



IRAP - Fostering Excellence and Innovation

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ABSTRACT BOOK





Number: **1**

Title: **Neural Network Interatomic Potentials For Nanomechanics Applications: Nanoindentation of body-centered cubic Molybdenum**

Project leader: **Stefanos Papanikolaou**

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IRAP project: **NOMATEN**

Group name: **Materials Structure, Informatics and Function**

Accurate characterization of materials through computational nano-mechanical tests on a large scale requires precise interatomic potentials to predict the energies and forces of atoms at the quantum mechanical level. In this study, we aim to develop robust Neural Network Interatomic Potentials (NNIP) tailored for the molecular dynamics (MD) nanoindentation simulations of single element crystalline body-centered cubic (BCC) metals. We focus on molybdenum (Mo), a promising material for applications in extreme environments at elevated temperature. Nanoindentation simulations with three existing potentials [an embedded atom method (EAM) potential, a gaussian approximation potential (GAP), and a tabulated GAP (tabGAP) potential] predict different dislocation nucleation mechanisms, and are hampered by the absence of essential information on the shear stress at the sample's surface in the elastic region. To address such deficiencies, we employed a similarity measurement protocol to assess the dataset of the GAP potential, identifying the specific missing configurations to capture the behavior of the indented sample. Crucial among those are, first, the generalized stacking fault (GSF) configurations featuring a dumbbell interstitial on the surface to cover dislocation cores, and second, high-temperature configurations incorporating a frozen layer of atoms to simulate the contact of the indenter tip with the sample. The modifications made to the dataset produce a NNIP with favourable results regarding the dislocation nucleation mechanisms, realistic generalized stacking fault energy (GSFE) curves, and an informative energy landscape for the atoms on the surface of the sample during the nanoindentation. All these features contribute to the reliability of our NNIP for realistic simulations of nano-indentation and the study of nano-mechanics.



Number: 2

Title: **Cocaine and sugar processing by the mouse brain**

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IRAP project: **BRAINCITY – Centre of Excellence for Neural Plasticity and Brain Disorders**

Group name: **Laboratory of Neuronal Plasticity**

Sweet food is highly desirable for animals as it typically contains calories necessary for survival. Its consumption triggers pleasant feelings, making sweet food a reward for them. Addictive substances such as cocaine also induce positive experiences, but their effects primarily rely on their pharmacological properties. Nevertheless, it is believed that they are processed by similar brain circuitry as tasty food. In the current study, we investigated the effects of initial and prolonged exposure to addictive and natural substances on the entire mouse brain. To address this question, we employed a single-cell whole-brain imaging approach to identify patterns of activation following acute and prolonged exposure to natural and addictive rewards. Cocaine intraperitoneal injections served as our model for addictive rewards, while sucrose self-administration mimicked the natural reward. After the behavioral training, we immunohistochemically labeled c-Fos protein, a widely used marker of neuronal activation. Using microscopy, we captured images of these samples and created a brain map highlighting specific c-Fos-positive neurons associated with these rewards. We found that both cocaine and sweet water exposure led to rapid excitation of distant parts of the brain. Particularly strong activation was observed in structures within the reward system, such as the nucleus accumbens and the amygdala complex. Furthermore, we identified structures selectively activated by addictive rewards (e.g., the visual cortex) and natural ones (e.g., the olfactory system). This comprehensive mapping of c-Fos expression enabled us to establish a general pattern of brain activation following both natural and addictive treatments. Through functional connectivity analysis, we uncovered alterations in the brain's modularity following exposure to these rewards. This modularity remained stable during prolonged sucrose intake but not during cocaine consumption.



Number: 3

Title: **Gravitational anomaly in NdAlSi**

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IRAP project: **MagTop – International Centre for Interfacing Magnetism and Superconductivity with Topological Matter**

Group name: **Weyl Group (ON6.6.6)**

Quantum anomalies are the breakdowns of classical conservation laws that occur in quantum-field theory description of a physical system. They appear in relativistic field theories of chiral fermions and are expected to lead to anomalous transport properties in Weyl semimetals. This includes a chiral anomaly, which is a violation of the chiral current conservation that takes place when a Weyl semimetal is subjected to parallel electric and magnetic fields. A charge pumping between Weyl points of opposite chirality causes the chiral magnetic effect that has been extensively studied with electrical transport. On the other hand, if the thermal gradient, instead of the electrical field, is applied along the magnetic field, then as a consequence of the gravitational (also called the thermal chiral) anomaly an energy pumping occurs within a pair of Weyl cones. As a result, this is expected to generate anomalous heat current contributing to the thermal conductivity. We report an increase of both the magneto-electric and magneto-thermal conductivities in semi-classical regime of the magnetic Weyl semimetal NdAlSi. We also show that the anomalous electric and heat currents, which occur due to the chiral magnetic effect and gravitational anomalies respectively, are still linked by a 170 years old relation called the Wiedemann-Franz law.



Number: 4

Title: **Balancing the Push–Pull Effect on the Synthesis and Fluorescent Properties of New ESIPT Dyes for Thin Film Applications**

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IRAP project: **ICRI-BioM – International Centre for Research on Innovative Biobased Materials**

Group name: **Nanomaterial group - junior group**

The development of functional materials exploiting excited-state intramolecular proton transfer (ESIPT) requires a deep understanding of the push–pull balance on their reactivity, emission mechanism, and response to the surrounding environment. In this study, we focused on the model 2-(2-hydroxyphenyl)benzothiazole (HBT) core, and we have developed a simplified synthetic pathway to obtain two new ESIPT dyes with amide groups at the para or meta positions of the phenolic ring. We studied the impact of the geometry of the push–pull system for the two HBT isomers, unraveling that it strongly influenced their reactivity patterns and fluorescence emission. The ESIPT emission of the new molecules in the solution was affected by the solvent polarity, transitioning from pure keto to pure enol emission as the solvent polarity was increased. In the spin-coated films, the intermolecular interactions generated by the push–pull balance and the molecular shape of the deposited materials were also found to be essential for defining their morphology and the related emissive properties. Furthermore, these features were tuned by applying thermal annealing or by changing the solvent used for thin film deposition. The combination of both strategies was employed to provide a more favorable molecular ordering and to increase the fluorescence quantum yield of the neat films by 150%.



Number: 5

Title: **Machine learning classification of mental disorders from resting state EEG - a preliminary study**

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IRAP project: **BRAINCITY – Centre of Excellence for Neural Plasticity and Brain Disorders**

Group name: **Laboratory of Neurophysiology of Mind**

Presently, diagnosis of mental disorders is based on subjective methods, like self-reported behavioral symptoms. In the search of objective, biophysical indicators for psychological disorders, machine learning (ML) classification based on electroencephalography (EEG) data was suggested in the current literature. This approach is very promising, reported accuracies fall in the range of 75-95%. However, current studies focus mainly on comparing people suffering from single disorder with healthy controls, while in reality, psychiatric diagnosis is a multicategorical choice. Moreover, these results were obtained on small sample sizes, which poses a danger of overfitting. From the psychiatric hospital's archival database, we obtained about 14000 resting-state EEG signals of psychiatric patients diagnosed with a wide range of disorders, which enables training of multicategorical choice algorithms on sufficient sample. In this poster, I present results of a preliminary experiment on this data. As the EEG signal is complex and irregular, one of the most important steps in its analysis is feature extraction and selection. We tested the importance of different EEG features in distinguishing between different groups of disorders and tested performance of different state-of-art classification algorithms, using selected feature set. We plan to develop a multicategorical classifier, and train it on this data. Results from this preliminary experiment could serve as a baseline for evaluation of multicategorical classification algorithms, as the literature about ML classification between different disorders is scarce.



Number: 6

Title: **Dissipative evolution of quantum Gaussian states**

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IRAP project: **ICTQT – International Centre for Theory of Quantum Technologies**

Group name: **Quantum Open Systems in Relation to Quantum Optics Group**

Recent works on quantum resource theories of non-Gaussianity, which are based upon the type of tools available in contemporary experimental settings, put Gaussian states and their convex combinations on equal footing. Motivated by this, in this article, we derive a model of dissipative time evolution based on unitary Lindblad operators. While it does not preserve the set of Gaussian states, it preserves the set of their convex combinations, i.e. so-called quantum Gaussian states. As we demonstrate, the considered evolution proves useful both as a description for random scattering and as a tool in dissipator engineering.



Number: 7

Title: **Quantized Spin Pumping in Topological Ferromagnetic-Superconducting Nanowires**

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IRAP project: **MagTop – International Centre for Interfacing Magnetism and Superconductivity with Topological Matter**

Group name: **Dirac Group (ON6.4)**

Semiconducting nanowires with strong spin-orbit coupling in the presence of induced superconductivity and ferromagnetism can support Majorana zero modes. We study the pumping due to the precession of the magnetization in single-subband nanowires and show that spin pumping is robustly quantized when the hybrid nanowire is in the topologically nontrivial phase, whereas charge pumping is not quantized. Moreover, there exists one-to-one correspondence between the quantized conductance, entropy change and spin pumping in long topologically nontrivial nanowires but these observables are uncorrelated in the case of accidental zero-energy Andreev bound states in the trivial phase. Thus, we conclude that observation of correlated and quantized peaks in the conductance, entropy change and spin pumping would provide strong evidence of Majorana zero modes, and we elaborate how topological Majorana zero modes can be distinguished from quasi-Majorana modes potentially created by a smooth tunnel barrier at the lead-nanowire interface. Finally, we discuss peculiar interference effects affecting the spin pumping in short nanowires at very low energies.



Number: 8

Title: **Bridging the Gap from Materials Modeling to Experiments: Simulating Multicomponent Solid Solution Alloys and Metallic Glasses**

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IRAP project: **NOMATEN**

Group name: **Complexity in Functional Materials**

We utilize molecular dynamics (MD) simulations to investigate strengthening mechanisms in high-entropy alloys (HEAs). Our study is focused on the plastic deformation by dislocation dynamics, during nanoindentation test, and the development of a novel approach for glass formation via a hybrid Monte Carlo and MD approach. We identify distinctive plasticity mechanisms leading to exceptional strength, characterized by stacking fault widths and notable dislocation roughness, and the impact of chemical disorder on strengthening. Our findings propose an innovative strategy for enhancing the strength of multicomponent random solid solution alloys (RSS) through the manipulation of stacking fault width and element-based chemical disorder, represented as a hardening factor. Additionally, we delve into the study of metallic glass systems by enabling the generation of equilibrated samples at temperatures below the conventional glass transition achievable through conventional methods. Utilizing realistic interatomic potentials, we investigate the kinetics, thermodynamics, and rheological behavior of metallic glasses within the ultrastable glass regime. Our results shed light on the temperature-dependent configurational entropy, opening avenues for theoretical studies of complex metallic glasses and their comparison with experimental observations. Furthermore, our research delves into the plasticity mechanisms of RSS alloys during nanoindentation tests. We conduct a comprehensive analysis of dynamic deformation processes, defect nucleation and evolution, stress-strain behavior, and surface morphology mapping, facilitating comparisons with experimental data and electron microscopy images. We observe that RSS alloys exhibit localized lattice strain and distortion, augmenting material resistance to deformation and impeding dislocation mobility. Remarkably, equiatomic RSS alloys display a notable suppression of the plastic zone size, hinting at an optimal hardening response. This work offers a promising pathway for MD-based material design in complex, multi-component alloys, tailored to engineer novel materials suited for extreme operating conditions.



Number: 9

Title: **Functional Polymers and Materials for a Sustainable Future**

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IRAP project: **ICRI-BioM – International Centre for Research on Innovative Biobased Materials**

Group name: **Biomaterial group - senior group**

The research conducted by the Polymers and Biomaterials (PolyBioMat) group focused on sustainable waste valorisation to address environmental pollution, infectious diseases, greenhouse gas emissions, and energy crises. One significant area of interest involves the exploration of Brewer's spent grain (BSG) for various applications; A multi-product biorefinery process was established to extract different biomaterials (including protein, lignin, hemicellulose, and nanocellulose) from BSG. These compounds were then employed in creating nanocomposite films, exhibiting promising characteristics such as bioactivity, mechanical strength, and barrier properties as alternatives to conventional plastics. The synthesis of graphene quantum dots (GQDs) and reduced graphene oxide (rGO) from BSG is another important topic of interest. BSG-derived GQDs with ZnO nanoparticles showed antibacterial efficacy against the Methicillin-resistant *Staphylococcus aureus* (MRSA) isolated from actual wound specimens. Furthermore, rGO is integrated into alginate-based hydrogels for addressing infectious in the field of bone tissue engineering. In the domain of dental pulp infection treatment, injectable hydrogels composed of chitosan and liposomes loaded with curcumin and α -tocopherol were developed. Curcumin and α -tocopherol exhibited antioxidant, antibacterial, and anti-inflammatory properties. The hydrogels demonstrated potential in terms of rheological properties, thermal stability, biodegradability, and biocompatibility, making them suitable for regenerative dentistry. Another ongoing research activity involves the valorisation of agricultural wastes for the fabrication of 2D materials (including rGO, MXene, metal-organic frameworks, and GQDs), and bioderived polymers (including chitosan, PHA, etc). These 2D materials and biopolymers will be used for various biomedical applications including tissues engineering, regenerative medicine, and biosensors. Overall, the findings of the PolyBioMat group contribute significantly to fostering a more sustainable and inclusive healthcare system, promoting green production, advancing circular bioeconomy practices, and enhancing waste management strategies.



Number: **10**

Title: **Spin Pumping and Inverse Spin Hall Effect in Pb_{1-x}Sn_xSe/Ni₈₁Fe₁₉, Ni₈₁Fe₁₉/Pt and SnTe/Ni₈₁Fe₁₉ Bilayer Thin Films**

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IRAP project: **MagTop – International Centre for Interfacing Magnetism and Superconductivity with Topological Matter**

Group name: **Group of Characterization and Processing (ON6.3)**

Spin Pumping and Inverse Spin Hall Effect in Pb_{1-x}Sn_xSe/Ni₈₁Fe₁₉, Ni₈₁Fe₁₉/Pt and SnTe/Ni₈₁Fe₁₉ Bilayer Thin Films

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In the realm of magnonic devices [1], a critical component lies in the detection of magnon signals and their conversion into electrical signals. One particularly effective method for achieving this is through spin pumping [2], leveraging the inverse spin Hall effect (ISHE) phenomena. Topological materials, with their pronounced spin-orbit coupling and spin-polarized surface states [3], stand out as prime candidates for generating pure spin currents. Notably, topological crystalline insulators (TCI) like SnTe [4] and Pb_{1-x}Sn_xSe [5] possess surface states protected by crystalline symmetry, making them intriguing for spin pumping applications. Nevertheless, spin pumping in these TCIs remains relatively unexplored. Moreover, investigating low-temperature (< 20 K) spin pumping in TCIs has become imperative in superconductor spintronics [6]. We present broadband spin pumping and ISHE experiments conducted on Ni₈₁Fe₁₉/Pt, Pb_{1-x}Sn_xSe/Ni₈₁Fe₁₉, and SnTe/ Ni₈₁Fe₁₉ systems in a temperature range of 300-4 K and frequency range of 2–12 GHz. We observed systematic shifts in ferromagnetic resonance fields, amplitude variations, and linewidth changes as functions of frequency and temperature. Notably, we find that spin mixing conductance and spin hall angle values exhibit pronounced temperature dependencies. These findings hold significant implications for the utilization of TCIs as spin sink layers in the realms of magnonics and superconducting spintronics applications. References: [1] A. V. Chumak, et al., Nat. phys. 11, 453 (2015). [2] Y. Tserkovnyak, et al., PRL 88, 117601 (2002). [3] M. Jamali et al., Nano Lett., 15 7126 (2015). [4] A. Sulich et al., J. Mater. Chem. C 10 3139 (2022). [5] A. Kazakov et al., PRB 103, 245307 (2021). [6] K. Jeon, et al., Nat. Mater. 17, 499 (2018). We acknowledge support from the Foundation for Polish Science through the IRA Programme financed by EU within SG OP Programme and National Science Center in Poland under the grant number UMO-2020/38/E/ST3/00578.



Number: **11**

Title: **MMP-9 mediates behavioral alterations following bacteria-like inflammation in early life**

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IRAP project: **BRAINCITY – Centre of Excellence for Neural Plasticity and Brain Disorders**

Group name: **Laboratory of Neurobiology**

Various external challenges (e.g., inflammation) during key stages of the nervous system development may contribute to such neurodevelopmental disorders (NDDs) as Autism Spectrum Disorders, ADHD, or schizophrenia. The NDDs tend to last throughout patient's lifetime and may affect different behavioral domains, including emotions, memory, and sociability. Herein, we have investigated the role of matrix metalloproteinase-9 (MMP-9) an extracellular protease-a key player in plasticity, in this process. We decided to focus on the significant period of neurodevelopment – exuberant synaptogenesis, which occurs around postnatal day 7 in mice. During this key stage, we challenged the immune system of C57/BL6 mice with either a single injection of lipopolysaccharide (LPS, 0.05 mg/kg, i.p.) to mimic bacterial infection or physiological saline as a control. Two hours and after the administration serum levels of TNF- α , IL-6, IFN- γ , CCL-5, IL-10, and TIMP-1 were elevated in both sexes in comparison to saline-treated control, as shown with Luminex[®] immunoassay. Additionally, in males (and not females) elevated levels of MMP-9 were observed in serum and the cerebral cortex, as shown also with gel zymography approach. To further study the role of MMP-9 we conducted a behavioral assessment of adult wild-type animals (MMP-9 WT) and their littermates lacking MMP-9 (MMP-9 KO) after LPS injection in P7. WT males after the immune challenge were less interested in a social odor from unknown animals, while females were more interested in the unknown social object. Interestingly, this effect was not observed in MMP-9 KO animals. In aggregate, the presented results suggest, that MMP-9 is involved in behavioral deficits after immune activation during the critical stage of neurodevelopment. The exact molecular mechanism needs further investigation.



Number: **12**

Title: **Development of novel porous materials and application for energy storage**

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IRAP project: **ENSEMBLE3 – Centre of Excellence for nanophotonics, advanced Materials and novel crystal growth-Based technologies**

Group name: **Functional Material Technology**

Our group at Ensemble3 is responsible for the development of porous organic materials as covalent organic frameworks (COFs) in the direction of energy storage applications over the world. COF is a type of porous crystalline material whose ease of preparation, functionality, and modularity make it a powerful platform for the development of molecular devices in many (bio)engineering fields, including energy storage such as battery and fuel cell. Recently, we are developing (I) novel ionic COFs for fuel cell applications, (II) 2D charge-transfer (CT) complexed assembly of 1D oligo(squaraine-co-pyrene) with tetracyanoquinodimethane (TCNQ) for semiconductor application, and (III) porous graphite oxide from the heating treatment of polyimide-COFs for battery application. These results to date are presented separately below: (I) Novel ionic COFs were synthesized by two methods; one is that pyridine, quinoline, or triazole groups on the pore wall or frame of COFs were produced as salt, and other is that synthesis of novel salt-building block and the salt-linked COFs were prepared. As the result, their BET surface areas are from 300 to 2000 m²/g, pore sizes are mesopores, their proton conductivities are more than 10⁻³ S/cm at 130 °C under unhumidified condition. (II) 1D oligo(squaraine-co-pyrene) were synthesized from the condensation reaction of squaric acid and diaminopyrene in the presence of TCNQ. The obtained oligomer was self-assembly organized. The aggregation structures were changed by the feed ratio of TCNQ relative to the pyrene moieties in preparing oligomers. As a result, the obtained oligomers have BET surface area and pore size (>300 m²/g and mesopores), electron-conductivity is more than 10⁻³ S/cm at room temperature, which is highest as compared with recently reported that of pyrene-TCNQ complex (10⁻¹²) at room temperature. (III) According to ref.3, polyimide-linked COFs were synthesized, and their pellet were heated at 1400 °C for 20 h. As a result, the obtained mesoporous graphite oxide was highest conductivity (100 S/cm) as compared with that of commercial graphite oxide (10⁻³ S/cm). 1. Nagai, A. "Covalent Organic Frameworks" Pan Stanford Publishing, published this book in 2020 (ISBN: 978-981-4800-87-7). 2. Nagai, A. et al. Angew. Chem. Int. Ed. 2012, 51, 2612, Angew. Chem. Int. Ed. 2013, 52, 2017, J. Am. Chem. Sci. 2013, 135, 546. 3. Nagai, A. et al. Chemistry of Materials, 2021, 33, 818.



Number: **13**

Title: **Description of topological and altermagnetic systems via first-principle modeling**

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IRAP project: **MagTop – International Centre for Interfacing Magnetism and Superconductivity with Topological Matter**

Group name: **Group of Physics of Majoranas (ON6.5)**

Using first-principle modeling, we investigate the k-space topology for bulk, 2D systems, interfaces, nanowires and curved systems. The k-space topology appears in the presence of band inversion, with the wave functions of the conduction and valence having opposite parity. As a result, surface states with Dirac points and new properties rise in topological compounds. Recently, we discovered that the BCS superconductors Nb₃Ge and Nb₃Sn show Dirac surface states [1]. Among the topological insulators, we have the Z₂ insulator with band inversion at the Γ point protected by time-reversal symmetry, the topological crystalline insulator where the band inversion is protected by the combination of time-reversal and crystal symmetry, and the Quantum spin Hall phase where the conductance is quantized to a value of $2e^2/h$. Among the topological semimetals, we have studied semimetals with semiDirac points protected by non-symmorphic symmetries[2,3], Weyl and Dirac semimetals. When we break the time-reversal symmetry, other topological phases can take place as the Quantum anomalous Hall effect and the axion insulator where the conductance is half-quantized on both surfaces[4]. We have engineered new topological phases as the flat band in curved Weyl semimetal[5]. We have predicted QSH phases in new materials [6]. We have investigated how to tune other physical properties as the sign of the Anomalous Hall effect [7]. Finally, we investigated the recent form of magnetism named „altermagnetism” [8]and we are going towards the study of the interplay between k-space topology and altermagnetism [9]. [1] R. M. Sattigeri, G. Cuono, G. Hussain et al, and C. Autieri (in manuscript, 2023). [2] Physical Review Materials 3 (9), 095004 (2019). [3] npj Quantum Materials 6 (1), 1-7 (2021). [4] Phys. Rev. B 107, 125102 (2023) [5] Physical Review X 11 (3), 031017 (2021). [6] Adv. Electron. Mater. 9, 2300156 (2023); Phys. Rev. B 106, 245149 (2022). [7] Physical Review Letters 127 (12), 127202 (2021); Phys. Rev. B 107, 085102 (2023). [8] J. Magn. Magn. Mat. 586, 171163, (2023);arXiv:2308.08416 accepted in Phys. Rev. B. (2023). [9] Phys. Rev. B 108, 075150 (2023); R. M. Sattigeri, G. Cuono, C. Autieri, arXiv:2307.10146 (2023).



Number: **14**

Title: **Prelude to Malignancy: A Gene Expression Signature in Normal Mammary Gland from Breast Cancer Patients Suggests Pre-tumorous Alterations and Is Associated with Adverse Outcomes**

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IRAP project: **LM 3P**

Group name: **Research Group: Mosaicism for autosomal post-zygotic mutation**

Breast cancer recurrence and mortality continue to pose a substantial health challenge, despite advances in early detection and treatment strategies. Decisions regarding therapeutic management primarily rely on the examination of the primary tumor and the surrounding normal mammary gland excised during surgery, however, the portion of the breast surrounding the tumor that usually stays intact, holds promise of prognostic value. Nonetheless, a comprehensive understanding of the gene expression profiles in these tissues and their relationship to patient outcomes is lacking. We examined the transcriptomic profiles of 242 samples of breast tumors, and paired uninvolved mammary gland samples, collected at both distal (1.5-5 cm) and proximal (UMP, at least 1 cm and always in a shorter distance than corresponding UMD) locations from the primary lesions of 83 patients with unfavorable outcomes. Control mammary gland samples from 53 plastic surgery individuals without a history of cancer were also included. Gene expression profiling was conducted using a custom panel of 634 genes, associated with breast cancer progression and metastasis. Statistical analyses were performed to identify molecular signatures and their significant associations with the clinical outcomes of the patients. An exclusive subgroup was identified within both the UM and control samples, marked by a unique pattern of gene expression, including keratins, cell adhesion proteins, and tumor suppressor genes. Disrupted epithelial, cell adhesion-related processes and alterations in estrogen signaling were revealed by enrichment analysis, and the identified subgroup was additionally associated with elevated mortality. The strong association of this subgroup with mortality, but not recurrence, may suggest that this subgroup's characteristics were more related to the overall systemic aggressiveness of the disease (thus, mortality) rather than the likelihood of the disease coming back (recurrence). This study reveals the presence of a disturbed, pre-tumorigenic environment with the seemingly normal mammary gland of breast cancer patients with adverse outcomes. Integrating molecular assessment of non-malignant mammary tissue into disease management strategies could enhance personalized patient care.



Number: **15**

Title: **Photosensor development for dark matter searches and medical application**

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IRAP project: **AstroCeNT – Particle Astrophysics Science and Technology Centre**

Group name: **Ultrapure SiPMs and Associated Readout Electronics Group**

We develop ultra-pure photosensors based on Silicon Photo Multipliers (SiPMs) for experimental searches for new physics beyond the Standard Model, such as dark matter direction and neutrino-less double beta decay. We also apply the same technology to medical devices based on SiPMs, such as a Positron Emission Tomography (PET) scanner. This ultra-pure photosensor enables us to search for the elusive signal from dark matter particles, which are hypothetical particles that never detected so far. The discovery of dark matter will cause revolutionary change in our understanding of our universe. With specific integrated electronics, SiPMs are also suitable for PET scanners. For our applications, the time resolution of the signal from SiPM plus the integrated electronics is important as well as the radio purity of the sensors. In collaboration with INFN Torino, the University of Cagliari, the University of Houston and Princeton, we will measure the time resolution in liquid argon.



Number: **16**

Title: **Towards Quantum Qubits with Topological Crystalline Insulators**

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IRAP project: **MagTop – International Centre for Interfacing Magnetism and Superconductivity with Topological Matter**

Group name: **Molecular Beam Epitaxy Group (ON6.2)**

The essential point for the realization of quantum computing (QC) is the fabrication of qubits resistant to noise and decoherence. The quest for an ideal material platform for qubit implementation stands as a pivotal challenge in quantum materials science. Up to now, only several material systems, including III-V semiconductors, have been thoroughly studied experimentally to overcome the decoherence issue. However, it was found that the level of disorder is still too high for qubit implementation. A solution to this problem is the realization of qubits based on other materials using, for example, topological crystalline insulators (TCIs) that possess all the necessary ingredients for qubit implementation, namely high spin-orbit coupling and a reduced role of charge disorder due to a high dielectric constant and topological protection. Thus, a new material platform based on TCIs can be used for the successful fabrication of semiconductor qubits. We fabricated high-quality epilayers and nanostructures of TCIs using molecular beam epitaxy. This technique allows the controllable growth of single-crystalline heterostructures with monolayer precision. Subsequent growth optimization, involving precisely tuned compositions, was achieved through multiple ex-situ structural techniques. Magneto-transport measurements conclusively demonstrated reduced carrier density and enhanced mobility. We attempted to induce superconductivity (SC) in grown structures through the SC-proximity effect. The quality of the interfaces is crucial for Cooper pair injection. Therefore, interfaces were characterized by transport means. Also, the band structure at the SC-semiconductor interface was probed using angle-resolved photoemission spectroscopy. Finally, we fabricated the gate using atomic layer deposition of hafnia on the TCI surface and tested the gating effect. In conclusion, our work represents significant progress in the advancement of quantum qubits based on TCIs. Further outline and challenges will be discussed.



Number: **17**

Title: **Hidden Chern number in non-Hermitian topological systems**

Project leader: **Wojciech Brzezicki**

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Authors: **Wojciech Brzezicki**

IRAP project: **MagTop – International Centre for Interfacing Magnetism and Superconductivity with Topological Matter**

Group name: **Group of Theory of Topological Matter (ON6.1)**

Our recent study of the signatures of dissipative end-modes in a postulated chain of superconducting oscillators called transmons, see Ref. [1], shows that it is feasible to realize dissipative topological states experimentally. What more, we have also shown that it is possible to generate long-range entanglement in such systems by designing proper time-evolution. Open quantum systems can be described by the Lindblad equation, yielding time-evolution of the density matrix. Nevertheless if we neglect quantum jumps, which we are allowed to do at zero temperature, the problem can be reduced to a time-independent Schrödinger equation with a non-Hermitian (NH) Hamiltonian. In our case the transmon-chain Hamiltonian has a non-trivial topology governed by the so-called hidden Chern number, describe in our earlier work [2]. Such an invariant assures that bulk-boundary correspondence always holds, which may not be a case in a generic NH system, putting us on a safe theoretical ground to postulate a measurement protocol to observe topological end-modes. This theoretical framework of the hidden Chern number was also used in an earlier work to describe lasing in the end-states of a coupled polariton chain [3], an artificial photonic crystal. [1] W. Brzezicki, M. Silveri, M. Płodzień, F. Massel, T. Hyart Phys. Rev. B 107, 115146 (2023) [2] W. Brzezicki, T. Hyart, Phys. Rev. B 100, 161105(R) (2019) [3] P. Comaron, V. Shahnazaryan, W. Brzezicki, T. Hyart, and M. Matuszewski, Phys. Rev. Research 2, 022051(R) (2020)



Number: **18**

Title: **Quantum technologies for optical communications**

Project leader: **Marcin Jarzyna**

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Authors: **Konrad Banaszek, Artur Czerwiński, Michał Jachura, Marcin Jarzyna, Mateusz Kucharczyk, Karol Łukanowski, Antoni Mikos-Nuszkiewicz**

IRAP project: **QOT – Quantum Optical Technologies**

Group name: **Quantum Technologies Laboratory**

The amount of data transmitted by satellites and space missions is restricted by the characteristics of the communication links. Standard radio links have limited bandwidth and the corresponding frequency band is highly regulated by various administrative bodies. A way to avoid these issues and improve the communication rates is to utilize optical frequencies, which, due to the existence of lasers, are characterized by vastly reduced losses and improved transmission bandwidth. On the other hand, for optical space links the issue of modulation power becomes critical as the power budget on the satellite is typically extremely constrained. Moreover, because of large distances over which such links operate, the received power is on the level of few photons per time slot. In such a regime quantum mechanical effects start to play a major role. They not only define the ultimate limits on the communication rates but also may allow to design novel detection strategies that improve the performance. Such quantum enhancement may be beneficial also in other contexts like multispan amplified fiber links which are the backbone of many communication networks, however, one has to include the impact of noise which may diametrically change the picture. A closely related topic is secure information transmission, in which information leakage to a third party is prevented. Quantum-enhanced technologies offer different protocols, such as quantum key distribution, with varying levels of security guaranteed by the laws of nature.



Number: **19**

Title: **Protein Conformational Changes as Driver of Innovations in Ophthalmology: From Structure to Diagnosis and Back**

Project leader: **Luca Gessa**

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Authors: **Luca Gessa, Nelam Kumar, Sathi Goswami, Łukasz Olejnik, Vineeta Kaushik, Humberto Fernandes**

IRAP project: **ICTER – International Center for Translational Eye Research**

Group name: **Integrated Structural Biology**

Phototransduction begins with the activation of visual pigments, which subsequently activate phosphodiesterase 6 (PDE6). This results in cGMP degradation, leading to the initiation of electrical current flow across the retina. Similarly, the visual cycle begins with the activation of visual pigments that are covalently bonded to 11-cis-retinal. Upon exposure to light, the chromophore isomerizes to all-trans-retinal, which is then released from the activated opsin. Given their vital roles in transmitting signals from photon arrival to electrical signals processed by the brain, protein dysfunctions in the phototransduction and visual cycle often lead to several diseases. However, these proteins also have the potential to be excellent biomarkers for evaluating retinal function and tracking treatment efficacy. Two applications in this field are two-photon imaging and optoretinography (ORG). While two-photon imaging can track natural fluorescent retinoid molecules and detect imbalances in the visual cycle, ORG enables the detection of nanometer-scale changes in photoreceptors upon light stimulus within milliseconds. However, the data's utility remains limited without identifying the molecular drivers behind these measurable or quantifiable change. In our studies, we harness structural biology methods to gain insights into and identify the molecular drivers of biomarkers detected by functional imaging systems or to develop direct measurements of their in-situ performance. In particular, we have improved the resolution of the retinol-binding protein 3 (RBP3) cryoEM structure and analyzed its conformational changes in solution, offering potential use in diabetic retinopathy diagnosis by direct quantification of RBP3 using two-photon imaging. Furthermore, we have obtained cryoEM tomograms of rod outer segments (ROS) in an attempt to identify PDE6 as the molecular driver of the photoreceptors' morphological changes upon light stimulus that underpins the ORG system.



Number: 20

Title: **Quantum sensors: dynamical modelling and data processing**

Project leader: **Jan Kolodynski**

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IRAP project: **QOT – Quantum Optical Technologies**

Group name: **Quantum Information and Inference Laboratory**

In order to benefit from quantum features that quantum sensors have to offer, we still need better dynamical models that describe their inner workings, as well as data-processing and control-theory tools to efficiently interpret their output signals and modify their evolution in real time. Within the Quantum Information and Inference Laboratory (QI²lab@QOTUW) we have successfully developed improved models of atomic and optomechanical devices, as well as sensors based on nitrogen-vacancy centres in diamond. On one hand, we have assessed what are the fundamental limits on their performance by adapting frameworks of quantum stochastic dynamics and resorting to methods of quantum information theory and quantum metrology. On the other, we have demonstrated how to unleash their full quantum potential by resorting to techniques of statistical inference, e.g. extended Kalman filters or approximate Bayesian computation, and by carefully engineering the active feedback with help of control theory tools, e.g. linear-quadratic regulators. Our results pave the way for a new generation of quantum sensors to come.



Number: **21**

Title: **New comprehensive method for multimodal single-cell data visualization**

Project leader: **Piotr Rutkowski**

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Authors: **Piotr Rutkowski, Marcin Tabaka**

IRAP project: **ICTER – International Center for Translational Eye Research**

Group name: **Computational Genomics Group**

The single-cell sequencing approaches allow researchers to uncover rare cell types, reveal the diversity of cell populations, and infer the developmental trajectories of cell lineages. Recent progress in developing multimodal single-cell techniques has enabled the study of complex biological systems and processes simultaneously at multiple layers of gene regulation. We propose a new comprehensive method for finding and visualizing developmental landscapes from multimodal data. Our approach is scalable to adapt to the growing dataset sizes and generalizable to include multiple layers of information per cell. When compared to state-of-the-art methods, we found an increase in execution speed by an order of magnitude for the 100,000-cell datasets. Further benchmarking was performed on simulated and biological multimodal datasets to test the accuracy and explainability of our method. The proposed algorithm could reconstruct developmental trajectories, including the rare cell state transitions, and a general structure from noisy data better than other methods giving deeper understanding of regulatory mechanisms driving developmental changes.



Number: 22

Title: **A Novel Instance of Unbounded Quantum Advantage**

Project leader: **Sumit Rout**

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IRAP project: **ICTQT – International Centre for Theory of Quantum Technologies**

Group name: **New Quantum Resources Group**

Prepare and measure scenarios that involve computing the minimum communication required between distant parties in order to perform the distributed computation of functions are often considered to explore the advantage of quantum systems over classical systems as carriers of information. In this work, we have considered the extension of communication complexity to relations through communication-based tasks between two players, Alice and Bob, who receive inputs and have access to a one-way communication channel. For each such input, Bob has to yield an output such that it satisfies the given relation without any error. The class of relations we have considered is induced by a distributed clique labelling problem. We consider two variants: 1) the receiver outputs an answer satisfying the relation - the traditional communication complexity of relations (CCR) and 2) the receiver has non-zero probabilities of outputting every valid answer satisfying the relation (equivalently, the relation can be fully reconstructed), that we denote the strong communication complexity of the relation (S-CCR). We prove that for the specific class of relations considered here when the players do not share any resources, there is no quantum advantage in the CCR task for any graph. On the other hand, we show that there exist, classes of graphs for which the separation between one-way classical and quantum communication in the S-CCR task grows boundlessly with the order of the graph m , specifically, the quantum complexity is $O(1)$ while the classical complexity is $\Omega(\log m)$. Secondly, we prove a lower bound (that is linear in the number of cliques) on the amount of shared randomness necessary to overcome the separation in the scenario of restricted communication and connect this to the existence of Orthogonal Arrays. Finally, we highlight some applications of this task to semi-device-independent dimension witnessing as well as to the detection of Mutually Unbiased Bases.



Number: **23**

Title: **Advances in entanglement catalysis**

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IRAP project: **QOT – Quantum Optical Technologies**

Group name: **Quantum Resources and Information Laboratory**

In chemistry, a catalyst is a substance which enables a chemical reaction or increases its rate, while remaining unchanged in the process. Instead of chemical reactions, quantum catalysis enhances our ability to convert quantum states into each other under physical constraints. The nature of the constraints depends on the problem under study, and can arise, e.g., from energy preservation. We summarize the most recent advances of quantum catalysis, focusing on transitions between entangled states.



Number: **24**

Title: **Rydberg atoms for quantum signal processing and transduction**

Project leader: **Michał Parniak**

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IRAP project: **QOT – Quantum Optical Technologies**

Group name: **Quantum Optical Devices Laboratory**

Microwave fields in conventional scenarios are detected using superheterodyne techniques. Photon counting at the microwave level presents immense challenges and can only be realized with advanced superconducting, cryogenic circuits operating at dilution refrigerator temperatures. On the other hand counting of optical photons can be facilitated with astounding efficiency, low dark-count rate and timing precision. The advantages of optical detectors for microwave photon counting can be leveraged using upconversion. In our experiment we have used Rydberg atoms for this purpose. Remarkably, Rydberg atoms couple well to both microwave and optical photons, therefore a parametric process can be facilitated with good efficiency. We have also discovered that room-temperature atomic vapor, even though they are an intrinsically hot and noisy system, can support the upconversion processing maintaining its low-noise characteristics. We have designed a process in which all pump fields address different transitions than the upconverted photon, therefore minimizing noise down to the level of single photons. We have shown upconversion and detection of microwave room-temperature thermal background radiation, with intrinsic upconverter noise reaching down to single Kelvins of noise-equivalent temperature. We observed second-order thermal character of radiations, as well as its two-photon interference with a coherent microwave tone. Our results elucidate the prospect of atom-based devices (which in the next step should be enhanced via cavity effects) coupled with photon counters acting as ultra-precise and quite unique microwave detectors. Further applications include coupling easily with terahertz fields for uniquely precise sensing and metrological SI-referenced sensitivity thanks to methods based on Autler-Townes splitting. Overall, Rydberg sensors we develop hold multiple advantages and prospects for commercial development via advanced quantum science.



Number: 25

Title: **Quantum Memory-based optical processor for communication and metrology**

Project leader: **Mateusz Mazelanik**

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Authors: **Mateusz Mazelanik, Michał Lipka, Adam Leszczyński, Bartosz Niewelt, Stanisław Kurzyna, Marcin Jastrzębski, Jan Nowosielski, Michał Parniak, Wojciech Wasilewski**

IRAP project: **QOT – Quantum Optical Technologies**

Group name: **Quantum Memories Laboratory**

We demonstrate optical quantum memory with built-in processing capabilities. The memory employs an inhomogeneously-broadened cold-atomic medium that allows controllable absorption and reemission of light pulses. The absorption process maps the light pulses onto atomic coherence that can be manipulated by using additional magnetic or optical fields. This way we can virtually modulate the stored light and release it on demand. Within this framework, we have been able to demonstrate a far-field temporal imaging (Fourier Transform) protocol working in a previously unreachable regime of ultranarrowband light. We achieved 1 MHz bandwidth with a resolution



Number: **26**

Title: **In-situ and ex-situ study on structural evolution of graphite in nuclear reactors**

Project leader: **Magdalena Gawęda**

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IRAP project: **NOMATEN**

Group name: **Material Characterization**

The aim of this work was to describe behaviour of graphite under the conditions of Gen-IV nuclear reactors, particularly high-temperature gas-cooled reactors (HTGR). This is crucial for addressing the energy crisis by developing safe, reliable, and efficient reactor materials. The materials used in HTGR, especially graphite, must exhibit high radiation tolerance and temperature resistance, as graphite serves both as a moderator and a structural component for hexagonal prisms. The comparative structural analysis was conducted on three types of nuclear graphite providing detailed insights into processes related to structural deterioration that could lead to component failure. Commercial graphites IG-110 and NBG-17, along with in-house NCBJ laboratory material, were irradiated with 150 keV He⁺ and Ar⁺ ions at 400 °C, and fluence up to 2E17 ion/cm², and subsequently analysed using Raman spectroscopy. The first stage of study focused on ex-situ structural evolution induced by increasing levels of irradiation. The results revealed a gradual deterioration following an expected three-stage progression. Up to the fluence of 3E14 ion/cm² (Ar⁺) and 3E16 ion/cm² (He⁺), the material maintained its structural integrity, to further transfer into nanocrystalline graphite and eventually deteriorate into amorphous carbon. The core of the second stage aimed to provide detailed information on the structural behaviour of defected nuclear graphite under high-temperature conditions. Previously irradiated samples were analysed in-situ using high-temperature Raman spectroscopy at up to 900 °C. With increasing temperature, a structural transition towards nano- up to submicron-sized grains was observed. It clearly depicted its opposite effect to radiation, preventing deterioration and facilitating structural rearrangement. Acknowledgments: The authors acknowledge support from the European Regional Development Fund via the Foundation for Polish Science IRAP program grant No. MAB PLUS/2018/8.



Number: 27

Title: **Cancer and Cellular Senescence – two complementary stress models to study turnover and quality control of mitochondrial respiratory complexes.**

Project leader: **Karolina Szczepanowska**

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Authors: **Hanna Salmonowicz, Mahdi S. Mahdi, Karolina Szczepanowska**

IRAP project: **ReMedy – Regenerative Mechanisms for Health**

Group name: **Szczepanowska Group - Laboratory of Metabolic Quality Control**

Maintenance and turnover of macromolecular complexes constitute a great challenge to the cells, particularly under stress that alters protein homeostasis. Mitochondrial respiratory complexes (OXPHOS) are central machinery responsible for energy production and key elements interconnecting distinct metabolic pathways. We want to understand how cells maintain these elaborate yet damage-prone molecular machines over time and whether they can do it in a sustainable way. We are also curious how the upkeep and re-purposing of the OXPHOS system entangle in the cell fate decisions. To get insight into the OXPHOS quality control mechanisms and their physiological relevance, we decided to focus on two disease models, cancer and cellular senescence, in which the burden of genotoxic stress directs the cell toward two completely opposite fates. Hyperproliferation and cell cycle arrest featuring respective pathological states impose strikingly different contexts on the highly organized OXPHOS system by altering the balance between synthesis and degradation of its individual protein components. Meanwhile, repurposing OXPHOS toward anabolic or catabolic function can potentially associate with different damage patterns. Using a combination of molecular biology and proteomic approaches on parallel cell culture models, we trace OXPHOS assembly/degradation patterns and investigate the underlying mechanisms. Our results indicate that both cancer and senescent cells show a highly imbalanced abundance of individual structural subunits of respiratory complexes and a loss of coherency between gene expression and protein levels. Dysregulation of OXPHOS components is accompanied by changes in subunit distribution toward distinct macromolecular assemblies that are not only persistent but also featured by model-specific patterns. Furthermore, our preliminary data suggest that cancer and senescent cells can preferentially rely on intramitochondrial protein quality control system, proteases and chaperons, to ensure appropriate turnover and maintenance of respiratory complexes.



Number: **28**

Title: **Acoustic Newtonian Noise estimates in Virgo and beyond**

Project leader: **Tomasz Bulik**

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Authors: **Tomasz Bulik, Mariusz Suchenek, Marek Cieřlar, Mateusz Pietrzak**

IRAP project: **AstroCeNT – Particle Astrophysics Science and Technology Centre**

Group name: **Seismic Sensors Group**

The acoustic Newtonian noise estimates in future gravitational wave detectors like Einstein Telescope ET or Cosmic Explorer (third-generation wave detectors) are presented in the poster. The Virgo acoustic noise reveals that the sensitivity requirements for the next-generation wave detectors are very demanding. The acoustic Newtonian noise can not be neglected. We have developed noise estimates for future gravity wave detectors based on measurement data from the acoustic microphone network at VIRGO and theoretical estimates of Newtonian noise. We conclude that in order to mitigate acoustic Newtonian noise, one needs either very quiet detectors or small, well insulated halls.



Number: **29**

Title: **Interdisciplinary research on cancer diagnosis and therapy at NOMATEN**

Project leader: **Marek Pruszyński**

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IRAP project: **NOMATEN**

Group name: **Nover Radiopharmaceuticals for Medical Purposes**

The Radiopharmaceuticals Group at NOMATEN Centre of Excellence (CoE) performs interdisciplinary research on cancer diagnosis and therapy. Most of the studies focus on design and synthesis of molecular radiopharmaceuticals for personalized medicine via: i) looking for new production routes of commercial and also potentially applicable new radionuclides in research reactor (Maria) and soon installed at NCBJ (CERAD centre) IBA Cyclone XP 30 cyclotron; ii) target's material preparation and its irradiation in reactor or cyclotron, radiochemical separation of interested radionuclide and target material recovery; iii) labeling of biomolecules (monoclonal antibodies and their fragments, peptides etc) with radionuclides via chelators or prosthetic groups; iv) development of multimodal nanomaterials for diagnostic and therapeutic applications in medicine; v) preclinical in vitro and in vivo evaluation of developed compounds and materials. Part of the work is related to research on external radiotherapy, especially with the use of in-house (Department of Nuclear Equipment and Techniques) built electron accelerators and apoptosis, necrosis, cell-signaling etc. in cancerous cells after external radiotherapy, including also FLASH that is an emerging approach in cancer treatment. The results of these studies will improve portfolio of nuclear medicine in terms of imaging, prognostic and therapeutic novel strategies to defeat cancer. Research is performed in collaboration with Commissariat à l'énergie atomique et aux énergies alternatives (CEA, France) and Teknologian Tutkimuskeskus VTT Oy (VTT, Finland). Close collaboration with Radioisotope Centre POLATOM at National Centre for Nuclear Research, the worldwide known manufacturer of radiopharmaceuticals enables translation of developed radiopharmaceuticals into clinical studies and their further commercialization. The Radiopharmaceuticals Group at NOMATEN CoE intends to further strengthen joint work and synergistic effects. NOMATEN is also actively looking for external collaborations at industrial, national and international level, including Horizon Europe and Euratom instruments.



Number: 30

Title: **Loss of chromosome Y is associated with changes in genome-wide DNA methylation profiles of immune cells in patients with Alzheimer's disease**

Project leader: **Marcin Jąkalowski**

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IRAP project: **LM 3P**

Group name: **Research Group: Computational Biology – Chromatin structures reflecting cellular states**

Loss of chromosome Y (LOY) is the most common form of clonal mosaicism in males. Presence of this phenomenon is most pronounced in leukocytes and increases with age. LOY is also associated with an increased risk for disease and mortality. Within a single cell, LOY is an event leading to a complete loss of chromosome Y and causes disappearance of almost 2% of the male haploid nuclear genome. This should in turn lead to changes in DNA's compaction and its rearrangement in the cell's nucleus and hence alter the epigenetic processes that influence gene expression. Among these are DNA methylation, histone modifications, as well as higher level 3-dimensional structures such as topologically associating domains. Significantly reduced DNA methylation levels were found to coincide with low Y levels. Our previous research showed that LOY has a clear transcriptional effect in leukocytes, and it is associated with dysregulation of multiple genes. Many of these are involved in immune functions. Moreover, we found that levels of LOY in leukocytes were varying dependent on the investigated cell type but had the highest range of values in granulocytes and monocytes. These two cell types make up the major human blood fractions and play key roles in inflammatory and anti-microbial defense processes. Alzheimer disease (AD), the most common chronic neurodegenerative disorder and cause of dementia in the elderly, is a major public health problem worldwide. Losing chromosome Y is associated with higher risks of AD. Disruption in the inflammatory signals has also been documented to be implicated AD. Here we aimed at investigating the epigenetic effect of LOY in leukocytes in the Alzheimer's disease. We generated a broad set of DNA methylation data representing AD patients and healthy controls. All these had their LOY levels estimated that allowed to further divide them into LOY and non-LOY groups. We confirmed the involvement of dysregulated genes (both at the level of DNA methylation, as well as bulk and single-cell RNA expression) in immune processes and found these to be abnormally activated in LOY. Additionally, we show that LOY-associated epigenetic changes are much more pronounced in AD when compared to controls.



Number: **31**

Title: **Development of materials for extreme applications - Gen. IV nuclear reactors.**

Project leader: **Łukasz Kurpaska**

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IRAP project: **NOMATEN**

Group name: **Functional Properties**

Materials for future nuclear energy systems must operate under more extreme conditions than those in current Gen II or Gen III systems. These conditions include higher temperatures, higher dpa, and more corrosive environments. Further, the chemical environment of all Gen IV systems will be more severe than current LWRs (Light Water Reactors), due to a combination of coolant aggressiveness and the higher operating temperature. The higher fluxes combined with longer lifetimes present an even greater challenge to material performance. New structural materials and fuels with greater resistance to severe environments are required if these systems are going to be built. In the frame of the Functional Properties group, which is a part of the NOMATEN Center of Excellence, National Center for Nuclear Research, we study radiation damage resistance of new materials, which the international community has selected as critical for developing Gen. IV technologies. This includes studies on martensitic-ferritic steels, amorphous alumina coatings, nickel-based and zirconium alloys, and high entropy alloys. We also manufacture new materials by using Arc Melting and Spark Plasma Sintering techniques and test them in extreme conditions. Close collaboration with numerical teams of the CoE allows us to understand the importance of each element in the microstructure and the fundamental mechanisms associated with deformation and radiation damage.



Number: **32**

Title: **Fetal Birth Weight Prediction using Multimodal Data**

Project leader: **Przemysław Korzeniowski**

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IRAP project: **Sano – Centre for New Methods in Computational Diagnostics and Personalised Therapy**

Group name: **Health Informatics**

Accurate prediction of fetal weight at birth is essential for effective perinatal care, particularly in the context of antenatal management, which involves determining the timing and mode of delivery. The current standard of care involves performing a prenatal ultrasound 24 hours prior to delivery. However, this task presents challenges as it requires acquiring high-quality images, which becomes difficult during advanced pregnancy due to the lack of amniotic fluid. In this paper, we present a novel method that automatically predicts fetal birth weight by using fetal ultrasound video scans and clinical data. Our proposed method is based on a Transformer-based approach that combines a Residual Transformer Module with a Dynamic Affine Feature Map Transform. This method leverages tabular clinical data to evaluate $2D+t$ spatio-temporal features in fetal ultrasound video scans. Development and evaluation were carried out on a clinical set comprising 582 2D fetal ultrasound videos and clinical records of pregnancies from 194 patients performed less than 24 hours before delivery. Our results show that our method outperforms several state-of-the-art automatic methods and estimates fetal birth weight with an accuracy comparable to human experts. Hence, automatic measurements obtained by our method can reduce the risk of errors inherent in manual measurements. Observer studies suggest that our approach may be used as an aid for less experienced clinicians to predict fetal birth weight before delivery, optimizing perinatal care regardless of the available expertise.



Number: **33**

Title: **STOC-T – new tool for structural and functional studies of the retinal tissue**

Project leader: **Piotr Węgrzyn**

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IRAP project: **ICTER – International Center for Translational Eye Research**

Group name: **Physical Optics and Biophotonics**

In this poster, we introduce a cutting-edge retinal in vivo imaging method known as Spatio-Temporal Optical Coherence Tomography (STOC-T) developed at ICTER and present recent results. This technique demonstrates exceptional proficiency in acquiring high-quality structural and functional images of both the human and mouse retina. The structural imaging component provides expansive field-of-view images of the retinal and choroidal microstructures, offering high-resolution details across all dimensions. The functional capabilities of STOC-T enable the implementation of optoretinography, a novel approach for assessing the retinal tissue's response to external light stimulation. Optoretinography (ORG) offers an objective means to quantify photoreceptor responses, distinguishing it from conventional techniques such as ERG and EEG. STOC-T combines cutting-edge optical engineering, swept-source lasers, sophisticated signal processing algorithms, and ultrafast cameras. Simultaneously, its design has been meticulously optimized to facilitate the seamless translation of this technique into clinical settings.



Number: **34**

Title: **Generative AI: A Promising Future Amidst Emerging Concerns**

Project leader: **Ahmed Abdeen Hamed**

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IRAP project: **Sano – Centre for New Methods in Computational Diagnostics and Personalised Therapy**

Group name: **Clinical Data Science**

In an era where Generative AI takes center stage, the world finds itself divided into two distinct camps. On one side, there are the optimists who recognize the immense potential of this technology and eagerly seek ways to harness it for the greater good. On the other side, skeptics remain cautious, diligently seeking validation and conducting assessments to understand how this new paradigm might impact our lives. This division has spurred a compelling drive to establish policies, guidelines, and best practices. These efforts aim to establish trust in the capabilities of Generative AI while ensuring responsible usage. Ultimately, they pave the way for new opportunities to flourish and encourage the responsible adoption of this transformative technology.



Number: **35**

Title: **A seismic sensor prototype based fiber optic cable for seismic noise mitigation in VIRGO**

Project leader: **Mariusz Suchenek**

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IRAP project: **AstroCeNT – Particle Astrophysics Science and Technology Centre**

Group name: **Electronics and Data Acquisition and Processing Group**

Distributed acoustic sensing (DAS) technology uses every point of fiber optic cable as a virtual seismometer. A sequence of laser pulses injected into the optic cable is used as the probe signal to record the returned Rayleigh scattered lights. In principle, the returned scattered lights from fiber optic cable are recorded and further digitally processed to detect seismic events. We developed a seismic sensor prototype that uses an electrically modified SFP module, fiber optic cable, an optical circulator, and a data acquisition system with SoC Xilinx and an analog-digital converter. An appropriate signal processing algorithm can consider every point on the fiber optic cable as a virtual seismometer. The signal observed with the prototype sensor shows good agreement with the signal from the geophone. We plan to replace the existing seismic array based on geophones in VIRGO with the one developed with fiber optic cable.



Number: 36

Title: **Depletion of neurodegeneration-associated protein, TDP-43, perturbs cellular energymetabolism in motor neurons**

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Authors: **Ismail Gbadamosi, Ali Jawaid**

IRAP project: **BRAINCITY – Centre of Excellence for Neural Plasticity and Brain Disorders**

Group name: **Laboratory for Translational Research in Neuropsych**

Amyotrophic lateral sclerosis (ALS) and frontotemporal lobar degeneration (FTLD) are two incurable neurodegenerative disorders (NDDs) with considerable clinical and molecular overlaps. Cytoplasmic mislocalization and aggregation of protein TDP-43 in neurons and glia is the molecular hallmark of a majority of ALS and FTLD cases. Clinically, metabolic conditions that are conventionally considered unfavourable, such as type 2 diabetes mellitus and dyslipidaemia, are associated with better prognosis in ALS and FTLD. To ascertain whether changes in metabolism are critically linked to neurodegeneration in these TDP-43 proteinopathies, we depleted TDP-43 via RNA interference in NSC34 mouse motor neurons followed by a comprehensive cellular metabolic profiling. Transcriptomic analyses revealed increased expression of genes related to glucose transport, glycolysis, pyruvate metabolism and AMPK signalling following TDP-43 depletion. Functional metabolic assays confirmed that TDP-43knockdown increased glucose uptake and glycolysis, as well as oxidative phosphorylation in NSC34 cells resulting in the exacerbated generation of reactive species. An overall increase in glycolytic flux and oxygen consumption upon TDP-43 knockdown was further confirmed by metabolic flux analysis. Finally, we showed that defects in cellular energy sensing are likely responsible for these metabolic changes as indicated by the dysregulated activity of the cellular energy sensor, AMPK. Taken together, these results reveal that TDP-43 loss-of-function, a prodromal event in TDP-43-associated NDDs, is associated with a constellation of cellular metabolic perturbations suggestive of hypermetabolism and impaired energy sensing. Characterization of metabolic changes in NSC34 cells after TDP-43 aggregation followed by in vivo/ex vivo validations are the subjects of our ongoing investigations.



Number: **37**

Title: **Targeted gene delivery: strategies for changing the viral tropism**

Project leader: **Jagoda Płaczekiewicz, Kordecka Katarzyna**

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Authors: **Jagoda Płaczekiewicz, Katarzyna Kordecka, Lucyna Piórkowska, Samuel Du, Krzysztof Palczewski, Anna Postuszny, Andrzej T. Foik**

IRAP project: **ICTER – International Center for Translational Eye Research**

Group name: **Ophthalmic Biology Group**

Vision provides a highly informative perception of the external environment in humans, enabling smooth and precisely directed interaction with the surrounding and distant world. This makes vision a sense crucial for human welfare. Recently, viral gene therapies delivering fully functional copies of genes in order to replace defective ones or optogenetic tools appeared to be the most effective ways to restore vision. Rabies virus (RV) is used in neurobiology for retrograde tracing due to its way of infection from postsynaptic to presynaptic cells. RV, however, is also an attractive candidate for gene delivery, as it can provide fast and high expression of transgenes that can be potentially used in gene therapy of degenerative diseases. Genetic modifications of the envelope glycoprotein (G) can impact the selectivity of RV infections, and such modification has been successfully applied to manipulate RV in the TVA/EnvA system. Therefore, pseudotyping of G-deleted RV (RVΔG) with a properly designed chimeric G protein, can restrict RV infection to specific cell types. We aimed to develop a novel proof-of-concept approach to therapeutic gene delivery using a modified Rabies virus (RV) as a vector specific to different types of remaining cells within a degenerated retina. In the aim of effective infection of cones, and ON-bipolar cells we created pseudotyped viral vectors carrying genes coding proteins crucial for these cells' function, Rod-derived Cone Viability Factor (RdCVF), and Leucine Rich Repeat, Ig-Like And Transmembrane Domains 3 (LRIT3), respectively. After intravitreal administration to the mice retina, immunohistochemical analysis of eyes cross sections, revealed that our pseudotyping approach enables modified viral particles to infect specific types of cells within the retina. Funding: The International Centre for Translational Eye Research (MAB/2019/12) project is carried out within the International Research Agendas programme of the Foundation for Polish Science co-financed by the European Union under the European Regional Development Fund. National Science Center, Poland (2019/34/E/NZ5/00434) National Science Center, Poland (2020/39/D/NZ4/01881) National Science Center, Poland (2022/47/B/NZ5/03023)



Number: 38

Title: **Tunable magnon-phonon polaritons at around 1.0 THz**

Project leader: **Marcin Białek**

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IRAP project: **CENTERA – Center for Terahertz Research and Applications**

Group name: **Lab 6 and WG6**

In the recent decade there is growth of interest in light-matter coupling in magnetic materials. It is motivated by potential applications in quantum technologies as well as by interesting physics, like observation of dissipative coupling. However, this research is mostly done with ferromagnets in the microwave the range. The antiferromagnetic resonance in the terahertz (THz) range is much less explored because there are challenges in constructing cavities of high quality factor. Hematite (α -Fe₂O₃) and nickel oxide (NiO) are perfect candidates for magnon-photon coupling, because their antiferromagnetic resonance is characterised by very narrow linewidths, fast dependence of their frequencies on temperature around room temperature and very high Néel temperature. Coupling magnons with phonons might enhance magnon-photon coupling because of much higher electric dipolar moments than magnetic ones. Such hybrid excitations offer new possibilities of tuning magnetic excitations in antiferromagnets.



Number: **39**

Title: **Pioneering Cancer Immunotherapy: A Breakthrough from ICCVS,**

University of Gdansk, Poland

Project leader: **Sachin Kote**

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Magdalena Pilch, Martyna Muszczek, Ted Hupp, Natalia Marek- Trzonkowska

IRAP project: **ICCVS – International Centre for Cancer Vaccine Science**

Group name: **Clinical Peptidomics Group**

The International Centre for Cancer Vaccine Science (ICCVS) at the University of Gdansk, Poland, stands at the forefront of a groundbreaking era in cancer research. Our dedicated team has undertaken comprehensive research that promises to revolutionize cancer treatment through personalized therapeutic cancer vaccines.

Clinical Peptidomics A New Frontier 🌀 At ICCVS, we proudly introduce the innovative realm of Clinical Peptidomics. Leveraging cutting-edge mass spectrometry technology and pioneering peptidomics approaches, we are reshaping the landscape of cellular therapies and advancing translational research. We aim to establish robust, high-throughput peptidome profiling pipelines for clinical materials. These pipelines will not only drive biomarker discovery but also foster the development of diagnostic tools and personalized therapies, bringing us closer to the dream of precise and effective cancer treatments. 💡 Innovation That Shapes Tomorrow 🚀 Our journey is marked by innovation, with seven (7) European Patent Office (EPO) applications encompassing a spectrum of groundbreaking techniques. These patents include immunopeptidomics and neoantigen discovery (EP23182549.8 and EP23182546.4), serum peptidomics from both human and non-human biofluids (EP22216500.3, EP22216509.4, EP22216488.1), tissue extracellular peptidomics (EP23182547.2), intracellular peptidomics (EP23167220.5), and quantitative proteomics research dedicated to enhancing health, environment, and safety.



Number: 40

Title: **Scientific computing at AstroCeNT**

Project leader: **Piotr Gawron**

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Authors: **Mikołaj Boroński, Marek Bukowicki, Mateusz Denys, Aleksander Gautier, Piotr Gawron, Manish Kumar Gupta, Barbara Jasiulis-Góldyn, Emilia Kaczmarczyk, Piotr Kalaczyński, Aleksandra Krawiec, Wojciech Rogala, Tomasz Rybotycki, Mateusz Stępnia, Marek Wiejak, Magdalena Wiercioch, Marcin Wierzbiński**

IRAP project: **AstroCeNT – Particle Astrophysics Science and Technology Centre**

Group name: **Scientific Computing & Information Technology Group**

AstroCeNT's mission is to explore the hidden Universe. This mission is implemented by, among others, the development of tools required for gravitational waves and dark matter detection. One of the tools needed in astroparticle physics research is scientific computing. The activities of AstroCeNT's Scientific Computing & Information Technology Group cover: currently widely used traditional computing, and forward-looking — non von Neumann computing. The areas of traditional computing we employ a variety of data analysis tools such as e.g. machine learning. The non von Neumann computing research is focussed on quantum and neuromorphic computing paradigms. AstroCeNT is a member of LUMI-Q project that aims to deploy a new European quantum computer and integrate it with the most powerful High Performance Computing systems in Europe. Our task will be to show how satellite data and information acquired by the future Einstein Telescope can be processed in a hybrid HPC–quantum system. During the implementation of the AstroCeNT IRAP project our research was focussed on applications of neural networks for gravitational waves signals analysis and position reconstruction of events in argon dark matter detector. We have also successfully applied modern computational tools and libraries in order to model direct dark matter detection using Monte Carlo methods. We have studied causality in auxiliary channels of gravitational waves detectors data. Additionally, we have studied a variety of applications of quantum machine learning techniques for Earth observation data analysis. Here we summarize our past activities and plans for the future.



Number: **41**

Title: **Plasmonic Crystals Oscillating at Terahertz Frequencies**

Project leader: **Pavlo Sai**

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Authors: **Maxym Dub, Pavlo Sai, Vadym Korotev, Wojciech Knap**

IRAP project: **CENTERA – Center for Terahertz Research and Applications**

Group name: **Lab 1 and WG1**

We present a comprehensive study the diverse phases of terahertz (THz) plasmonic crystals. Our research focuses on the electrically controlled modulation of plasmonic crystal phases by manipulating the charge carrier density profile through gate voltage application to gated cavities. Through a combination of experimental and theoretical investigations, we explore the resonant behavior of THz 2D plasmons and identify two distinct phases of plasmonic crystals: the delocalized phase and the localized phase. Intriguingly, we discover that the resonant frequency of plasmonic crystals in the localized phase exhibits an unexpected sensitivity to the gate voltage. We attribute this phenomenon to the specific contraction of the conductive profile of the 2DEG in the ungated region, known as the edge gate effect. While our study focuses on plasmons in AlGa_N/Ga_N grating-gate structures, our findings possess a general nature and are applicable to other semiconductor-based plasmonic crystal configurations. By demonstrating the electrically tunable transition between different phases of THz plasmonic crystals, our work represents a significant advancement towards a deeper understanding of THz plasma physics and the development of all-electrically tunable devices for THz optoelectronics.



Number: **42**

Title: **Compact and Cost-effective Silicon Technology Based Terahertz Devices**

Project leader: **Dmytro BUT**

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IRAP project: **CENTERA – Center for Terahertz Research and Applications**

Group name: **Lab 3 and WG3**

We shortly present the state of silicon complementary metal-oxide-semiconductor (Si CMOS)-based electronic sources and detectors developed for the THz frequency range by the WG3 group at the CENTERA laboratory. Si CMOS technology has taken the lead in digital applications due to its high level of integration, mass production capability, reliability, and well-developed building-block approach. The continuous development of Si CMOS devices has already contributed to a paradigm shift, enabling Si CMOS to operate in the tens of GHz range. By using special design approaches, we can effectively adapt this technology also to the THz range. Implementing an efficient antenna for the THz integrated detector is one of the main challenges in the device development process. Si CMOS TeraFET detectors commonly use planar antennas, and these devices demonstrate broadband operation with a nearly flat frequency response up to a few THz. Another common solution is patch antennas with on-chip ground planes that can be adapted to specific frequencies with a 10% bandwidth relative to the central frequency. The noise voltage for the TeraFET detectors is approximately $8 \text{ nV}/\sqrt{\text{Hz}}$. We also present antenna-coupled push-push oscillators that employ the Colpitts configuration and emit up to $75 \text{ }\mu\text{W}$ at 254 GHz (harmonic oscillator) and $325 \text{ }\mu\text{W}$ at 260 GHz (fundamental oscillator) into the propagated beam. The combination of this source and the substrate-lens coupled detectors allows the realization of optical emitter-detector systems that exhibit an input power-related signal-to-noise ratio above 70 dB in the direct detection regime for a one Hz equivalent noise bandwidth. The availability of compact CMOS-based components enables the realization of compact and cost-effective silicon technology based devices enabling multiple applications. For example, the direct link between the emitter and detector (point-to-point connection, line-of-sight, etc.) can be employed for raster-scan imaging systems as well as for wireless data transmission. It also finds a place in more advanced research setups as a part of the scattering-type scanning near-field optical microscopy (s-SNOM) operating in THz range.



Number: **43**

Title: **A linear program for testing nonclassicality, its implementation, and an application**

Project leader: **Vinicius Pretti Rossi**

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IRAP project: **ICTQT – International Centre for Theory of Quantum Technologies**

Group name: **Foundational Underpinnings of Quantum Technologies Group**

A well-motivated method for demonstrating that an experiment resists any classical explanation is to show that its statistics violate generalized noncontextuality. We formulate this problem as a linear program and provide an open-source implementation of it which tests whether or not any given prepare-measure experiment is classically-explainable in this sense. If it is not, the implementation computes the minimal amount of noise that must be added such that a noncontextual ontological model does exist and then provides this model. We then apply this program to the investigation of the robustness of contextuality to partially dephasing noise in a scenario related to state discrimination (for which contextuality is a resource). We find that a vanishing amount of coherence is sufficient to demonstrate the failure of noncontextuality in this scenario, and we give a proof of contextuality that is robust to arbitrary amounts of partially dephasing noise. This is in stark contrast to partially depolarizing noise, which is always sufficient to destroy contextuality.



Number: **44**

Title: **DETECTING NK CELL SERIAL KILLERS – FLOW CYTOMETRY ASSAY**

Project leader: **Ines Papak**

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IRAP project: **ICCVS – International Centre for Cancer Vaccine Science**

Group name: **Cancer Immunology Group**

NK cells have a unique ability to repeatedly target and kill infected or cancerous cells. This phenomenon occurs in situations like severe viral infections or within solid tumors when there are more targets than available NK cells. Once activated, NK cells initiate target cell elimination by releasing their cytotoxic granule contents, leading to the exposure of CD107a, also referred to as lysosomal-associated membrane protein 1 (LAMP-1), on the cell surface. We have developed a methodology employing CD107a antibodies labeled with distinct fluorophores, combined with flow cytometry and cell sorting, to precisely identify and isolate NK cells capable of performing multiple attacks. In summary, our method represents a useful tool for studying NK cells with serial killing properties, such as the evaluation of the cytotoxic potential of NK cells serial killers in scenarios like non-small cell lung cancer. NK cells demonstrating this serial killing capacity hold greater potential as therapeutic targets for cellular immunotherapies, in contrast to NK cells that undergo degranulation only once.



Number: 45

Title: **Post-Zygotic Chromosomal Aberrations in Non-Cancerous Bladder Urothelium**

Project leader: **Wiktoria Stankowska**

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Authors: **Wiktoria Stankowska**

IRAP project: **LM 3P**

Group name: **Research Group: Loss of chromosome Y and human disease**

Introduction: As people age, tissues become susceptible to colonization by mutant clones carrying driver mutations, including those in cancer genes. Bladder cancer, originating from the urothelium, exhibits one of the highest mutation burdens among major cancer types, showcasing a diverse landscape of driver mutations. However, the scope of chromosomal aberrations within the normal urothelium remains poorly understood. These aberrations might confer a growth advantage, promoting clonal expansions that may represent early events in carcinogenesis. Our study focused on post-zygotic chromosomal aberrations in a cohort of 67 bladder cancer donors, with a concentration on non-cancerous samples. Methods: We employed SNP microarrays followed by the application of the Mosaic Chromosomal Alteration Caller (MoChA) for sensitive detection of copy number aberrations (loss and gains) and copy-neutral aberrations (CN-LOH) at > 5% cell fraction. Results: The bladder cancer cohort encompassed 485 samples (145 cancerous, 277 non-cancerous, and 63 blood) and yielded a total of 480 post-zygotic manually curated aberrations (with a conservative estimate) across 34 donors (45%), within 64 non-cancerous samples. Notably, recurrent regions revealed 16 aberration hotspots, indicating recurring aberrations in genes commonly associated with bladder cancer. These included well-known oncogenes like RAF1 and FGFR1, as well as tumor suppressors like TP53 and PTEN. Moreover, loss of chromosome Y (LOY) was present in 30%, 19%, and 30% of cancerous, non-cancerous, and blood samples, respectively, using a very conservative threshold of 10% of cells with LOY. Conclusion: Our findings point to a high prevalence of post-zygotic chromosomal aberrations in non-cancerous bladder tissue that might predispose individuals to bladder cancer.



Number: 46

Title: **Bell-nonclassicality Of a Single-photon**

Project leader: **Marek Żukowski**

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Authors: **Tamoghna Das, Marcin Karczewski , Antonio Mandarino, Marcin Markiewicz, Bianka Woloncewicz, Marek Żukowski**

IRAP project: **ICTQT – International Centre for Theory of Quantum Technologies**

Group name: **Multiphoton Quantum Optics for Quantum Information Group**

The Bell nonclassicality of a single-photon in superposition in two modes, aka “nonlocality of a single photon” is one of the most striking nonclassical phenomena discussed in the context of foundations of quantum physics. We show how to violate local realism with weak-field homodyne measurements for any superposition of one photon with the vacuum. Our modification of the previously proposed setups involves tunable beam splitters, and weak local oscillator fields. As photon-number-resolving measurements are now feasible, we use of the Clauser-Horne Bell inequalities for detection events defined by a fixed numbers of photons and we find a condition for optimal measurement settings leading to a maximal violation of local realism, this states that the reflectivity of the local beam splitter must be equal to the strength of the local oscillator field. We show that this condition holds not only for the vacuum–one-photon qubit input state, but also for the superposition of a photon pair with vacuum, which suggests its generality as a property of weak-field homodyne detection with photon-number resolution.



Number: **47**

Title: **Quantum Cybersecurity and Communication**

Project leader: **Akshata Shenoy**

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Authors: **Akshata Shenoy, Pedro Ruas-Diequez, H.S. Karthik, Giovanni Scala, Marcin Pawłowski**

IRAP project: **ICTQT – International Centre for Theory of Quantum Technologies**

Group name: **Quantum Cybersecurity and Communication Group**

We present the research endeavors of the Quantum Cybersecurity and Communication Group at the International Centre for Theory of Quantum Technologies, University of Gdańsk, Gdańsk. The focus of the group is to develop cutting-edge quantum solutions in communication scenarios and in tandem formulate optimized information-theoretic security protocols based on the fundamental aspects of quantum theory. Along with this, our group members work on a series of diverse topics not limited to characterization of multipartite correlations and their applications in communication tasks, device-independent quantum cryptography, technological aspects of space quantum communication, delayed choice experiments and their applications.



Number: 48

Title: **Light collection and detection technologies for dark matter searches and other applications**

Project leader: **Marcin Kuźniak**

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Authors: **Sarthak Choudhary, André Cortez, Theo Hugues, Marcin Kuźniak, Maciej Kuźwa, Grzegorz Nieradka, Michał Olszewski, Marek Walczak, Tadeusz Sworobowicz**

IRAP project: **AstroCeNT – Particle Astrophysics Science and Technology Centre**

Group name: **SiPM Systems for Astroparticle Physics and Medical Group**

Mysterious dark matter accounts for 23% of energy density of the Universe (five times more than ordinary matter) and yet its nature remains unknown. Weakly interacting massive particles (WIMPs) that have not yet been directly detected are a possible dark matter candidate. The search for WIMPs is carried out by international collaborations with large detectors located in underground laboratories (to eliminate the cosmic ray backgrounds). Interactions with WIMPs would manifest as faint flashes of light registered by these detectors. AstroCeNT researchers are part of the Global Argon Dark Matter Collaboration and leaders in R&D on novel light collection and detection schemes, which are key for such detectors. Our achievements on this front include, in particular: development and large scale tests of novel wavelength shifter materials and establishing a facility for characterization of modern 20 cm x 20 cm area silicon photomultiplier-based photodetector units, with sensitivity to single photons. These will be presented in the general context of dark matter searches, as well as well as non-scientific applications with potential for commercialization.



Number: 49

Title: **Robotic arm-based tracking for ophthalmic microscope system for live display of OCT cross-sections at the surgical tool tip**

Project leader: **Karol Karnowski**

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Authors: **Karol Karnowski, Piotr Ciągła, Krzysztof Gromada, Tomasz Piesio, Adam Kurek, Andrea Curatolo**

IRAP project: **ICTER – International Center for Translational Eye Research**

Group name: **Image-guided Devices for Ophthalmic Care**

Surgical procedures performed on delicate structures within the human eye require a high level of manual dexterity. However, current techniques, such as ophthalmic stereoscopes, may result in decreased treatment accuracy (due to limited depth perception) and reduced precision (due to natural hand tremors). Optical Coherence Tomography (OCT) can provide depth information on the specific ocular tissue of interest, thereby enhancing accuracy. However, a challenge lies in obtaining OCT depth scans in close proximity to the surgical tools' tips. To address this, we have developed an OCT system that can be seamlessly integrated with a surgical microscope. The system includes a robotic arm with a specialized holder for surgical tools, which improves the precision of the surgical procedure. Through careful calibration, the system can parse the position of the tool tip from the robotic arm subsystem to Labview control software. The system synchronously acquires a pair of OCT cross-section images: one along the tool and another perpendicular to it, placed directly at the tool tip. The position of OCT scan is updated at a rate of 200 Hz, while the image display – an average of five consecutive scans - is updated at 40 Hz. Our hardware and software solutions enable real-time tracking of the surgical tool tip, ensuring that the displayed OCT tomograms are always aligned with the tool's position. The real-time display of OCT images locked to the surgical tool tip has the potential to significantly enhance the accuracy of ophthalmic procedures. Additionally, the assistance provided by the robotic arm can mitigate the impact of the surgeon's hand tremor, resulting in improved surgical precision.



Number: 50

Title: **High-Performance Computing Tools for Computational Medicine**

Project leader: **Karol Zajac**

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Authors: **Karol Zajac, Marek Kasztelnik, Jan Meizner, Piotr Nowakowski, Bartosz Baliś, Albert Kuźma, Taras Zhyhulin, Krzysztof Gądek, Adam Nowak, Mikołaj Bul, Konrad Czerepak, Maciej Malawski**

IRAP project: **Sano – Centre for New Methods in Computational Diagnostics and Personalised Therapy**

Group name: **Extreme-scale Data and Computing**

Today's computational research landscape presents unique challenges, particularly in the context of big data analysis and generative AI-driven decision support systems. These challenges often necessitate the utilization of specialized computational frameworks available through supercomputing centers. However, for clinicians and researchers, interfacing with such infrastructures can be a complex endeavour, marked by administrative and technical hurdles when transferring substantial input data or extracting publishable results. Our solution involves the development of a versatile computational toolkit that caters to the needs of researchers in various domains, transcending the medical field. This toolkit empowers users to seamlessly execute computations on high-performance computing (HPC) resources while directly accessing data stored in external repositories like the DataVerse platform. The user-friendly toolkit provides a set of user interfaces for designing, launching and monitoring execution (eg. processing patient cohorts) and is supplemented by a set of monitoring tools, facilitating optimal resource allocation. Additionally, it offers a set of monitoring tools that facilitate efficient resource allocation. Notably, our platform also enables the direct publication of results generated through HPC, optionally involving a verification step that allows human researchers to curate specific results for inclusion in the final dataset. The computational medicine toolkit is developed in the context of the InSilicoWorld project, where it is used to process intensive computational tasks for various research applications in medicine (including research of osteoporosis, angiological disorders, COVID-19 and others).



Number: **51**

Title: **An orthogonal O,S -CKA monomer for the introduction of thioester and/or thionoester functionalities by radical polymerization**

Project leader: **Sylwia Wróbel**

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Authors: **Marlena Pięta, Vishal B. Purohit, Sylwia Wróbel, Joanna Pietrasik, Piotr Paneth, Christopher M. Plummer**

IRAP project: **ICRI-BioM – International Centre for Research on Innovative Biobased Materials**

Group name: **Polymer chemistry group - junior group**

Copolymerization of conventional monomers with cyclic monomers undergoing radical ring-opening polymerization (rROP) is a promising tool for obtaining (bio)degradable polymers. Cyclic ketene acetals (CKA) and cyclic thionoesters allow this method to introduce ester and thioester groups, respectively, which can be degraded under various conditions.¹ We have obtained a sulfur analogue of a known monomer of the CKA class, which undergoes radical ring-opening homo- and copolymerization with a number of classic monomers, introducing a thiono- or thioester function or a mixture of the above into the polymer skeleton.² The obtained results are the first example of the introduction of a repeating thionoester unit directly by radical copolymerization. We present experimental research and computational analysis. Acknowledgements: This research was conducted as part of the International Research Agendas PLUS Programme of the Foundation for Polish Science, co-financed by the European Union under the European Regional Development Fund (MAB PLUS/2019/11). 1. (a) A. Tardy, J. Nicolas, D. Gigmes, C. Lefay, Y. Guillaneuf, *Chem. Rev.* 2017, 117, 1319–1406, (b) V. B. Purohit, M. Pięta, J. Pietrasik and C. M. Plummer, *Polym. Chem.*, 2022, 13, 4858–4878. 2. M. Pięta, V. B. Purohit, P. Paneth, J. Pietrasik, L. Li, C. M. Plummer, *Polym. Chem.* 2023, 14, 3872–3880.



Number: **52**

Title: **The Quest For Dark Matter: From The Big Bang To Our Laboratories**

Project leader: **Andrew Cheek**

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Authors: **Leszek Roszkowski, Andrew Cheek, Jacek Osiński, Sebastian Trojanowski**

IRAP project: **AstroCeNT – Particle Astrophysics Science and Technology Centre**

Group name: **Particle Astrophysics Group**

This poster will describe how our group contributes to the global search for dark matter, a hypothesized form of matter that is the cornerstone of modern cosmology and astrophysics. We work on particle explanations for dark matter, focusing on its production in the early universe, observational signals in existing and future experiments and how it may lead to solutions to other problems in modern physics.



Number: **53**

Title: **Non-Reciprocal Approach in Charging Quantum Batteries**

Project leader: **Paweł Mazurek**

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Authors: **Borhan Ahmadi, Paweł Mazurek, Paweł Horodecki, Shabir Barzanjeh**

IRAP project: **ICTQT – International Centre for Theory of Quantum Technologies**

Group name: **New Quantum Resources and Thermodynamics Group**

Non-reciprocal approach has found many promising applications in distinct fields of quantum technologies. Here, we examine its application in the performance improvement of charging process of a quantum battery. By breaking the symmetry of the evolution we activate nonreciprocal flow of energy from the quantum charger to the quantum which allows for considerable enhancement of accumulation of energy in the quantum battery. To establish the non-reciprocity in the evolution of the charging process we use a waveguide connecting the charger to the battery. We prove that when no dissipation is present in the charging process, non-reciprocity causes a substantial increase in the energy of the battery by 4 times and interestingly the positive effect remains noticeable even when the dissipation rates of energy of the charger and the battery increase. Therefore, the waveguide-enabled non-reciprocal approach constitutes a reliable alternative to the standard, waveguide-free setting. Importantly, the non-reciprocal approach optimal operation is achieved in the stationary limit, eliminating the need for fine time-control of the evolution parameters.