

Foreword

C²TN - Radiation for Science and Society

We are very pleased to walk you through C²TN's scientific, technical, education, training and services endeavors and achievements of 2018!

C²TN, acronym for “Centro de Ciências e Tecnologias Nucleares” is an interdisciplinary Research Unit of Instituto Superior Técnico (IST), Universidade de Lisboa, established in 2013, located in Campus Tecnológico e Nuclear. It groups several tens of researchers (physicists, chemists, biologists, geologists, among others) recognized internationally as the Portuguese experts in matters related to Nuclear Sciences and Technologies and applications of Ionizing Radiation. This stems from the unique combination of C²TN's knowledge, skills and competence with its experimental facilities.

Indeed, C²TN has specialized scientific equipment, laboratories and infrastructures, some unique in Portugal, used as nodes in research networks: Laboratories for Synthesis & Characterization of Materials (licensed to handle radioisotopes), including at Low Temperature and High Magnetic Fields; facilities for Synthesis, Characterization & Preclinical Evaluation of Radioactive Tools for Nuclear Molecular Imaging and Therapy; Clean Rooms; Luminescence, Radiocarbon and Tritium Dating; Spectroscopy facilities – Mössbauer, X-ray fluorescence, Inductively Coupled Plasma Mass Spectrometer; alpha and gamma spectrometry laboratories; liquid scintillation counters; irradiation facilities for metrological verification of radiation detection equipment; linear electron accelerator; and access to Tandem and Van de Graaff accelerators and a Gamma Irradiation Unit, located in the Campus.

During 2018, C²TN strengthened its role in the Portuguese Scientific and Technology System and in the international arena. The main axes of activities undertaken aimed at strengthening C²TN's excellence in RD&I and to reinforce:

- ✧ Internationalization, pursuing the collaboration with reference institutions worldwide, in European platforms, international organizations and networks, nurturing new links and consolidating existing ones;
- ✧ Engagement of young researchers, students and stakeholders in Portugal and abroad, fostering new collaborations between C²TN and RD&I and academic institutions, hospitals, municipalities, environmental, industrial, energy and services companies;
- ✧ Outreach, dissemination and communication of Science and its activities.

C²TN's motto “Radiation for Science and Society” highlights the outstanding contributions of C²TN to several societal challenges, namely:

- Better management of cancer and neurodegenerative diseases with more effective and personalized diagnosis and treatments;

- Assessment of detrimental effects due to the exposure to ionizing radiation of patients and medical staff, aiming at the Quality and Safety of health care;
- Radiological and nuclear emergency response and preparedness;
- Prevention of infectious diseases and outbreaks;
- Improving the air quality and reducing the carbon footprint;
- Environmental protection, management of natural resources and global changes;
- Sustainable agro-industry and food safety;
- Cultural Heritage leverage and safeguard;
- Advanced materials for applications in physics and engineering, electronic sensors and devices, energy conversion, cybersecurity and medical applications.

During 2018, a number of C²TN's members, previously holding Post-Doc fellowships, were hired as researchers with a fixed term contract, under the new Government policy on scientific research employment and the corresponding newly approved Decree-Law; although not removing the precarious contractual link of those researchers, the aforementioned policy partially attenuates the uncertainties that affect the sustainability of part of C²TN's human resources.

Outreach activities expanded and consolidated during 2018 with intense participation at national and regional level.

Building on the success of the previous meeting, the wealth and pluridisciplinarity of C²TN's activities were exhibited during the 2nd C²TN Annual Meeting, held in December of 2018, with the participation of external experts.

The highlights of C²TN's activities during 2018, detailed in the sequence, follow closely its structure, namely the organization in 6 interdisciplinary Groups:

ES – Solid State: New Materials with Unconventional Electrical and Magnetic properties and characterization using Low Temperature and High Magnetic Field Techniques

NET – Nuclear Engineering and Techniques: Nuclear Physics, Geo-environments and Cultural Heritage using neutrons, radioactive nuclei and ion beams

RPS – Radiation Protection and Safety: Dosimetry, Radiobiology, Environmental Radioactivity, Radioecology, Radioactive Waste and Metrology

RS – Radiopharmaceutical Sciences: Nuclear Tools for Molecular Imaging and Theranostics

REI – Environmental Processes: Archaeological Material Culture and Macromolecular Materials using Nuclear Analytical Techniques and Ionizing Radiation

QEf – f-Element Chemistry

with the RD&I activities synergistically interwoven into 3 Thematic Strands: i) Advanced Materials ii) Radiopharmaceutical Sciences and Health Physics iii) Earth Systems, Radioactivity & Cultural Heritage.

The most important asset of C²TN is its members.

The Executive Commission would like to acknowledge and thank all C²TN members for their efforts, contributions and accomplishments that made possible the positive journey throughout 2018!

C²TN Executive Commission

Pedro Vaz
(President)

Fernanda Margaça
(Vice-President)

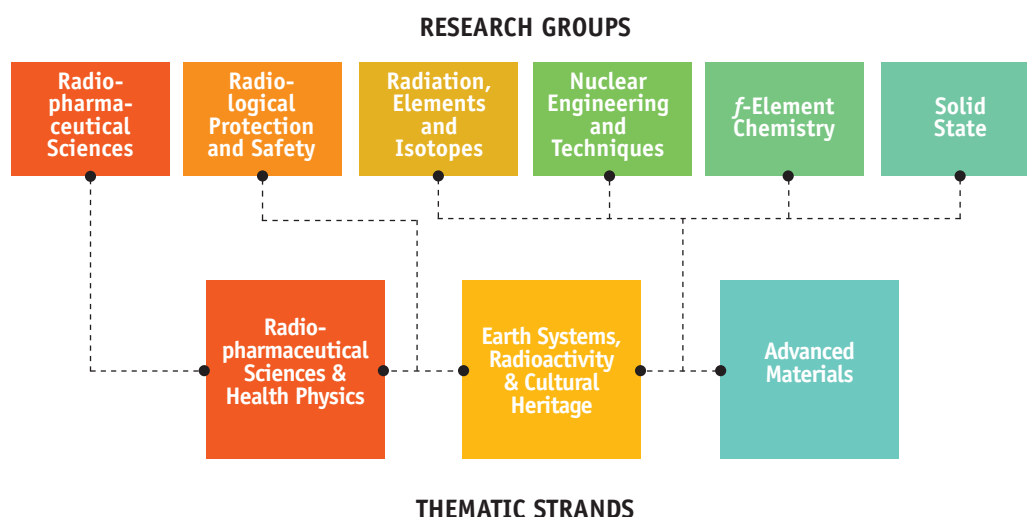
Dulce Belo
(Vogal)

C²TN Organization and Coordination

Considering the complementary know-how, common interests and facilities, the C²TN members are organized in six Research Groups: Radiopharmaceutical Sciences (RS), Radiological Protection and Safety (RPS), Radiation, Elements and Isotopes (REI), Nuclear Engineering and Techniques (NET), *f*-Element Chemistry (QEf) and Solid State (SS). For the period 2015-2020, the 6 groups of scientists will converge and collaborate on 3 main Thematic Strands (TS):



Scheme 1 shows the C²TN research groups and their contribution to the three Thematic Strands. Within these TS the role of the groups is well established and the overall research objectives are in line and nicely intersect with the EU Horizon 2020 initiative.



The Research Group Coordinators are:

RS – António Rocha Paulo; RPS – Pedro Vaz; REI – Maria de Fátima Araújo;
NET – Maria Isabel Dias; QEf – João Paulo Leal; ES – Manuel Leite de Almeida

The Thematic Strands Coordinators are:

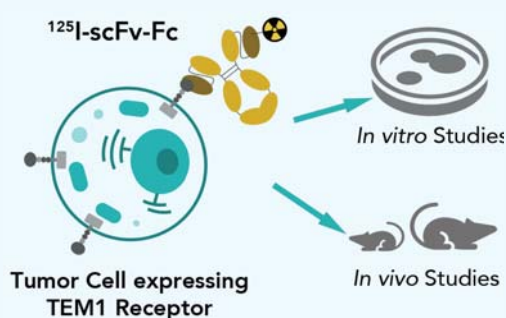
RSHP – António Rocha Paulo; ESRCH – Maria Isabel Prudêncio;
AM – Manuel Leite de Almeida

Thematic Strands

Scientific Report 2018

Radiopharmaceutical Sciences and Health Physics (RSHP)

Researchers of the RSHP thematic strand applied their know-how, techniques and infrastructures to carry out research on Radiopharmaceutical Sciences, Radiation Protection and Dosimetry, Biological Effects of Ionizing Radiation (IR) and Metrology, aiming to contribute to the following major topics:



RADIOLABELED ANTIBODY FRAGMENTS FOR TARGETING OF THE TEM1 RECEPTOR

The endosialin/TEM1 receptor is a suitable target for antibody-mediated therapy due to its minimal expression in normal healthy tissues and its overexpression in several human solid cancers. The preclinical evaluation of a small panel of antibody fragments – scFv-Fc – targeting the TEM1 receptor was undertaken after radiolabeling with ^{125}I . A preliminary screening to identify the most promising fragments was followed by an extensive in vitro characterization in cell lines expressing either the human or the murine receptors, assessing binding affinities and specificity towards

the TEM1 receptor. Biodistribution studies in tumor-bearing mice were also performed, paving the way for further investigations on the pre-targeting approach to this receptor, using radiometals and clickable chelators already developed by the Radiopharmaceutical Sciences Group.

EVALUATION OF HIGH-Z MATERIALS AS RADIOSENSITIZERS

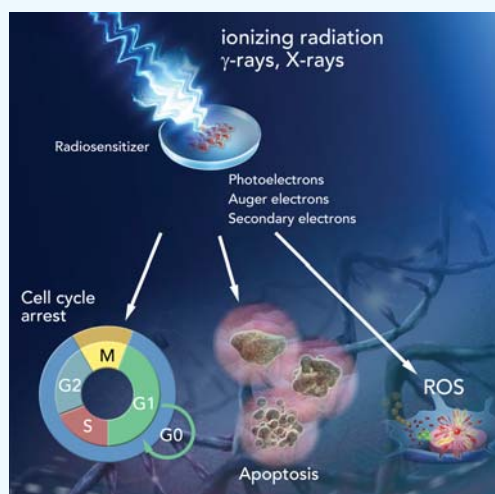
The main challenges of radiation therapy of cancer are the side effects of ionizing radiation in surrounding healthy tissues and the acquired resistance of tumor cells to radiation. One approach to enhance the efficacy of radiotherapy is the use of radiosensitizers to selectively increase the dose at the tumor site. High-Z (atomic number) materials have emerged as new tools in oncology to improve cancer therapy, based on their radiosensitizing capabilities. Using the CTN irradiation facilities, we have studied the effect of different types of electromagnetic radiation on U87 glioblastoma cells pre-loaded with iodinated molecules or gold nanoparticles, as radiosensitizers. In general, the presence

- ❄ Design, Synthesis and Pre-Clinical Evaluation of Radioactive Tools for Molecular Imaging and Theranostics;
- ❄ Evaluation of Biological Effects of Ionizing Radiation;
- ❄ Medical Dosimetry and Metrology of Ionizing Radiation.

The scientific output of the RSHP team was: 36 papers in peer-reviewed journals, 1 book chapter, 5 proceedings, 12 lectures in conferences, 1 Ph.D., 7 M.Sc. and 4 graduation theses. The team has participated in the organization of 2 international conferences and summer schools. The team's research work has been supported by European and FCT competitive funding, with a noteworthy rate of approval of R&D projects (ca. 1 M€) in the 2017-FCT call. There was also a high degree of internationalization with participation in European Union Technology Platforms and Networks, namely MELODI, EURADOS NERIS-TP, IGD-TP and EURAMET, several COST actions and the MCurie ITN MEDICIS-Promed.

Highlights of the R&D activities performed during 2018 are presented below.

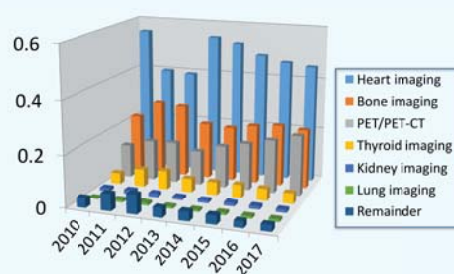
of the radiosensitizers led to an enhanced radiocytotoxicity, most probably due to an increase on ROS production, cell cycle alterations and induction of apoptosis.



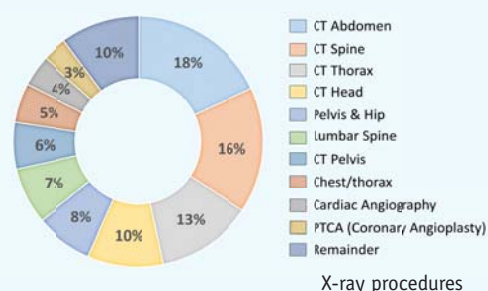
RADIATION EXPOSURE OF THE PORTUGUESE POPULATION IN RADIO-DIAGNOSTIC PROCEDURES (X-RAY AND NUCLEAR MEDICINE EXAMS)

The use of ionizing radiation (IR) in medical imaging has drastically improved diagnostic outcomes, but has also resulted in an increase of the exposure of the

population to man-made IR. This is a cause of concern, both from a radiation protection and Public Health perspectives. To address this issue, this work studied the exposure of the Portuguese population to IR due to radio-diagnostic procedures (x-ray and nuclear medicine exams) in the 2013-2017 period. The estimated total collective dose due to nuclear medicine exams was of 0.088 mSv/person in 2013 and 0.090 mSv/person in 2017.



Nuclear medicine exams



X-ray procedures

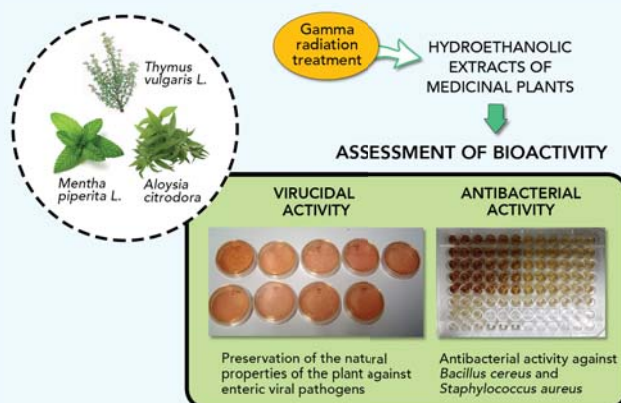
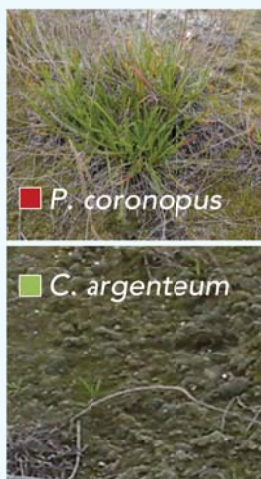
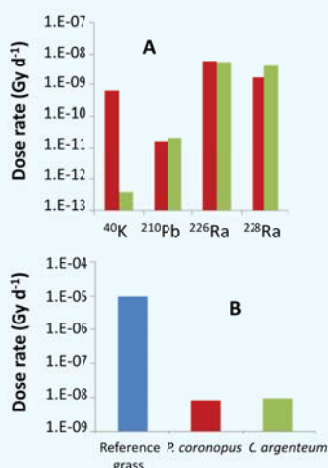
Earth Systems, Radioactivity and Cultural Heritage (ESRCH)

During 2018, the scientific output of the ESRCH team included the publication of 48 papers in peer-reviewed journals, 9 book chapters, 18 international conference proceedings, 8 invited and 32 contributed lectures in international conferences and the completion of 3 PhD and 8 MSc theses. Team members have also given 15 seminars and were responsible for 15 courses given in universities and polytechnical schools, along with the participation in 22 scientific committees of evaluation panels.

The team research has been supported by EC (LIFE, ERA-MIN, Interreg Sudoe and Interreg Mediterranean), FCT, IAEA, and bilateral projects. Overall, ESRCH team has participated in 6 European research contracts, 2 bilateral research projects, 5 research contracts with IAEA, 5 research projects funded by FCT and 3 industrial research contracts.

TRANSFER AND RELATED DOSE ASSESSMENT OF NATURAL RADIONUCLIDES IN PLANTS AND MOSSES GROWING ON A PHOSPHOGYPSUM STOCKPILE IN PORTUGAL

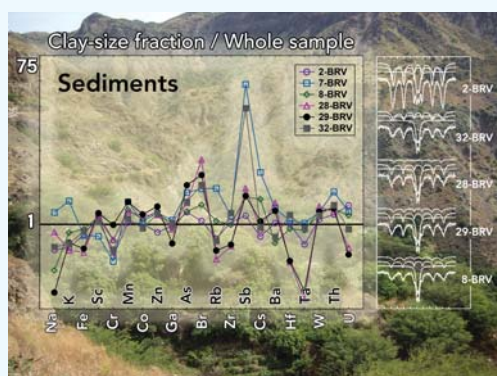
A PG stockpile in the south bank of Tejo estuary, where herbaceous plants (*Plantago coronopus*) and moss (*Bryum argenteum*) grow, was used as a natural laboratory. Internal doses are similar to external doses in herbaceous plants, but can exceed 2 orders of magnitude in moss. The estimated doses are in the order of the natural background for ICRP reference wild grass ($< 0.01 \text{ mGy d}^{-1}$).



ANTIMICROBIAL ACTIVITY OF IRRADIATED AROMATIC AND MEDICINAL PLANTS

A new extraction approach as a process to improve value to aromatic plants as bio-active agents was evaluated. The gamma radiation treatment up to a dose of 10 kGy promotes the antibacterial activity and preserves the virucidal potential on the hydroalcoholic extracts of studied plant species.

A significant participation in the scientific and technical activities of European Union Technology Platforms and Networks, namely ALLIANCE, IGD-TP and NERIS, and in the COST ACTIONS CA16109 and ES1407 has also taken place. During 2018, the team has also prepared and submitted several common projects under calls from EC, FCT, Interreg Sudoe and Horizon 2020. Two contracts were established with private companies. The ESRCH team has also prepared one patent, along with the development of a new algorithm and one prototype during 2018. In order to promote and disseminate the work developed within this thematic strand, ESRCH members participated in 12 different events, namely performances and exhibitions, that were held in Portugal and abroad.

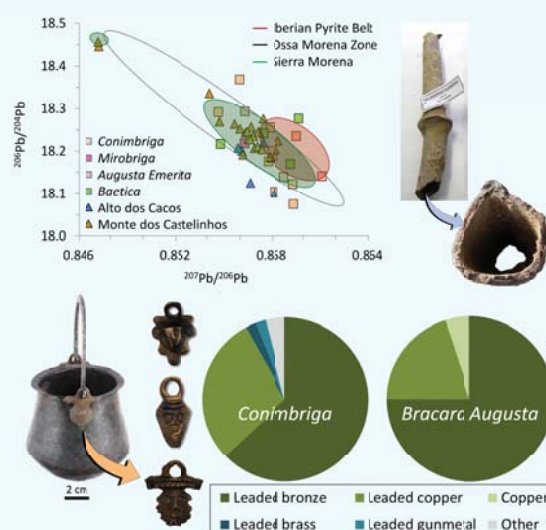


CHARACTERIZATION OF CLAY-SIZED FRACTION OF VOLCANIC SOILS USED FOR AGRICULTURE – BRAVA ISLAND (CAPE VERDE)

Mössbauer spectroscopy and INAA revealed high concentrations of As, Br and Sb in the clay-size fraction, where only Fe(III) occurs and all the Fe oxides are nano-sized. The significant amounts of these elements and vitreous phases in fine particles of soils contribute to their mobility/ accumulation in plants.

LEAD AND COPPER IN WESTERN PROVINCES OF THE ROMAN EMPIRE: PROVENANCE, PRODUCTION AND USE

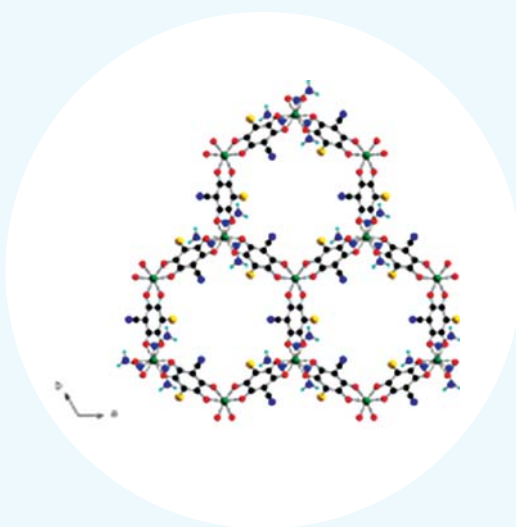
Archaeometallurgical research was focused in collections from Conimbriga, Augusta Emerita and Mirobriga (Lusitania) and Bracara Augusta (Galaecia). Elemental and isotopic composition of hydraulic systems assigned raw materials to the Iberian Pyrite Belt (argentiferous jarosite) and Sierra Morena/Ossa Morena Zone (galena). In general, recycling practises became common during the Empire, suggesting a technology strongly influenced by economic factors.



Advanced Materials (AM)

The research activities under this thematic strand have been focused in different advanced materials, with emphasis on multifunctional and unconventional electrical and magnetic materials, with potential applications in the fields of electronic and optoelectronics, health, catalysis and energy. These activities were possible thanks to a valuable combination of a wide range of complementary techniques existing at C²TN for both preparation and characterization of materials, enabling to address current challenges in materials science research and contributing to the establishment of more detailed correlations between the structure and the physical properties.

A significant part of the activities in this area has been possible by the operation and development of infrastructures and research tools, rare or even unique at national level, which have been placed open at the benefit of a large external community through an extensive network of scientific collaborations. These facilities include materials modification by ion implantation, neutrons, gama and electron irradiation, several ion beam techniques for elemental composition analysis and the Low Temperatures and High Magnetic Field Laboratory with facilities for the study of electrical transport, magnetic properties of materials and Mössbauer spectroscopy.



DEVELOPMENT OF CHITOSAN-BASED MATRICES BY RADIATION TECHNOLOGIES FOR BIOMEDICAL APPLICATIONS

Chitosan-based matrices with poly(vinyl pyrrolidone) (PVP) were obtained by gamma irradiation from a Co-60 source. Radiation dose, copolymer concentration and synthesis procedure were found to tailor matrix porosity and surface roughness, giving materials with enhanced properties to be applied as skin substitute capable of tissue regeneration.

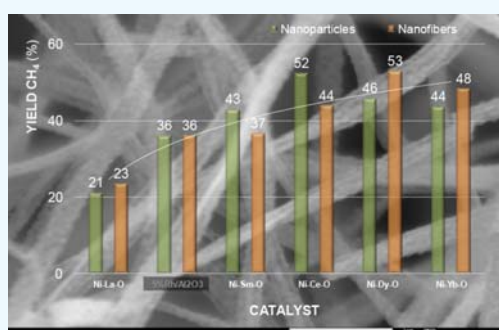
MULTIFUNCTIONAL MATERIALS

Mössbauer spectroscopy was used as a key technique to study the role of electron charge transfer and magnetic ordering of the Fe cations on a material combining conducting and magnetic electrons and based on anilate coordination polymer.



During 2018, the scientific output of the team involved in Advanced Materials studies was: 44 papers in peer-reviewed journals, 3 book chapters, 3 proceedings, 7 invited and 19 contributed lectures in conferences, 1 PhD, 3 MSc and 1 graduated completed theses, and 2 patents. The team research has been supported by European, FCT and bilateral projects, with several new projects being secured this year. The team has participated in the organization of 2 conferences and workshops and 1 international training courses. A significant participation in the scientific and technical activities of European Union Technology Platforms and Networks, namely COST ACTIONS CA15128 CM1105, TD1004 has also taken place. During 2018 the team has also prepared and submitted several common projects under calls from EC, FCT, CERN-FCT, and Horizon 2020.

The activities had contributions from different research groups (ES, ETN, QEf, and REI) as more detailed described in their reports. The following major achievements in 2018 are highlighted.

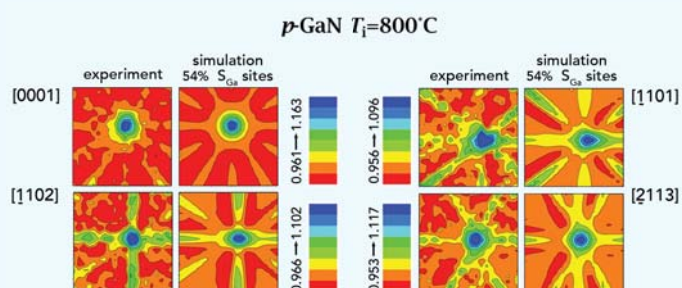


NANOSTRUCTURED COMPOUNDS CONTAINING *f*-BLOCK ELEMENTS AND VALORIZATION OF CO₂ AS FEEDSTOCK

Nanostructured bimetallic oxides containing 4*f*-block elements (La, Ce, Pr, Sm, Dy, and Yb) and nickel supported on silica and alumina obtained by electrospinning, when tested as catalysts for the methanation of CO₂ were found to exhibit enhanced activity and selectivity towards the production of methane and stability on the gaseous stream.

AMPHOTERIC BEHAVIOUR OF BE AS DOPANT IN GAN

The amphoteric nature of Be in p-GaN, n-GaN and as-grown n-d-GaN was revealed using the β -emission channeling technique with implanted radioactive ¹¹Be (13.8s). Results show a balance of substitutional Be_s vs interstitial Be_i depending on doping type and implantation temperature.



Radiopharmaceutical Sciences Group

MISSION AND OBJECTIVES

The main research activities of the Radiopharmaceutical Sciences Group (RSG) aim at the development of innovative target-specific radiopharmaceuticals for Positron Emission Tomography (PET) or Single Photon Emission Computed Tomography (SPECT) Imaging and Targeted Radionuclide Therapy (TRT), for the diagnosis and/or treatment of oncological, cardiovascular or neurodegenerative diseases. Owing to its translational potential, this research field contributes towards the rise of molecular and personalized medicine. The group is a key partner of renowned national/international institutions involved in radionuclide production, nuclear medicine and biomedical research due to its rare combination of radiopharmaceutical chemistry expertise with preclinical evaluation skills. There is also an active collaboration with national and international research groups and biotech companies engaged in the discovery and development of novel drugs. The RSG provides also advanced training to students and young scientists on Radiopharmaceutical Sciences and Medicinal Chemistry, being a partner of the Marie-Sklodowska Curie ITN “MEDICIS-Promed” led by CERN and the PhD program “ChemMedTrain” coordinated by the Universities of Coimbra and Lisboa.

MAIN ACHIEVEMENTS

1 NOVEL MOLECULAR IMAGING TOOLS FOR CYSTIC FIBROSIS

The aim of the project is to bring forward a novel molecular imaging approach to cystic fibrosis (CF) through the development of specific anti-CF transmembrane conductance regulator (CFTR) radioprobes. The validation of novel anti-CFTR antibody fragments using biochemical techniques revealed detection of CFTR protein. However, cellular uptake studies using the antibodies as radioprobes did not reveal differences in two CFTR-expressing cell lines (normal and mutated). These results paved the way to explore the use of different antibody formats for CFTR imaging. Based on the phage display technology, we are currently selecting and expressing smaller antibody fragments against CFTR for further radiolabelling and evaluation of their ability to recognize the protein in the cellular environment.

2 BIFUNCTIONAL ¹¹¹IN-COMPLEXES FOR BREAST CANCER THERANOSTICS

We have explored an approach that combines two different biological targeting moieties, an estrogen receptor (ER) ligand (LXXLL peptide or estradiol derivative) and a nuclear-targeting moiety (the DNA intercalating agent acridine orange, AO, or a peptidic nuclear localizing sequence), in a single ¹¹¹In-hybrid compound for dual targeting of breast

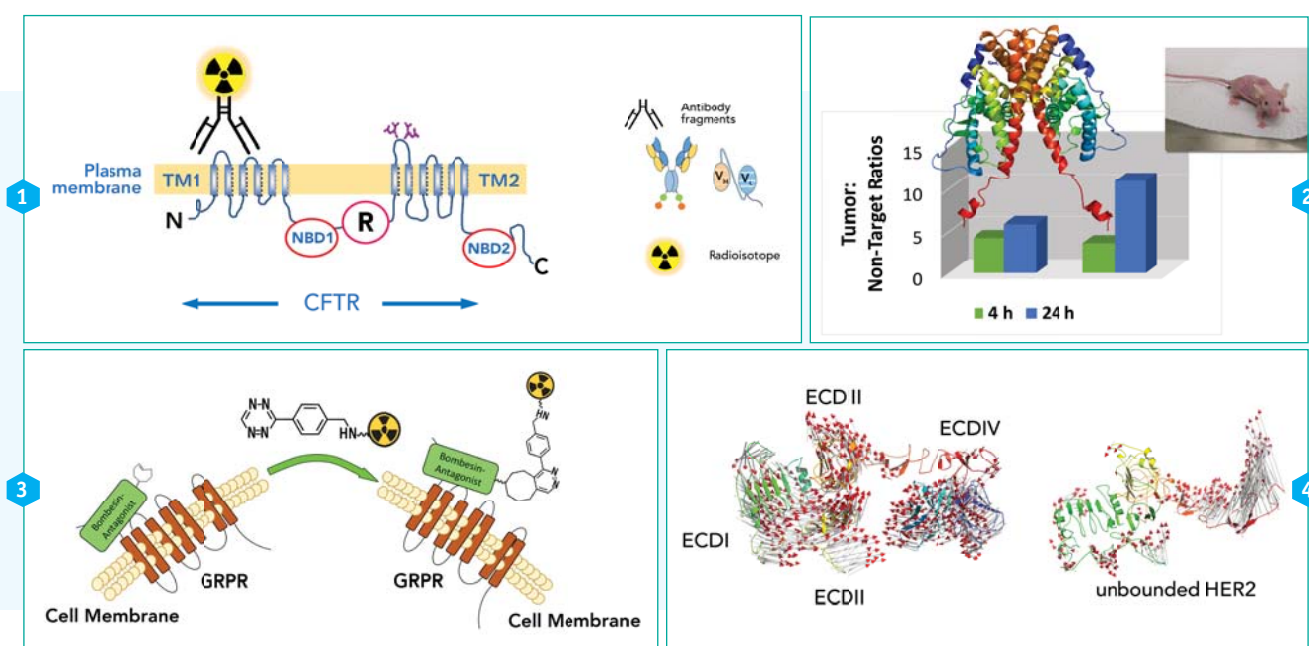
cancer (BC) cells. Evaluation of the ^{111}In -dual conjugates in MCF-7 cells demonstrated high nuclear internalization (> 50%); in tumor-bearing mice, their biodistribution profile was also quite promising, with high *in vivo* stability, fast blood clearance and high uptake in ER rich organs and MCF-7 xenografts. The favourable tumor/non-target tissue radio-activity ratios suggest the potential of these new bifunctional radioconjugates for the development of theranostic agents.

3 CLICKABLE BOMBESIN ANTAGONISTS FOR PROSTATE CANCER THERANOSTICS

The pretargeting approach based on peptide receptor antagonists might allow a more selective and efficient delivery of radionuclides to tumor sites. Towards this goal, we have studied IEDDA click reactions of a trans-cyclooctene (TCO)-containing gastrin-releasing peptide receptor (GRPR) antagonist (bombesin derivative, BBN) with a small library of clickable ^{111}In -labelled DOTA derivatives carrying a tetrazine (Tz) group. The most promising ^{111}In -complex showed increased cellular uptake when human prostate PC3 cells were previously incubated with the antagonist, revealing the occurrence of a click reaction with the BBN antagonist interacting with the GRPR on the cell surface. Future studies will confirm whether these results can be translated *in vivo* using prostate cancer xenografts in mice.

4 NOVEL SYNTHETIC PEPTIDES FOR INTERFERING WITH THE RANK-TRAF6 PATHWAY

The RANK-TRAF6 pathway is involved in cancer development and progression, namely in breast cancer. One of the potential ways to inhibit this pathway is to block the interaction of TRAF6 with RANK using decoy peptides, which will lead to an antiproliferative activity in cancer cell lines. We have assessed the stability of the interaction of TRAF6 with five different peptides and determined their binding affinity by *in silico* studies. Based on those results, we have identified the most promising sequences with ability to interfere with the RANK-TRAF6 interaction. These peptides were prepared by Fmoc solid-phase peptide synthesis, purified by RP-HPLC and characterized by ESI-MS and Circular Dichroism. The evaluation of their antiproliferative activity in specific cancer cell lines is currently underway.



4 (A) HER2:scFv complex; (B) unbound HER2

Radiological Protection and Safety Group

MISSION AND OBJECTIVES

The Radiological Protection and Safety Group is a unique research group in Portugal, undertaking fundamental and applied research activities addressing multidisciplinary, cross-cutting and leading edge topics in:

- ⦿ Dosimetry and Radiobiology,
- ⦿ Environmental Radioactivity and Radioecology,
- ⦿ Radioactive Waste,
- ⦿ Metrology,
- ⦿ Nuclear and radiological emergencies and accidents.

The objectives of the Group's activities encompass i) the deployment of unique scientific and technical expertise, skills and competence in radiological protection and safety in Portugal ii) keeping abreast of the state-of-the-art in scientific and technical topics and in international regulations and safety standards in radiation protection and radiation safety iii) higher education and training of students and professionals and the supervision of PhD or MSc students iv) the provision of scientific advice to the Portuguese stakeholders in policies and issues related to the application of ionizing radiations and radioisotopes v) raising the awareness about hot topics and multidisciplinary issues associated to the biological effects arising from the medical, industrial and environmental exposures to ionizing radiation of workers, patients and members of the public.

The GPSR researchers use laboratory infrastructures and equipment and state-of-the-art radiobiology, radioanalytical, dosimetry and metrology techniques. They master computational techniques, namely Monte Carlo simulations and modelling, in support of radiological protection activities related to medical, occupational and environmental exposures.

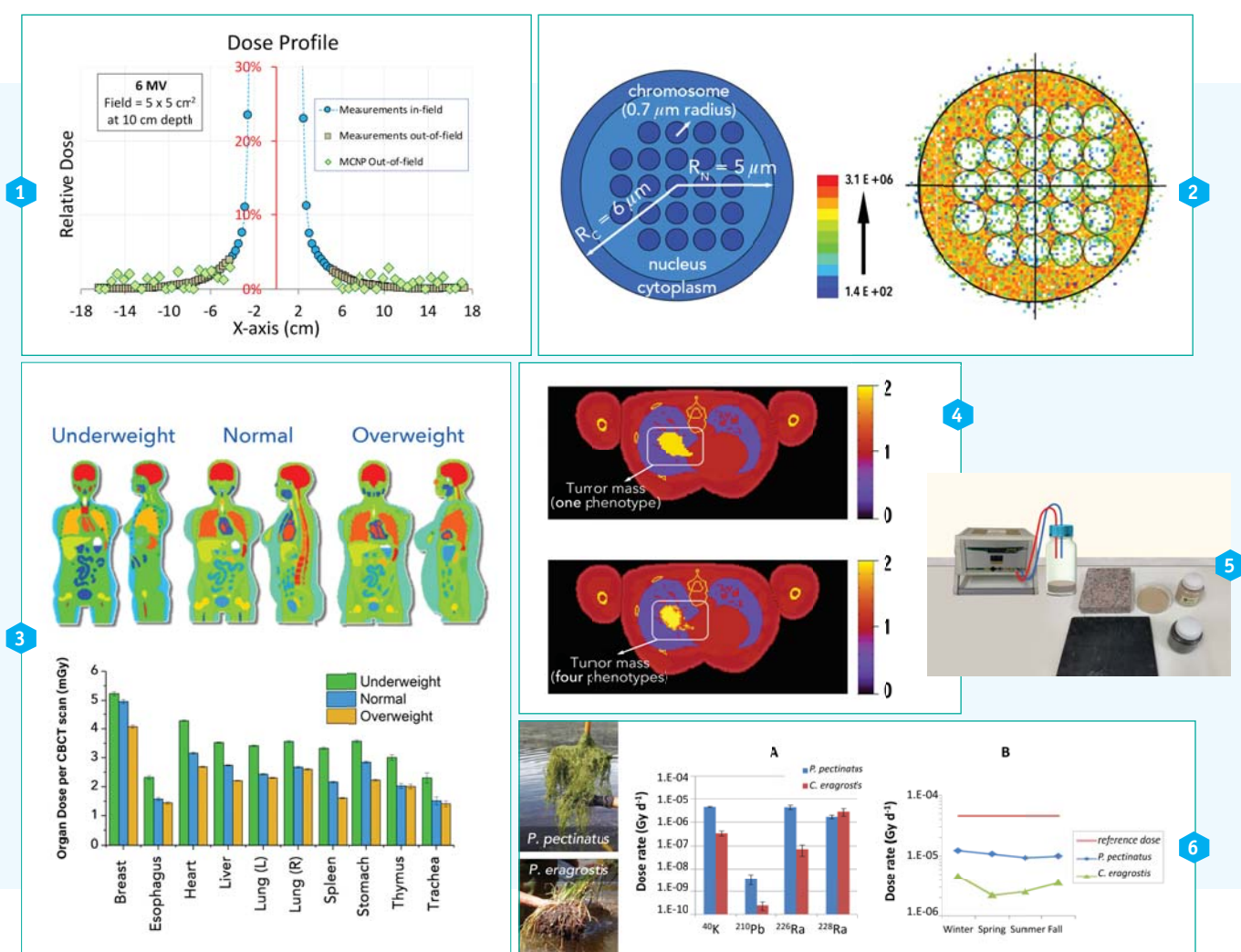
Throughout 2018, the Group's activities featured a high degree of internationalization and:

- ⦿ Were sustained by the participation in R&D projects funded by the European Union (EU) HORIZON 2020 Programmes, by EURAMET (European Association of National Metrology Institutes), by the FCT, or in collaboration with CERN and other research centres in Europe.
- ⦿ Included the participation in the EU Technological and Research Platforms MELODI (Multidisciplinary European Low Dose Research), EURADOS (European Radiation

Dosimetry Group) IGD-TP (Implementing Geological Disposal of Radioactive Waste), NERIS-TP (Preparedness for Nuclear and Radiological Emergency Response and Recovery) and Alliance (European Radioecology Alliance).

- Fostered collaborative links with Portuguese research groups, academia, hospitals and other stakeholders in Radiation Protection, in the framework of scientific projects and academic, education and training activities.

MAIN ACHIEVEMENTS



- Radiation therapy of paediatric patients – modelling radiotherapy Linacs and computing out-of-field doses
- Dosimetric assessment in critical sub-cellular volumes (cytoplasm, nucleus and chromosome) for accurate survival cell vs dose response curves evaluation
- Organ doses due to Cone Beam Computer Tomography (CBCT) imaging in Image Guided Radiation Therapy (IGRT) using patient-dependent voxel phantoms.
- Nanodosimetry and targeted radiotherapy – Dosimetric assessment in different tumor sub-volumes with Auger electron-emitting radionuclides
- Radon and thoron exhalation rates from building materials
- Radiation dose assessment in aquatic and emergent plants in Tejo river

Radiation, Elements and Isotopes Group



MISSION AND OBJECTIVES

GREI is an interdisciplinary group with expertise on nuclear related analytical techniques focusing in Environment Studies, Cultural Heritage and Materials Sciences. The group operates an Ionizing Radiation Facility with gamma and e-beam sources and other facilities dedicated to: elemental, isotopic and trace element determinations, radiocarbon dating; microbiological and chemical analysis of radiation effects in products; and MeV ion microbeam analytical techniques. Major research fields are: environmental pollution; palaeoenvironmental evolution and climate changes; water quality, protection and management; wastewater treatment; provenance, manufacturing technologies and chronological framework of ancient artefacts; materials processing by ionizing radiation for biomedical and industrial applications.

MAIN ACHIEVEMENTS

1 CHRONOLOGICAL SILVER ALLOYS COMPOSITION DURING THE 4TH DYNASTY; COINS VERSUS JEWELRY

Portuguese silver coins from the 15th-17th centuries were analysed by non-destructive PIXE technique to determine major, minor and trace elements of the silver alloys which allowed to: 1. establish a chronological framework of the silver alloy used, the silver ore provenance and metallurgical procedures; 2. differentiate production centers (Lisbon and Oporto); 3. allow comparison with coeval Portuguese silver objects, namely Indo-Portuguese silver jewellery from the Ancient Art Nacional Museum (MNAA); 4. help for detecting forgeries.

The work was performed in collaboration, using coin collections from the Portuguese Mint House (ICNM – Imprensa Nacional Casa da Moeda) and from the Bank of Portugal (BdP).

2 RADIOLYTIC DEGRADATION MECHANISMS OF CORK WASTEWATER POLLUTANTS

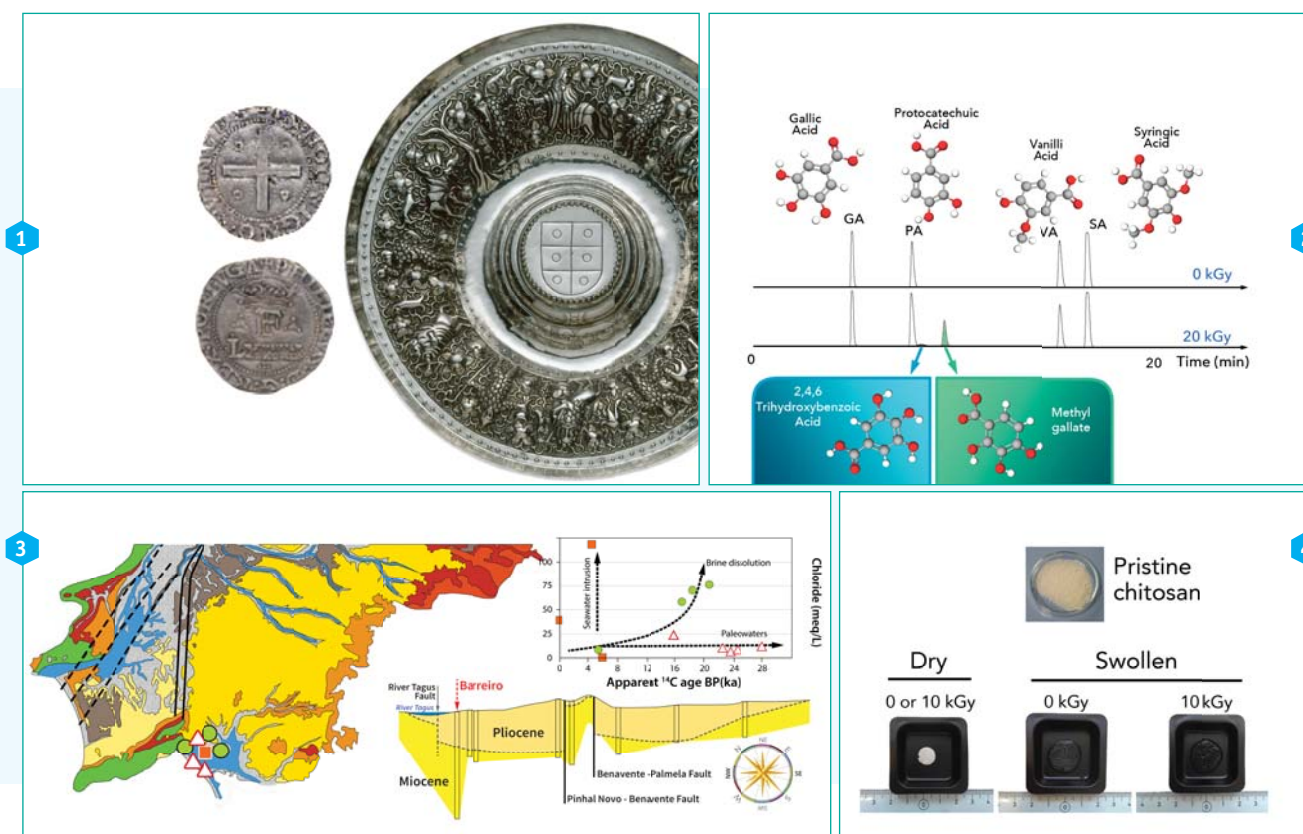
The feasibility of gamma irradiation treatments to degrade four phenolic compounds (gallic acid, protocatechuic acid, vanillic acid and syringic acid) present in cork wastewaters was investigated in isolated and mixture aqueous solutions under different pH's and irradiation atmosphere conditions. Degradation rates were 50% higher for the treated solutions at 20 kGy under aeration and at natural pH. Two different compounds were identified as radiolytic products, and their fragmentation pathways were proposed. Results highlighted that ionizing radiation could be used as clean technology, without the addition of chemicals, for pollutants degradation using doses of 20 kGy.

3 COASTAL AQUIFERS – DEGRADATION AND CLIMATIC CHANGES FINGERPRINTS

The continuous decrease of recharge in semi-arid and arid regions leads to a strong groundwater mineralization, enhanced by higher evaporation rates. The impact in the groundwater systems due to over exploitation was investigated in coastal aquifers (Cape Verde, Tunisia, Morocco and Portugal). Results obtained revealed: an increase of land extent by seawater intrusion and a clear influence of marine aerosol; a deficiency of water management together with increase needs for Human supply resulting in serious degradation of water resources; the presence of old groundwater (± 4000 years BP) indicating recharge under different climatic conditions (Santiago Island, Cape Verde).

4 DEVELOPMENT OF CHITOSAN-BASED MATRICES BY RADIATION TECHNOLOGIES FOR BIOMEDICAL APPLICATIONS

Research aims to engineer chitosan-based matrices using ionizing radiation for skin substitute capable of tissue regeneration. Radiation processing avoids the use of initiators/solvents and enables preparation with simultaneous sterilisation. Several chitosan-based matrices with poly(vinyl pyrrolidone) (PVP) were obtained by gamma irradiation from a Co-60 source. The in vitro cellular viability and proliferation of fibroblasts provided information on biocompatibility and ability to assist skin regeneration. Results show that radiation dose, copolymer concentration and synthesis procedure tailor matrix porosity and surface roughness. Chitosan/PVP (5%) matrices irradiated at 10 kGy present the higher cellular viability. In vivo studies are ongoing.



Nuclear Engineering and Techniques Group



MISSION AND OBJECTIVES

The Nuclear Engineering and Techniques research group (NET) explores the uses of nuclear and related techniques within a high range of scientific fields. The group develops advanced materials using unique radioactive beams and nuclear techniques at ISOLDE-CERN, being responsible for the maintenance and development of the experimental Portuguese infrastructure built by CTN teams at that infrastructure. The group is also interested in the study of the violation of the mean field description of exotic nuclei, the development of state-of-the-art software for X-ray analytical methods and establishment/application of quantitative instrumental speciation methods, mainly for PIXE, and the modal identification of dynamical systems under operational conditions as a viable alternative to traditional approaches. NET also probes the interaction of radiation with matter upon emission and detection of the radiation, providing unique information regarding the structural, electronic, magnetic and dynamical local properties. In addition, NET group develops innovative research on earth sciences and cultural heritage (characterization, provenance and luminescence absolute dating) in close relation with museums and other public/ private entities. Regarding health and environmental issues, NET focuses on the study of low activity samples of long-lived isotopes in collaboration with hospitals and other C²TN groups, and research on air pollution assessment and on the transition to a low carbon economy. Education and training is also a major mission of NET group, being encompassed in several PhD and MSc programs. Another challenge of NET group is the development of a policy of linking knowledge with action for effective societal responses to persistent problems of the various level of scientific intervention of NET, aiming to make academic research more relevant to other types of organizations and practitioners. We try that research be problem driven rather than concept centric.

MAIN ACHIEVEMENTS

TUNNELLING IONIZATION PROCESSES INDUCED IN CHARGED UP ION BEAM IRRADIATED MATERIALS

Enhancement emission of X-ray by irradiated charged materials, known since the 1970s is not yet fully explained. Experimental results obtained in 2018 lead to the proposal of a tunnelling ionization model (represented here), which allows explaining all qualitative details of the process. In short, an aggregation of ions generates a potential well represented by the curve in brown may emerge, which action on the atomic potential, leads to a result presented by the curve in green. Grey arrows represent tunnelling transitions. (Reis & Chaves, 2018).

2 LUMINESCENCE DATING AND COMPOSITIONAL STUDIES OF CERAMICS FROM ANTEQUERA MEGALITHIC LANDSCAPE (UNESCO WORLD HERITAGE)

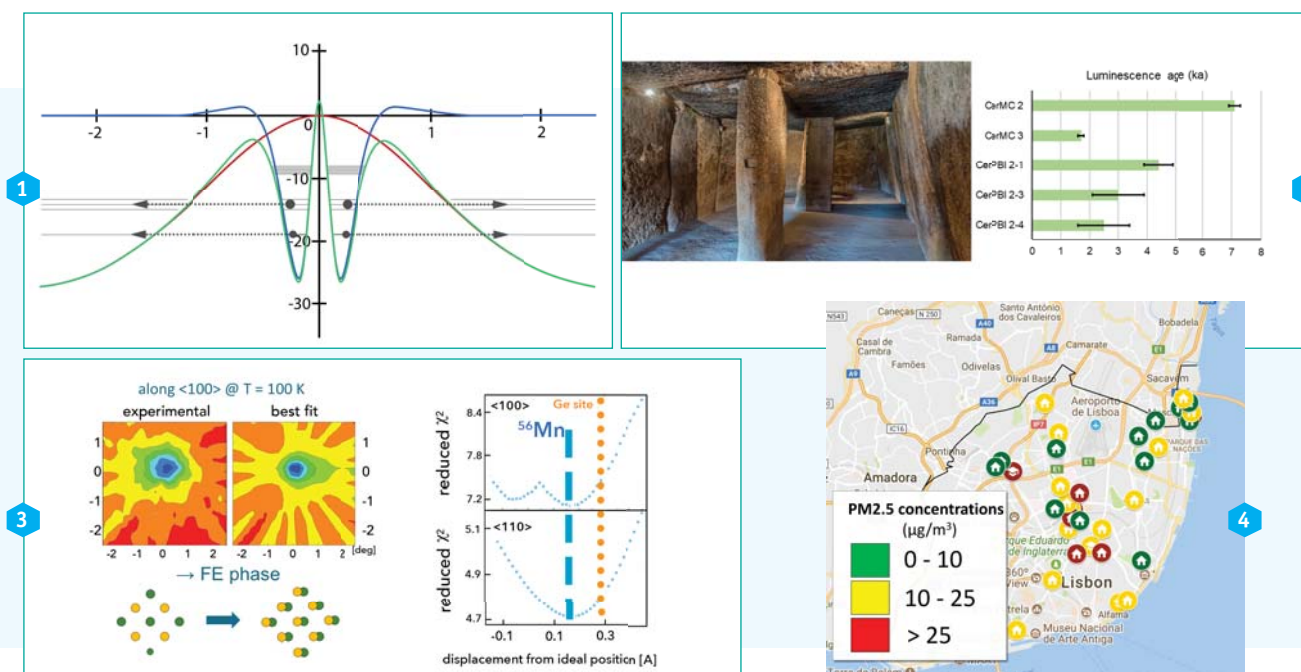
Luminescence, geochemical and mineralogical studies helps on establishing chronologies, provenance and production technologies of ceramics from Antequera Megalithic Landscape (UNESCO World Heritage). They have been mostly produced with calcite rich raw materials under low firing temperatures (Rogerio-Candelera et al., 2018). The luminescence ages are between $1,7 \pm 0,1$ ka and $7,1 \pm 0,2$ ka complementing archaeological data and establishing the chronological range of human occupation on Antequera Megalithic landscape.

3 FIRST STUDIES ON MUFERS ($\text{Ge}_{1-x}\text{Mn}_x\text{Te}$)

Multiferroic Rashba semiconductors (MUFERS) are novel quantum materials that couple ferromagnetism, ferroelectricity and the Rashba-Zeeman. $\text{Ge}_{1-x}\text{Mn}_x\text{Te}$, the model MUFERS, inherits its robust ferroelectricity and giant Rashba splitting from $\alpha\text{-GeTe}$, undergoing a ferroelectric and structural phase transition at T_c^{FE} with elongation along $\langle 111 \rangle$. A spontaneous ferroelectric dipole appears due to the displacement between the cation, Ge or Mn, and the anion Te sub-lattices. We probed this displacement with sub-Angstrom precision, below and above the ferroelectric transition, using β -emission channelling with implanted radioactive ^{56}Mn (2.6h). [L.M.C. Pereira, et al. CERN-INTC-2017-085 / INTC-P-526].

4 LIFE INDEX-AIR: ASSESSING CHILDREN EXPOSURE TO AIR POLLUTANTS

The time activity pattern survey for children living in Lisbon, developed within the LIFE Index-Air project (www.lifeindexair.net), showed that during the week they spend 89% of their time indoors - 55% in home, 27% in classrooms and 3.5% in vehicles. PM_{2.5-10} and PM₁₀ samples were collected in the indoor and outdoor of 40 homes, 5 schools and 4 transport to calculate the daily children exposure levels to PM components. PM_{2.5} concentrations measured in homes and schools from Lisbon differs ($\mu\text{g}\cdot\text{m}^{-3}$) showing that the level of the indoor air pollutants is the principal parameter for the assessment of the exposure, dose and burden of disease (E. Chalvatzaki, et al., 2018).



f-Element Chemistry Group

MISSION AND OBJECTIVES

The research activities of the QEf Group are centered in the study of the chemistry of lanthanides and actinides at fundamental and applied levels, with focus on topics of relevance in environmental, nuclear and materials sciences.

The activities comprise the synthesis of new *f*-element compounds and materials (complexes with new coordination environments, metal-organic frameworks, ionic liquids, nanostructured intermetallic compounds and bimetallic oxides), the examination of their properties, searching for unusual or enhanced behaviour, and reactivity and catalytic studies (activation of unsaturated and redox-active substrates, activation/elimination of major gaseous pollutants such as CO₂, CH₄ and N₂O, and production of value-added compounds such as CH₃OH). Studies on the recovery and separation from secondary sources of Rare Earth Elements (REEs), considered as critical materials by the European Commission, as well as other metal separations, are also carried out by the Group.

MAIN ACHIEVEMENTS

1 GAS-PHASE ACTIVATION OF HYDROCARBONS BY RARE EARTH AND ACTINIDE OXIDE NITRATE ANIONS

Trivalent rare earth (RE) tetranitrate anions, [M(NO₃)₄]⁻ (M = Sc, Y, Ln), are easily produced by electrospray ionization (ESI) and give rise to oxide nitrate anions, [MO(NO₃)₃]⁻, by collision induced dissociation (CID) in a quadrupole ion trap (QIT) that results in NO₂ elimination. For most of the REs, these oxide anions contain a radical oxygen and are highly reactive species. CID of [M(NO₃)₄]⁻ in the presence of ethane, ethene and benzene showed the formation of [M(OR)(NO₃)₃]⁻. These C-H activation reactions were also observed for [ThO(NO₃)₄]⁻ anions. These experimental studies bear interest in the long-standing search for systems that can activate methane.

2 NANOSTRUCTURED COMPOUNDS CONTAINING F-BLOCK ELEMENTS AND VALORIZATION OF CO₂ AS FEEDSTOCK

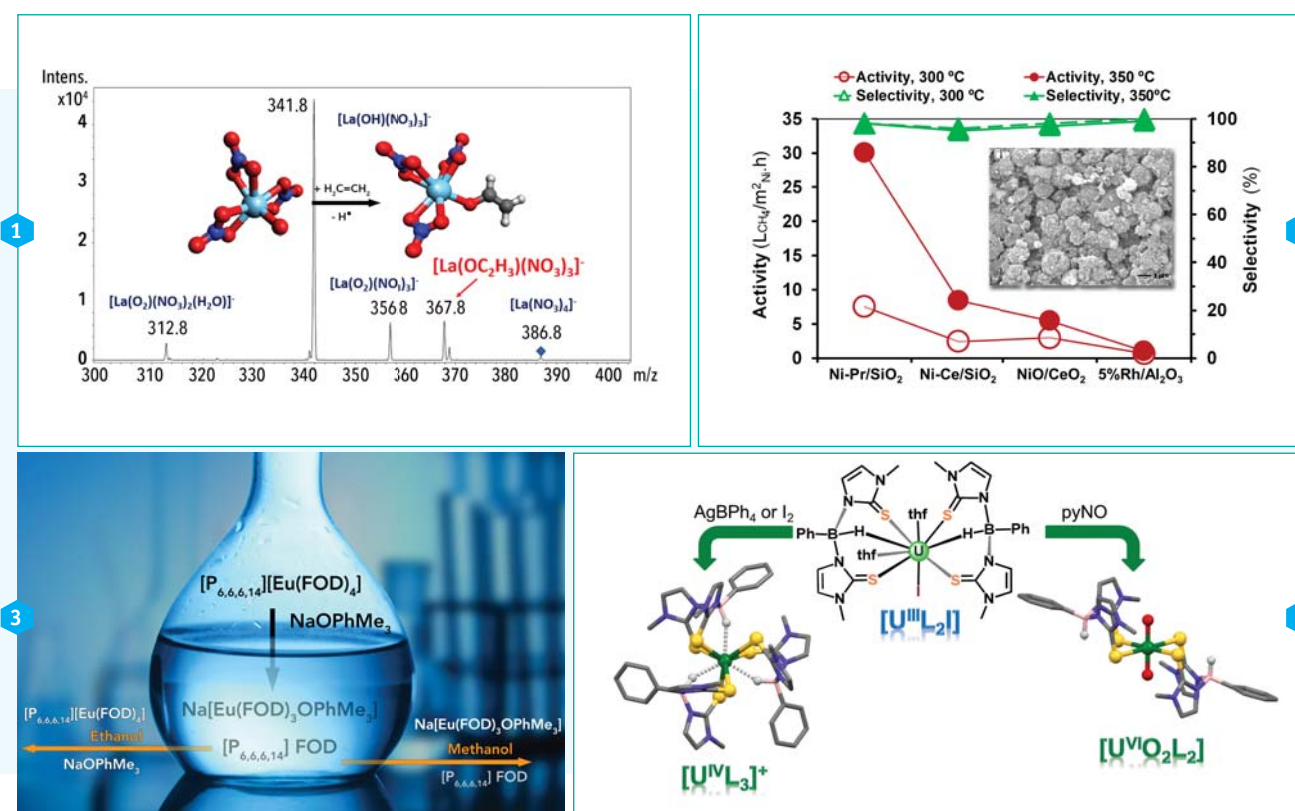
The work involves the preparation and characterization of nanostructured bimetallic oxides containing 4*f*-block elements (La, Ce, Pr, Sm, Dy, and Yb) and nickel supported on silica and alumina previously obtained by electrospinning. This is a reproducible and low cost route that enables the production of nanostructured materials, whose expected high surface areas and tunable surface properties bring benefits to their properties. They were tested as catalysts for the methanation of CO₂. Enhanced activity and selectivity towards the production of methane and stability on the gaseous stream are among the good results achieved in this work.

3 OPTICAL SENSORS

Based on the interaction of trihexyltetradecylphosphonium cation ($P_{6'6'6'14}$)⁺ with a β -diketonate (1,1,1,2,2,3,3-heptafluoro-7,7-dimethyloctane-4,6-dionate - FOD) of an Europium(III) tetrakis- β -diketonate complex, we found an equilibrium reaction with pronounced solvent effect between ethanol and methanol on Eu(III) luminescence, allowing detection and quantification of methanol in mixtures of both solvents (see Figure). The developed spectrofluorimetric method provides a faster and low-cost quality test to detect and quantify methanol with a limit detection of 15% (w/w).

4 NON-AQUEOUS URANIUM COORDINATION CHEMISTRY: URANIUM COMPLEXES SUPPORTED BY HYDROBIS(MERCAPTOIMIDAZOLYL)BORATES

The choice of the ancillary ligand is crucial for the stabilization of highly reactive metal complexes and for controlling their reactivity. Hydrobis(mercaptoimidazolyl)borate ligands are mono-anionic sulphur chelates that are able to stabilize neutral and cationic U(III) complexes. One-electron oxidation of the neutral U(III) complex $[U\{\kappa^3\text{-H,S,S'-H(Ph)B(tim}^{\text{Me}})_2\text{I(thf)}_2\}]$ (1) with AgBPh_4 or I_2 give the uranium tetravalent homoleptic compounds $[U\{\kappa^3\text{-H,S,S'-H(Ph)B(tim}^{\text{Me}})_2\}_3][X]$ ($X = \text{BPh}_4, \text{I}$) (Fig. 1). Treatment of 1 with pyridine-N oxide (pyNO) led to the formation of the uranyl complex $[UO_2\{\kappa^2\text{-S,S'-H(Ph)B(tim}^{\text{Me}})_2\}_2]$, while from the reaction of the cationic complex $[U\{\kappa^3\text{-H(Ph)B(tim}^{\text{Me}})_2\}_2(\text{thf})_3][\text{BPh}_4]$ with pyNO, the oxo-bridged U(IV) complex $[U\{\kappa^3\text{-H(Ph)B(tim}^{\text{Me}})_2\}_2(\text{pyNO})_2(\mu\text{-O})][\text{BPh}_4]_2$ was also obtained.



1 Structures and Mass Spectrum for the $[M(\text{OH})(\text{NO}_3)_3]^-$ reaction with $\text{CH}_2=\text{CH}_2$.

2 Activity and Selectivity of several catalysts for the methanation of CO_2 .

3 Calibration curve for methanol estimation in ethanol/methanol mixtures. χ is the molar fraction of methanol in ethanol.

4 Reactions of $[U^{\text{III}}\{\kappa^3\text{-H,S,S'-H(Ph)B(tim}^{\text{Me}})_2\}_2(\text{thf})_2]$ with oxidizing substrates.

Solid State Group

MISSION AND OBJECTIVES

The Solid State Group is a multidisciplinary research group focused on the study of selected new materials with unconventional electrical and magnetic properties. The group combines a wide range of expertise ranging from the synthetic chemistry of either molecular materials with transition metal complexes and electro active organic molecules or intermetallic compounds, to many different specialized solid state characterization techniques. Besides molecular synthesis, high temperature preparation and crystal growth and X-ray diffraction laboratories, the facilities developed maintained and operated by the group include the Low Temperature and High Magnetic Field Laboratory (LTHMFL). This laboratory unique in Portugal hosts different equipment for measurements at low temperatures down to 0.3 K and under high magnetic fields up to 18 T, including several magnetometers (SQUID, extraction and AC susceptibility) electronic transport and magnetotransport characterization and Mössbauer spectroscopy.

MAIN ACHIEVEMENTS

1 ANION DISORDER EFFECTS IN BILAYER MOLECULAR METALS

β'' -(CNB-EDT-TTF)₄BF₄ is a new member of the family of 2D metals with donor bilayer structure, presenting severe anion disorder. Electrical transport properties show metallic behaviour with localization effects below ~25 K. The large thermoelectric power S (~110 μ V/K) and its electrical conductivity $\sigma = 20$ S/cm at room temperature lead to a large power factor $S^2\sigma = 24$ μ W/K²m, placing these compounds as potential candidates for thermoelectric materials.

2 SLOW RELAXATION OF MAGNETIZATION IN MOLECULAR MATERIALS WITH d AND f ELECTRONS

A new series of Co(II) and Fe(II) complexes with strong magnetic anisotropy and large energy barriers for the magnetic relaxation and lanthanides complexes (Gd(III), Ho(III), Pr(III), and Er(III)) were characterised as single molecule magnets contributing to elucidate this behaviour.

3 CATION-ANION INTERACTIONS IN THE SPIN CROSSOVER PHENOMENON

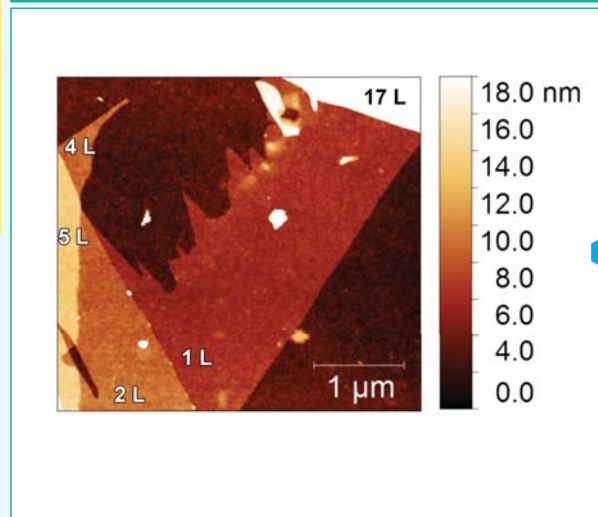
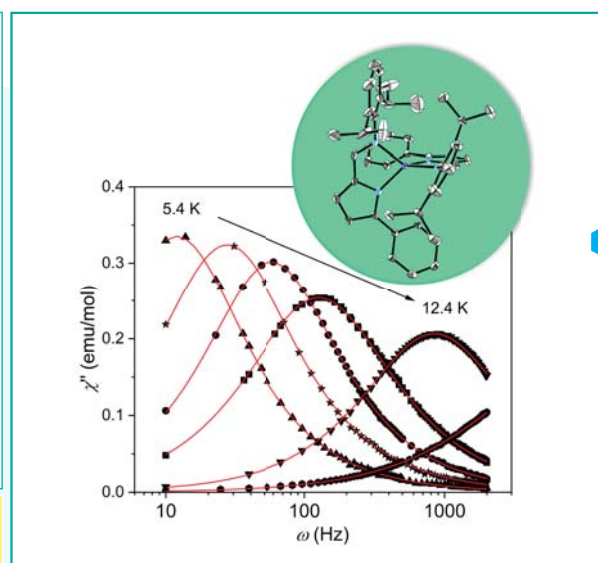
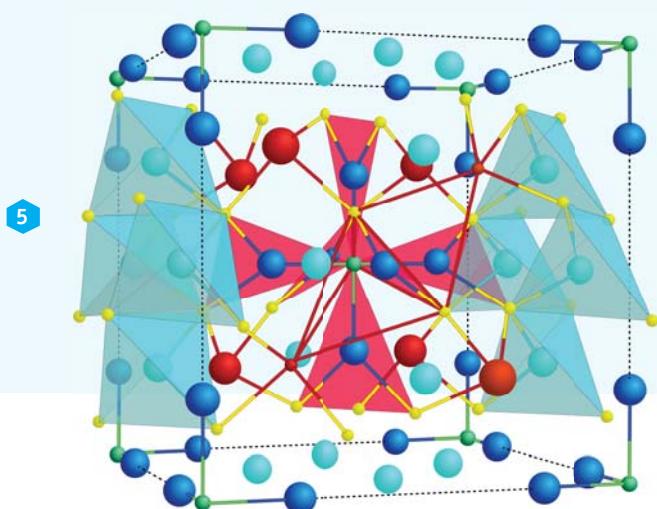
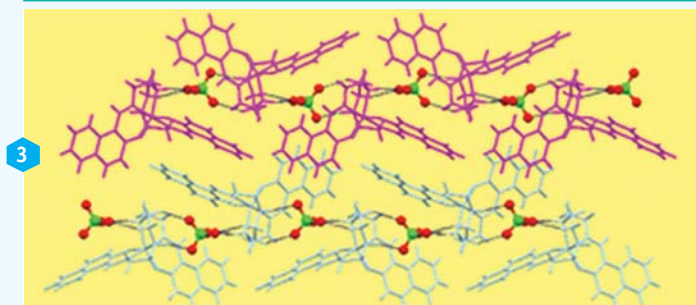
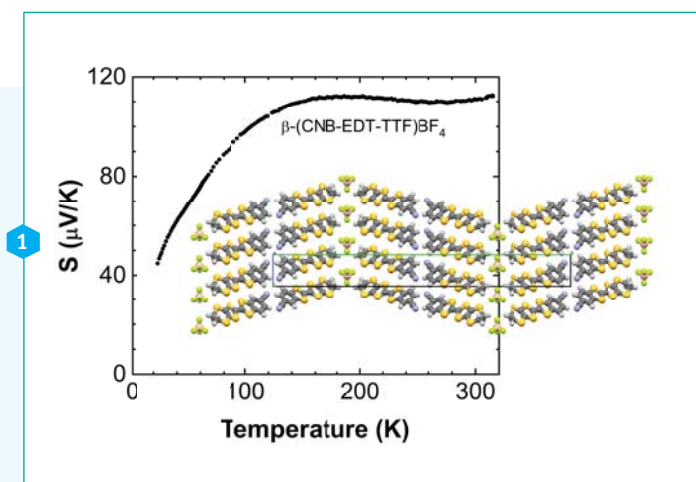
The study of six Fe(III) complexes with the closely related hexadentate ligands demonstrated the effects of crystal lattice rigidity and cation-anion interactions in the SCO behaviour.

4 2D MAGNETIC MATERIALS

Fe electronic state was determined by Mössbauer spectroscopy on a series of five isostructural layered magnetic coordination polymers based on Fe centres and different benzimidazole derivatives bearing a Cl, H, CH₃, Br or NH₂ side group.

5 NEW THERMOELECTRIC MATERIALS

The effect of composition on thermoelectric properties of tetrahedrites (Cu_{12-x}Co_xSb₄S_{13-y}Se_y) their oxidation behavior at high temperatures as well as glass ceramics Cu₂₀As₃₀Te₄₅, Cu₁₅As₃₀Te₅₅ and Cu₁₅As₂₅Te₆₅ were investigated and condition to achieve and preserve a high power factor were determined.



Outreach Group

MISSION AND OBJECTIVES

The C²TN's Outreach Group (GO) was formally created in 2018 with 3 main objectives:

- to promote and disseminate the relevance of the research, development and innovation activities and services provided by C²TN for the society and scientific communities, thus promoting the various aspects of scientific culture and knowledge;
- to increase the visibility of C²TN in national and international events and in social media;
- to encourage collaborative and cooperative links between C²TN and various stakeholders and actors in the academic, scientific, business, industrial and health fields.

GO works towards these objectives through:

- the organization and participation in seminars at schools, public libraries, scientific events, targeting different audiences;
- the coordination of guided visits to the infrastructures operated by C²TN members and the organization of "Open Days" dedicated to relevant topics related to C²TN activities that have a high social impact;
- the participation in summer internship programs organized by Ciência Viva,
- the organization of conferences and scientific workshops;
- the engagement in events of scientific relevance at the national and international levels.

GO's responsibilities also include the design, publication and release of promotional and informative material, such as, Activities Reports, pamphlets and posters. GO is in charge of C²TN's official website, social media accounts (such as Facebook, LinkedIn) and Blog, giving focus to all important and pertinent dates and events and also to the achievements of our researchers. Additionally, GO strengthens the bridge between C²TN members and other research centres, institutes, municipalities, schools and society in general, both at a national and international level, including IST's Communication Office and students associations. Finally, GO assists C²TN scientists in project submissions, contributes to the creation of new scientific networks and disseminates through the C²TN community new funding opportunities.

MAIN ACHIEVEMENTS

1 C²TN MARKETING PRODUCTS DESIGN

In 2018, GO designed and produced a set of communication and marketing products in order to disseminate C²TN and its activities, and to be presented and/or distributed in all

events that GO organized and participated. Moreover, the image of the Outreach Group was created to highlight the purpose of our activities: reaching the community to disseminate and show the importance and relevance of C²TN at the national and international levels.

2 “CIENTIFICAMENTE PROVÁVEL” PROGRAM

The “Cientificamente Provável” program aims at contributing to bridge the gap between primary and secondary education and higher education. In addition, this initiative aims at strengthening the young student’s motivation for acquiring knowledge and for pursuing higher education. C²TN established partnerships with Agrupamento de Escolas da Bobadela and Escola Secundária Fernão Mendes Pinto (Almada).

3 C²TN AT LOURES INSS

The GO was present on the 3rd edition of Loures InSS (a partnership between Câmara Municipal de Loures and Instituto Superior Técnico) that occurred at Parque Urbano de Santa Iria de Azóia in June 2018 (see Figure). The main objectives of this initiative were to convey good environmental and citizenship practices to the general public and to value the environmental potential of the city.

4 C²TN AT ENCONTRO CIÊNCIA 2018

The C²TN Outreach Group (GO) was present on the largest science meeting in Portugal in 2018, entitled “Science and Technology Summit in Portugal”, that was held at Lisbon, from 2nd to 4th of July.

5 C²TN AT NOITE EUROPEIA DOS INVESTIGADORES 2018

The 2018 edition of the initiative “Noite Europeia dos Investigadores” took place at the Museum of Natural History and Science and at Lisbon’s Botanical Garden (Lisbon’s University) on the 28th of September (see Figure). In that context, several activities were developed and promoted by the GO of C²TN as part of “C²TN’s contribution to the cities of tomorrow”.



- 1 C²TN's Outreach Group logo.
- 2 “Cientificamente Provável” program’s logo.
- 3 Photographic record of the event “Loures InSS”.
- 4 Photographic record of the event “Encontro Ciência 2018”.
- 5 Photographic record of the event “Noite Europeia dos Investigadores 2018”, including the successful “Science Dating powered by C²TN”.

C²TN Conferences at CTN Campus

During 2018, C²TN organized and hosted several scientific meetings, as well as a regular series of seminars by internal and external researchers.

MEETINGS

- ✧ EURADOS Annual Meeting 2018 (AM2018) & Winter School on “Application of physical and computational phantoms in dose assessment” / 5 to 8 February 2018, IST, Congress Centre, Lisbon (Portugal)
- ✧ 4th Conference on Small Animal Precision Image-Guided Radiotherapy / 12 to 14 March 2018, CTN-IST, Bobadela (Portugal)
- ✧ 48^{mes} Journées des Actinides (JdA2018) & 12th School on the Physics and Chemistry of the Actinides (12th SPCA) / 19 to 22 March 2018, CTN-IST, Bobadela (Portugal) & Hotel Golf Mar, Praia de Porto Novo (Portugal)
- ✧ ChemMat Doctoral Programme Workshop / 19 November 2018, CTN-IST, Bobadela (Portugal)
- ✧ Defense and Security Workshop / 21 November 2018, CTN-IST, Bobadela (Portugal)
- ✧ Workshop NRD Portugal / 7 December 2018, Escola Superior de Tecnologia da Saúde de Coimbra, Coimbra (Portugal)
- ✧ 2nd C²TN Workshop / 11 December 2018, CTN-IST, Bobadela (Portugal)

SEMINARS / Bobadela (CTN Auditorium), Loures Pole of IST (Portugal)



Prof. José Palma-Oliveira / [University of Lisbon, Lisbon \(Portugal\)](#) / 18 January
Conflict, Risk, and Resilience: A two-step process to overcome NIMBY and coordination failures



Bojan Petrovic / [Georgia Institute of Technology, Atlanta, GA \(USA\)](#) / 19 March
Modeling and simulations for nuclear science and engineering applications



Günther Dollinger / [Universität der Bundeswehr München \(Germany\)](#) / 22 March
Materials analysis by high energy heavy ions, focused protons, and low energy positrons



Paulo N. Martinho / [CQB, Faculdade de Ciências, Universidade de Lisboa \(Portugal\)](#) / 12 April
First-row transition-metal-based molecular sensors and molecular switches



Marta Ferraz Dias / [C²TN-IST, Universidade de Lisboa \(Portugal\)](#) / 4 October
What's next? ERC and Interreg Sudoe



Zaki Ajji / [Atomic Energy Commission, Department of Chemistry, Division of Analytical Chemistry, Damascus \(Syria\)](#) / 29 November
Current Status of Radiation Processing in Syria: Cultural Heritage Consolidation