by different methods (from electrodeposition to advanced lithography and reactive ion etching process combined with sputtering deposition techniques). The formation of nontrivial magnetic structures related to magnetic domain and domain wall formation is expected by the interplay between the magnetic exchange and different types of magnetic anisotropy energies. A complex morpho-structural and magnetic characterization will be performed. The propagation of the domain walls under different excitations will be investigated in order to be implemented in new spintronic and racetrack elements.

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16) **Designing methodologies for accurate determination of temperature in the closest neighborhood of magnetic nanoparticles in magnetic hyperthermia experiments** (C.Ş.I dr. Victor KUNCSER)

Magnetic relaxation phenomena in systems of magnetic nanoparticles are of topmost importance in magnetic hyperthermia. It is well known the present interest of magnetic hyperthermia in bio-medicine and especially in the localized cancer treatment. Although the main mechanisms involved in the magnetic hyperthermia are known, there are still two main limitations in the real control and monitoring of hyperthermia effects: (i) the presence of magnetic inter-particle interactions and (ii) the way of measuring the released heat in the tissue, based mainly on thermodynamic equilibrium methods. However, a much higher temperature at nanoparticle level is expected through the power transferred from the ac magnetic field to the nanoparticle system as compared to the temperature measured in the fluid media following the heat transfer from nanoparticles to the fluid. Having in mind the critical temperature control required in the localized hyperthermia treatment of malign cells, the knowledge of real temperature at the particles surfaces in contact with the targeted tissue is of crucial importance. While up to now there are no reports on reliable methodologies to provide this information, the present topic intends to overcome this challenging task.

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Direcţia: **Fizică teoretică şi computaţională**

1) **Ecuaţii de stare pentru stele neutronice** (C.Ş.I dr. Adriana RĂDUŢĂ)

Rezumat: Cu mase cuprinse între una şi două mase solare şi raze de ordinul a 10-14 km, stelele neutronice "adăpostesc" forme extreme ale materiei. Modul in care, pe o plajă ce acoperă cca. 15 ordine de mărime, presiunea materiei depinde de densitatea de energie determină majoritatea caracteristicilor

acestor stele şi compoziţia straturilor de diverse adâncimi. Această dependenţă, care poartă numele generic de ecuaţie de stare, este în mare măsură necunoscută, motivul fiind insuficienta cunoaştere a interacţiilor efective între hadroni. Scopul studiilor ce urmează să se desfăşoare este o mai bună înţelegere a proprietăţilor materiei comprimate şi a stelelor neutronice.
Cunoştinţe necesare: matematică, fizică (cuantică, statistică, nucleară), programare
Abilităţi necesare: apetit pentru cunoaştere, creativitate, putere de muncă, spirit critic, disciplină
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2) **Investigarea structurii nucleare pe linia de stabilitate protonică** (C.Ş.I dr. Doru-Sabin DELION)
Rezumat Investigarea nucleelor din zona de stabilitate protonică permite determinarea caracteristicilor câmpului nuclear mediu al nucleelor instabile prin studiul emisiei de protoni şi particule alfa din stările excitate rezultate în urma proceselor de dezintegrare beta plus. Acest fapt va permite determinarea precisă a secţiunilor de captură protonică legate de aşa-numitul "rp-process", care are o importanţă crucială în astrofizica formării elementelor.
În acest sens se vor face studii sistematice referitoare la
- procesele de emisie protonică, biprotonică şi alfa induse de dezintegrarea beta plus,
- constanta axial-vectoare care caractezizează interacţia slabă în această regiune, precum şi
- stările nucleare colective ale nucleelor din zona de stabilitate protonică, folosind metoda aproximaţiilor aleatoare pentru nuclee deformate.
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3) **The study of toroidal moments and supraconductibility in nanosystems and metamaterials** (prof.univ.dr. Iulia GHIU)
Rezumat: Superconductivity, a fascinating phenomenon where certain materials exhibit zero electrical resistance and expel magnetic fields below a critical temperature, has captivated scientists and engineers for over a century. While traditional superconductors required extremely low temperatures,

recent breakthroughs in high-temperature superconductors have ignited renewed interest and opened up exciting new possibilities for practical applications.

Superconductors, as well as other materials, like conductors and dielectrics, may be used in the construction of metamaterials, which are artificially engineered structures with unique electromagnetic properties not found in naturally occurring materials. In recent years, a specific type of metamaterial, those exhibiting toroidal moments, has garnered significant attention due to their intriguing physics and potential applications.

Toroidal moments, distinct from the familiar electric and magnetic dipoles, arise from poloidal currents flowing on the surface of a torus. These moments interact weakly with electromagnetic radiation, making them challenging to detect and manipulate. However, advancements in metamaterial design have enabled the realization of structures with strong toroidal responses, opening a new avenue for research and innovation.

During this project we shall study novel aspects of superconductivity and applications. We shall also investigate the quantum properties of nanostructures with toroidal moments, their mutual interaction, as well their interaction with external fields. We shall investigate the possibility to assemble them into metamaterials and study their properties. The toroidal moments of metamaterials and nanostructures may be directly manipulated by external charge and displacement currents, offering unique opportunities to control them. Furthermore, the absence of external fields makes them energy efficient and robust, being good candidates for memories and qubits.

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4) **Study of fundamental scalar particles in the Standard Model and beyond using rare event signatures with the ATLAS experiment** (C.Ş.I dr. Călin ALEXA)

Description: The candidate will participate to the operation of the ATLAS experiment during the last part of Run 3 (until 2026) and the cleaning and calibration of the recorded data to achieve optimal event reconstruction performances. An assessment of the methods developed for this purpose will then also be made to evaluate their viability in future operations in extreme pile-up conditions (Run 4) and how they can be adapted for that, where necessary. By the end of the Run 3 data-taking in 2026, a record 400 fb-1 dataset of inelastic proton-proton interactions at center-of-mass energies of 13 to 13.6 TeV should meanwhile become available. Following the discovery of the Higgs boson at LHC, this new dataset will allow unprecedented studies of the scalar sector of the physics landscape at the TeV scale, in particular whether other fundamental scalar particles may exist in addition to the observed boson, as would be the case in models of Supersymmetry or involving additional scalar SU(2) multiplets. The candidate will make an important contribution to this search program by analyzing events with rare signatures in the Standard Model, with production cross-sections under the picobarn scale, in the search of deviations with respect to Standard Model predictions in event counts or differential distributions. A strong emphasis will be given to the usage of modern techniques for data analysis and the development

of the corresponding software: columnar analysis, parallelism at every stage, continuous integration, advanced multivariate analysis and deep learning tools.

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5) **Strong gravity regime related research** (C.Ş.I dr. Octavian MICU)

There are four fundamental interactions that govern the Universe from the smallest to its largest scales. Three of the four interactions are quantised and combined together result in the Standard Model (of Particle Physics). The remaining one, a classical theory - as far as we know, is represented by gravity and it becomes comparable in strength with the other forces at Planck energies, approximately sixteen orders of magnitude above the TeV scale, which is the only scale reachable by particle colliders. This is why the gravitational interaction was only tested in the weak-field regime. At these (low) energies the perturbative results of general relativity are very well confirmed. However, during the recent years there are more and more experiments which allow the investigation of the gravitational interaction in stronger fields regimes. The strongest gravitational fields found in nature are in the cores of extremely dense objects. According to general relativity, when black holes form, the cores of these objects ultimately collapse down into a vanishing volume where the density becomes infinite. Such point-like sources for the gravitational field (singularities) are classically unacceptable and the hope is that some quantum effects will resolve this issue. An attempt to find solutions that evade the (most likely) unphysical singularities stemming from general relativity is represented by Bootstrapped Newtonian Gravity.

Proposed doctoral research: The interested student will contribute to further investigating theoretically the strong regime of gravity in a wide range of possible directions.

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6) **Turbulent transport in magnetized fusion plasmas: statistical and machine learning approaches** (prof.univ.dr. Virgil BĂRAN)

The turbulent transport in magnetized fusion plasmas will be characterized with the aid of a numerical code based on the statistical method of test-particles. The results of a large number of simulations will be compiled into a database, on which certain machine learning tools, such as neural networks, will be trained and tested. These tools will be extensively verified against experimental data and used to disentangle the intimate physical processes behind transport.

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7) **Cosmological applications of modified gravity theories** (prof.univ.dr. Virgil BĂRAN)

In the present cosmological context the current expansion of the Universe plays a fundamental role at the large scale structure, affecting the background dynamics and the emergence of complex astrophysical structures. The nature of this phenomenon is unknown, having different theoretical and technological implications in modern physics. Since general relativity theory by itself cannot explain different properties associated with the large-scale dynamics, new gravity theories need to be developed and studied from a theoretical perspective. The main aim of the present thesis is to explore possible theoretical scenarios, confronting the theoretical results with different astrophysical observations. After the experimental validation of the theoretical model, we focus on deducing the Hamiltonian analytical formulation, aiming towards a possible quantized theory of gravity.

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8) **Turbulent transport in magnetized fusion plasmas: statistical and machine learning approaches** (prof.univ.dr. Virgil BĂRAN)

The turbulent transport in magnetized fusion plasmas will be characterized with the aid of a numerical code based on the statistical method of test-particles. The results of a large number of simulations will be compiled into a database, on which certain machine learning tools, such as neural networks, will be trained and tested. These tools will be extensively verified against experimental data and used to disentangle the intimate physical processes behind transport.

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9) **Cosmological applications of modified gravity theories** (prof.univ.dr. Virgil BĂRAN)
In the present cosmological context the current expansion of the Universe plays a fundamental role at the large scale structure, affecting the background dynamics and the emergence of complex astrophysical structures. The nature of this phenomenon is unknown, having different theoretical and technological implications in modern physics. Since general relativity theory by itself cannot explain different properties associated with the large-scale dynamics, new gravity theories need to be developed and studied from a theoretical perspective. The main aim of the present thesis is to explore possible theoretical scenarios, confronting the theoretical results with different astrophysical observations. After the experimental validation of the theoretical model, we focus on deducing the Hamiltonian analytical formulation, aiming towards a possible quantized theory of gravity.
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10) **Machine Learning-Enhanced PIC Simulations for Plasma Physics** (prof.univ.dr. Virgil BĂRAN)
Numerical simulations of laser-plasma interactions are vital for advancing laser wakefield accelerators. We will employ standard Particle-In-Cell (PIC) codes enhanced with machine learning models. The PIC data will train surrogate models, creating efficient digital twins to reduce computational costs. Additionally, we will explore reinforcement learning algorithms to optimize and refine the qualities of the accelerated electron bunches and secondary sources. This integration aims to significantly improve simulation efficiency, offering a faster iteration alternative to classical PIC methods. By leveraging the abundance of data and modern computational power, this technique uses data-driven approaches to accelerate discovery in laser wakefield acceleration dynamics.
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11) **Transport and collective dynamics in nuclear and mesoscopic systems** (prof.univ.dr. Virgil BĂRAN)
We shall construct a microscopic model for the description of the dynamics of several many-body systems in term of coupled equations for one-body and two-body distribution functions and by considering various approximations for three-body distribution function. Through numerical simulations comparative analyses with the cases when the truncation takes place at the level of the two-body distribution function will be performed for various processes, including giant resonances and nuclear fragmentation.
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12) **Classical and quantum chaos in nonlinear systems** (prof.univ.dr. Virgil BĂRAN)
For Hamiltonian systems new features of the classical dynamics and of the corresponding quantum manifestation are explored, both through analytical and numerical methods, with focus on the correspondence between the structure of the classical phase-space and the quantum energy levels statistics. The dissipative systems and discrete maps, showing different routes for the transition to chaos, will be investigated from the perspective of phase transition and critical exponents associated to the quantities characterizing the chaotic dynamics.
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13) **Correlations and dissipation in the seismic networks** (prof.univ.dr. Virgil BĂRAN)
Our goal is to construct statistical and dynamical methods of investigation devoted to the earthquakes produced within several magnitude windows along several decades with the aim to reveal possible links between major events. Comparative studies for several seismic regions, including Vrancea, will be performed by accessing the existing data bases.
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14) **Common misconceptions and teaching approaches of modern concepts in theoretical physics** (prof.univ.dr. Virgil BĂRAN)
The recent advances in physics require a multi-faceted approach when teaching modern theoretical physics topics, such as quantum mechanics, statistical physics, electrodynamics, quantum information or quantum optics. The goal of the current thesis is to investigate the common misconceptions and learning difficulties of the bachelor and master students in the implementation of physics concepts related to theoretical physics disciplines with the aim to propose and test different teaching and remedial approaches. During the doctoral research stage, one will also benefit from the facilities offered by the quantum optics laboratory of the Faculty of Physics from University of Bucharest.
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15) **Nuclear theory calculations for effective weak axial coupling and rare decays** (C.Ş.I dr. Sabin STOICA)

Motivation: The study of weak interaction nuclear processes offers a practical and unique opportunity, for solving problems concerning the foundations of physics [1-2]. The thesis will focus on the study of nuclear beta decay and other weak interaction processes for physics beyond the standard model [1,2]. The research aims to give best-constrained predictions of neutrinoless double beta decay half-lives for candidates that are the focus of most of the state-of-the-art experiments of today. These candidates include neutrinoless double beta decay candidates in the A= 70-140 mass regions. The study of neutrinoless double beta decay includes tackling two major problems: i) the determination of the quenching of gA[3], and modelling concerning nuclear matrix elements [1,4]. The thesis is geared towards systematically tackling these problems. In addition, weak interaction processes can also aid the searches of dark matter, therefore such studies will also be done, an example being ref. [5].

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16) **Selection criteria and consistency conditions in general-relativistic models of classical and quantum cosmology** (C.Ş.I dr. Aurelian ISAR)

General-relativistic models of early-universe cosmology have been traditionally based on single-field theories, which are extremely difficult to generate consistently through model building starting from fundamental theories of nature such as string theory. Multifield cosmological models are much easier to connect to fundamental theories from a theoretical and conceptual perspective. Moreover, recent arguments [1-3] indicate that such theories should be preferred in any consistent theory of quantum gravity.

The current proposal uses a recent approach [4,5], where one uses a consistency condition (realized as a geometric partial differential equation) in order to select for good and acceptable models. The idea of dynamical consistency of models can be extended to higher orders, different model Lagrangeans and field content and "lifted" to the quantum level, where consistency conditions are expected to have important interpretations from the perspective of quantum information theory [6].

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Direcţia: **Optică, spectroscopie, plasmă şi laseri**

1) **Materiale compozite pentru aplicaţii în monitorizarea şi fotodegradarea poluanţilor din apă** (C.Ş.I dr. Mihaela BAIBARAC)
Descriere: Tema de cercetare are în vedere: i) monitorizarea prezenţei poluanţilor organici/anorganici în prezenţa materialelor plasmonice; ii) fotodegradarea poluanţilor organici, de tipul coloranţilor şi compuşilor utilizaţi în domeniul farmaceutic, în prezenţa unor materiale compozite pe bază de TiO_2 şi nanoparticule de carbon de tip nanotuburi de carbon, nanocoarne de carbon şi grafenă; şi iii) dezvoltarea unor membrane bazate pe policlorura de vinil (PVC) şi materiale compozite derivate din PVC pentru procese de filtrare efectuate în vederea eliminării poluanţilor organici/anorganici.
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2) **Plasmonic vortices: simulation, fabrication and applications** (prof.univ.dr. Daniela DRAGOMAN)
Abstract: Plasmonic vortices combine two domains of interest in optical research: optical vortices and surface plasmon polaritons. More precisely, optical vortices [1], i.e., light beams that carry an orbital angular momentum characterized by an integer topological charge, have been extensively studied in the context of communications, quantum computing, data processing, optical manipulation of nanoparticles, enhanced imaging sensitivity, and condensed matter characterization [2]. On the other hand, surface plasmon polaritons [3] are essential in subwavelength integrated optical devices and surface-enhanced spectroscopic techniques, due to the possibility of guiding and amplifying electromagnetic fields at dielectric-metal interfaces. As such, plasmonic vortices [4] are able to localize at subwavelength scale electromagnetic fields carrying optical angular momentum, offering promising perspectives for nanofocusing, increased near-field microscopy resolution, or enhanced light-matter interaction.

The aim of this doctoral grant is to simulate the generation, propagation and decay of plasmonic vortices, studying different methods to control the parameters of these optical beams, as well as to

propose novel applications starting from the recent experimental demonstrations of on-chip interferometers [5] or topological lattices of plasmonic merons based on optical spin-orbit interaction [6]. The fabrication of structures that can generate plasmonic vortices could be also envisaged, including the generation of compound vortices based on spiral nanoslits [7].

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3) **Particule accelerate cu laserul din ținte regenerabile** (C.Ş.I dr. Daniel URSESCU)

Accelerarea de particule cu laserul a fost investigată în ultimele decenii în vederea utilizării lor în aplicaţii. Principala lor proprietate complementară cu acceleratorii convenţionali este durata semnificativ mai scurtă a pachetului de particule încărcate electric. Proprietăţile au fost demonstrate în diferite experimente, cele mai multe operate cu doar câteva pulsuri pe oră. Unul din aspectele la care se lucrează în prezent este creşterea ratei de repetiţie atunci când aceste particule sunt produse. Deși sistemele laser sunt operate la rate de repetiție de la 1 puls pe minut la 10 Hz sau chiar 1 kHz, țintele solide folosite nu pot fi schimbate în același ritm susținut. De aceea, în ultimii ani se încearcă utilizarea de ținte regenerabile, de tip lichid pentru a creşte rata de producție de particule accelerate.

În această teză, vor fi investigate metode de producere şi caracterizare a unor ţinte lichide în vid şi interacţia pulsurilor laser cu astfel de ținte, pentru o mai bună înțelegere a limitărilor metodei şi pentru a optimiza sau a propune mecanisme de interacţie.

În acest sens, lucrarea va avea o componentă teoretică / de simulări şi una de dezvoltare experimentală pentru producerea de ioni şi controlul divergenţei acestora după ținta lichida. În partea teoretică, vor fi studiate diferite metode de reducere a divergenţei fascicolelor de protoni produse cu laserul, pornind de la folosirea unei micro-lentile tranziente pentru ioni [1], a unei spire [2] sau a unor fascicule de lumină structurate, de tip helicoidal [3]. Pe partea experimentală, va fi îmbunătățit un aranjament experimental existent în laboratorul de optică de la ELI-NP, ce conține microjeturi de apă în vid înalt (10^{-3} mbar) şi mai multe sisteme laser cu pulsuri de ns, ps sau fs, şi ulterior vor fi studiate diverse configurații pentru realizarea de pachete de protoni accelerați cu laserul cu proprietăţi îmbunătățite, folosind pulsuri ultrascurte complexe. În măsura posibilităților, studentul va participa la campanii la sistemul HPLS de la ELI-NP sau la alte facilități de cercetare.

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4) **Tomografia câmpului electromagnetic în focus pentru pulsuri ultrascurte şi ultraintense** (C.Ş.I dr. Daniel URSESCU)

Calificarea adecvată a distribuției intensității pulsurilor ultrascurte în planul focal necesită tehnici de metrologie specifice. Mai multe abordări au fost propuse pentru a obține informații despre intensitatea

maximă în focalizare [1], inclusiv ionizarea ionilor grei [2, 3], împrăștierea Compton [4] și accelerarea particulelor încărcate prin forțele ponderomotive și efectele acestora [5, 6, 7].
Cu toate acestea, pe lângă intensitatea maximă a impulsurilor, cunoașterea distribuției intensității lor în focalizare la putere maximă este esențială, mai ales pentru impulsurile care nu sunt perfect (super)gaussiene în spațiu și timp. Vom denumi acestea cu termenul pulsuri complexe (PC). Această categorie include impulsuri cu cuplaje spațio-temporale (STC), impulsuri cu front de undă elicoidal (HWP), impulsuri auto-modulate spectral (SMP) sau impulsuri multiple (MP).

Abordarea bazată pe forțele ponderomotive ar putea, în principiu, să ofere informații suplimentare legate de structura impulsurilor, așa cum este recunoscut și, din păcate, neexaminat, în rezultatele experimentale preliminare raportate [7].

În această teză, vor fi investigate metode de caracterizare de PC focalizate în vid, folosind o abordare mixtă teoretică şi experimentală.

În acest sens, lucrarea va avea o componentă teoretică / de simulări pentru propagarea pulsurilor ultrascurte în zona focala, în prezenţa unui sistem de obscurare cu dimensiuni comparabile cu dimensiunea petei focale sau a unuia care introduce modulaţii controlate în profilul colimat al fasciculului laser.

Pe partea de dezvoltare experimentală se vor efectua măsurători cu astfel de sisteme de obscurare. Pentru aceasta va fi folosit sistemul laser AVESTA existent în laboratorul de optică de la ELI-NP, şi instrumente aferente parte din acelaşi laborator. Partea de analiză a datelor se va orienta pe reconstrucţia unor detalii ale pulsului obţinute ca urmare a obscurării acestuia cu obiecte la poziţii diferite. În măsura posibilităților, studentul va participa la campanii la sistemul HPLS de la ELI-NP sau la alte facilități de cercetare.

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5) **Nanocomposite layers for microorganisms' decomposition by light-induced oxidation processes**
(C.Ş.I dr. Enikö GYÖRGY)

The objective of the thesis is the synthesis by laser techniques of hybrid photocatalysts composed of nano-carbon materials, heteroatom doped graphene and carbon nanotubes, and transition metal oxides. The morphology, composition, and structure down to the nanometer scale of the photocatalysts will be investigated by surface diagnostic techniques. Charge carrier generation under UV and visible light irradiation will be investigated by photocurrent measurements at the nanoscale through conducting AFM and photoelectrochemical measurements. The degradation of microorganisms will be monitorised by UV-visible spectroscopy. The final objective of the thesis is the production of nanocomposite layers with high photoactivity under both UV and visible light irradiation, ensuring relevant photocatalytic decomposition efficiency for the degradation of microorganisms in wastewater under simulated sun irradiation conditions.

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6) **Comparative studies on the liquid droplets coalescence at room temperature, in microgravity** (C.Ş.I dr. Mihail-Lucian PASCU)

Numerous challenging physical problems and technological processes are significantly influenced by gravity. A microgravity environment allows to study physical phenomena not hidden by the gravity forces. This is why microgravity or partial gravity research using parabolic flights, drop towers, sounding rockets or International Space Station conditions is attractive in basic science and technological explorations. The objectives of the PhD are the experimental data collection and interpretation of the liquids' coalescence in microgravity with comparation to 1g conditions, based on optical imaging techniques. This is part of an European Space Agency project recorded as DROPCOAL and its continuations, which are dedicated to the study of the coalescence of larger, "perfectly" spherical droplets of water and water solutions of Ethanol and Methylene Blue at 10-6g and in pendant positions. The main specific objectives of the thesis within are: (i) contributions at investigation in microgravity conditions of the coalescence of two pendant droplets in gaseous atmosphere containing two by two different liquids as mentioned above using: different drop sizes and variable droplet velocities and relative velocities (kinetic and geometric parameters of the collision); (ii) characterization of the conditions leading to different outcomes of binary droplets interactions, like rebound, coalescence, reflexive and elongating separation; (iii) development of theoretical and computational models for the main parameters that describe the drop coalescence under these conditions.

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Direcţia: **Fizică educaţională**

1) **Strategii didactice pentru predarea unor noţiuni cu implicare în dezvoltarea curricumului naţional la Fizică. Studiu de caz: Predarea surselor de energie neconvenţionale** (prof.univ.dr. Ştefan ANTOHE)
Ţinând seama de impactul existenţei Direcţiei de studiu ,,Fizică Educaţională" în cadrul Şcolii Doctorale de Fizică (ŞDF), la Universitatea din Bucureşti, direcţie unică la nivel naţional, demonstrat de peste 50 de profesori din învăţământul preuniversitar care au obţinut Titlul de Doctor în Fizică, şi expertiza Conducătorilor de doctorat din cadrul ŞDF, obiectivul temei propuse va fi elaborarea unui curs având ca tematică Noi surse de energie regenerabilă cu accent pe Conversia directă a energiei solare în energie electrică prin efect fotovoltaic.
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2) **Abordări comparative privind necesitatea predării coerente a Fizicii și Astrofizicii la nivel preuniversitar în Uniunea Europeană** (prof.univ.dr. Alexandru JIPA)
Studii recente derulate pe teritoriul statelor membre ale Uniunii Europene, dar și în Statele Unite ale Americii indică evoluții negative în privința ponderii pe care o au disciplinele subsumate domeniului ŞTIM (Științe, Tehnologii, Inginerie și Matematică)/STEM (Sciences, Technologies, Engineering, Mathematics), conținuturilor programelor și corelarea noțiunilor predate. Prea dese modificări în organizare, derulare și structura anului școlar afectează performanțele școlare, parcursuri academice posibile ale elevilor,

precum și corecta acoperire a cerințelor pe piața muncii, în domenii vitale, inclusiv în Medicină, mai ales în specializările complexe.

Chiar dacă tendința a fost observată și s-au încercat unele măsuri comune la nivelul Uniunii Europe (de exemplu, manifestările din 2013, 2020 ș.m.a.), măsurile în domeniu sunt semnificativ afectate de tendințe agresive actuale din Științele educație și din Științe politice.

Deși aparențele ar putea indica contrariul – argumentul de bază fiind legat de premiile obținute de elevi din România la diverse concursuri internaționale din domeniu – realitatea, la nivel național, este mult diferită. Aspecte similare se observă și în alte țări din Uniunea Europeană.

Tema propusă va permite o analiză a măsurilor necesare, educaționale, organizatorice și chiar financiare, pentru a se asigura coerența predării Fizicii, cu deosebire a Fizicii moderne – absentă în bună măsură din programele minimale, dar și din subiectele de la bacalaureat, cu deschiderea spre un subdomeniu de mare importanță științifică, și anume: Astrofizica. Teza de doctorat va trebui să semnaleze, pe baza investigațiilor făcute, declinul disciplinelor și efectele negative asupra progresului științific și tehnologic, precum și asupra echilibrului economic-social. Se va avea în vedere necesitatea unor programe clare și coerente, în acord cu dezvoltarea Științelor, susținerilor reciproce, stabilirea de teme comune de interes ș.a.

Discutarea situației la nivel național se va face și prin compararea cu situația din țările Uniunii Europene, cu luarea în considerare a tendințelor comune, a corelațiilor existente, cu raportare la fonduri și tradiții. Vor fi propuse îmbunătățiri pentru infrastructură și instrumentele specifice educației științifice în școli și cluburi ale elevilor, precum și pentru formarea inițială și continuă a formatorilor în domeniile de interes, inclusiv prin acordarea de burse, premii, prezență în mijloace de comunicare în masă și alte forme de sprijin pentru elevi, studenți, profesori și cercetători cu preocupări în domeniu.

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3) **Exploring and implementing new and engaging ways for teachingclassical mechanics concepts by employing modern technology and interactive methods** (prof.univ.dr. Valentin BARNA)

The subject aims at tackling new methods for describing and analyzing mechanics experiments, while making them attractive for students at high-school and faculty level. A series of interesting software/programs will be implemented for data acquisition, data analysis as well as elaborating 2D/3D virtual simulations. The proposed approach allows the candidate to employ the hi-tech skills and use of tools specific to new technologies in the didactic and research activity and to further advance such skills towards students, ensuring the innovative nature of learning. The aptitudes to manipulate new technologies anchor the instructional-educational process in the realities of our days and make it extremely attractive for students. The worth of these strategies is already confirmed by the value of the obtained results: rich and accurate data acquisition and straight-forward investigations, fast and efficient processing methods, very good overall disseminated results, the possibility to adapt these methods also for online classes, the excellent quality of observations and conclusions. The creation of a positive attitude towards the implementation of such methods leads additionally to the increase of satisfaction obtained as a result of the proposed activities. One of the main tangible consequences towards the educational process is that the student becomes responsible for his own learning process, with the

teacher having the role of facilitator. Thus, students can better build their own hypotheses, research and investigate to verify them, evaluate the research process looking for methods of improvement. By exploring the integration of these novel technology tools, alongside augmented reality and virtual reality, we shall definitely contribute to the advancement of the physics education field.

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4) **Special STEM methods for the design and improvement of physics experiments while incorporating modern advancements and ensuring alignment with educational goals** (prof.univ.dr. Valentin BARNA)

It is known that one of the biggest challenges for decision-makers in the education system is how the skills that the school forms fit with their social needs. As a result, the efforts regarding the development of a positive attitude regarding the adoption of STEM teaching methods by teachers, along with stimulating their desire to explore and discover new notions and didactic methods, to experience new things, are not insignificant. It is clear that the teacher's attitude towards the act of teaching and towards that approach has a crucial influence on how students will look at the concepts studied and even how they will later approach solving problems in everyday life. This theory is based on five basic principles: inspiring motivation, cognitive conflict, self-development, self-evaluation and consolidation of retention and transfer capacity. With the proposed study we target at several specific intentions: Developing new digitalized approaches to investigate and then explain physics phenomena via experimental methods as well as implementing simulations or virtual laboratories to improve students' comprehension of complicated physics concepts; Incorporate inquiry-based learning (IBL) strategies into physics instruction and assess their efficacy in enabling students to autonomously investigate and discover topics; Evaluate the common physics misunderstandings and enable teaching ways to confront and dismiss them; Create and examine advanced evaluation techniques that accurately test students' comprehension of physics ideas; Provide tools or initiatives to support physics instructors in their continued professional development and keep them up to date on best practices. Furthermore, all these proposed physics education aspects should definitely provide for students a better understanding of the analyzed physics phenomena.

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