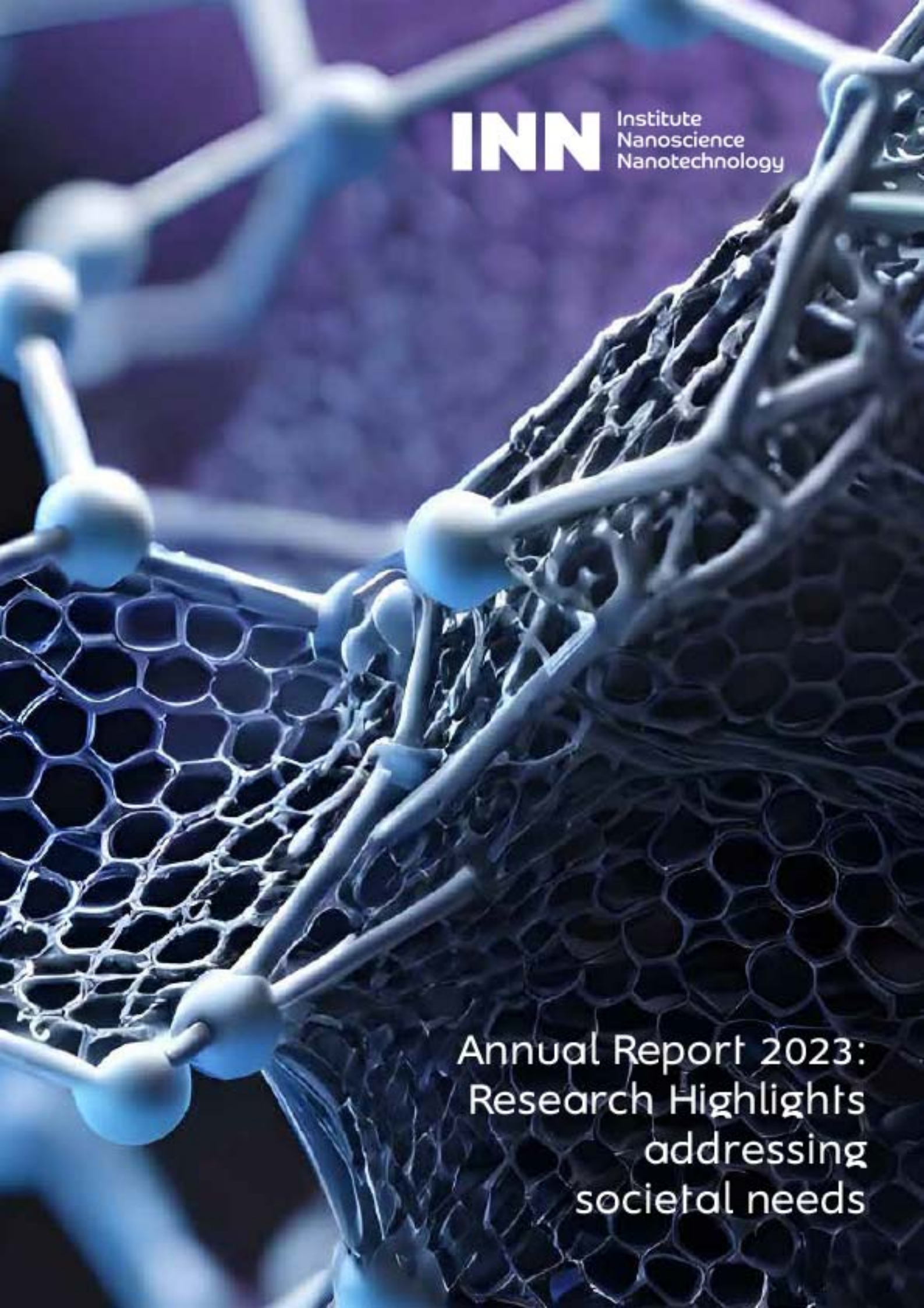

INN
Institute
Nanoscience
Nanotechnology
Annual Report 2023:
Research Highlights
addressing
societal needs

Table of contents

A note from Inn Director	3
Financials	4
INN at a glance	5
Scientific output	6
Lectures at INN	7
INN graduate student presentations	9
Excellent people & Infrastructures projects	10
ERC grants	10
Innovative training Networks	10
Individual Fellowships	11
Running Infrastructure projects	11
New projects in 2023	12
EU/Horizon	12
National Projects	12
Kick-off projects in first quarter of 2024	13
Spin-offs	14
Patents	16
Research Highlights addressing Societal Needs	17
Digital, Space, Defense & Security	19
Energy & Environment	25
Cultural Heritage	37
Quantum materials & technologies	41
Health & Agrofood	45
Fundamental Research	51

INN 2023 research highlights addressing societal needs and challenges



2023 has been a year of hard work and action for INN. Following the INN evaluation of 2022, the director, the Scientific Council and the researchers have devoted time to analyze the evaluation reports and work towards the recommendations to further promote excellence and advance the international status of INN.

Several Institute-wide, large proposals were submitted or prepared for submission: A WIDERA proposal, and two Emblematic Action proposals were submitted, the preparation of the Large Infrastructure proposal INNOVALTION-EL II has started, while in collaboration with the Industry Association HETIA a proposal for the Hellenic Chips Act Competence Center is in preparation.

Several large European Research Centers visited INN for presentations and collaborations including CSEM from Switzerland, CNR and others. Visits from large companies for collaborations mark the strong bonds of INN researchers with Greek and EU companies. INN researchers were active in many conference organizations, while INN and NCSR Demokritos hosted several international conferences and workshops co-organized by INN researchers.

In 2023 several tenure-track researchers were promoted to senior tenured positions, while several colleagues retired. Thus, a researcher recruiting and hiring plan is in preparation.

Realizing the need to communicate our research achievements to the general public, we started in 2022 with a report of research highlights for the general public.

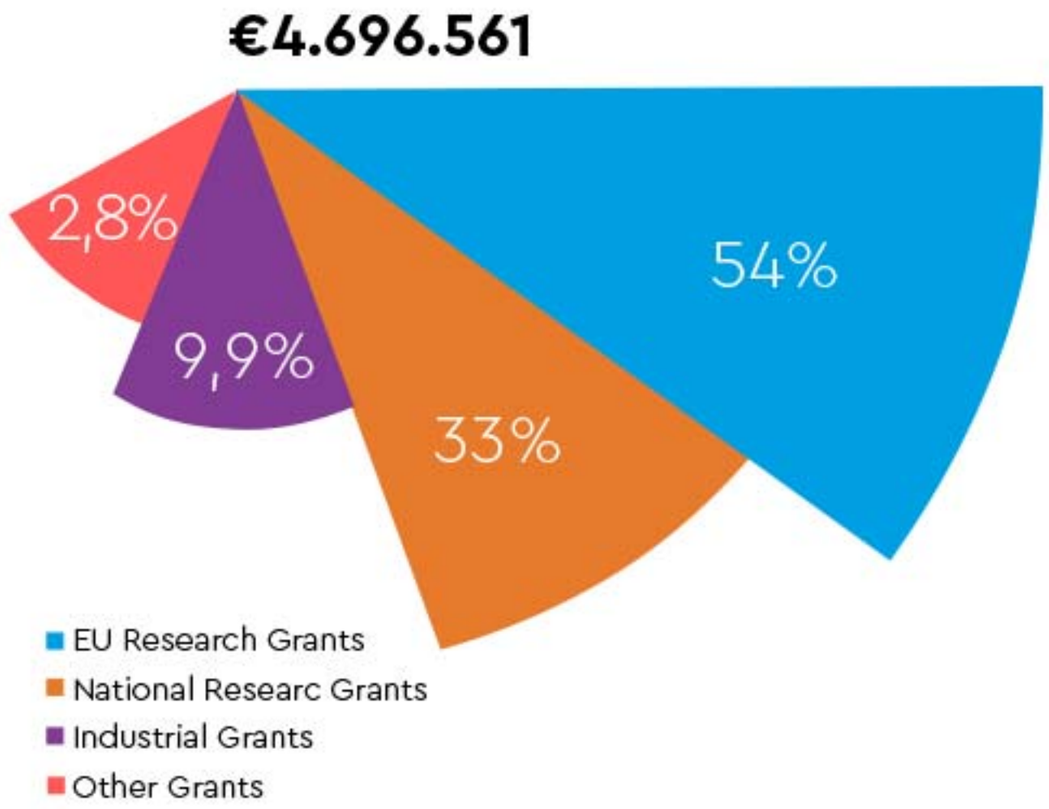
Following the success of the 2022 edition, we continue with the present 2023 edition. After a short presentation of the Institute, the report presents results addressing specific societal challenges, written in a language that can be grasped by the general public with some science background.

We thank you for reading and we are looking for your comments and suggestions for even better presented research highlights next year.

Sincerely
On behalf of the research, technical,
and administrative stuff

Evangelos Gogolides
INN Director

Financials



€2.549.487
EU Research Grants

€1.548.336
National Research Grants

€466.205
Industrial Grants

€132.533
Other funding

INN at a glance

293
People

72
Researchers

58
Postdocs

77
PhD Students

21
Administrative/ Technical

19
Lab Scientists

21
Master Thesis Students

25
Diploma Thesis/ Practical Training

213
Publications

11.480
Citations

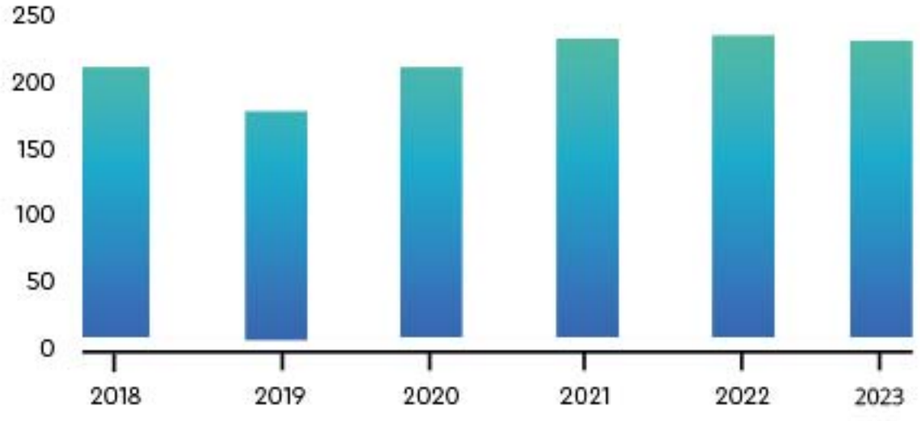
40
Running projects

10 Research + **1** Industrial
New Projects

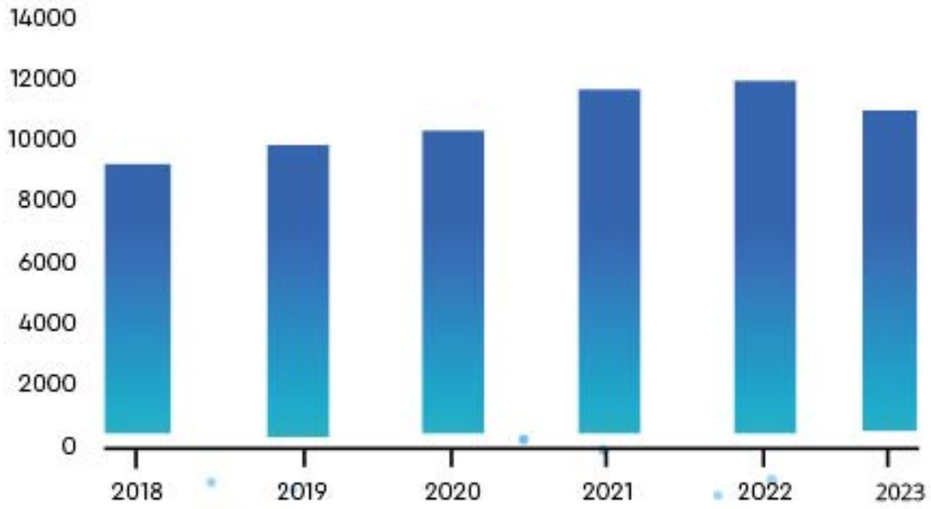
Scientific output

In particular, in 2023, this scientific work was reflected in a total of **213** articles in prestigious international scientific journals, **18** publications in conference proceedings, **62** chapters in books. Citations 11.480

INN Publications (per year)



INN Citations (per year)



Lectures at INN

Dr. Thomas Valentin
Centre Suisse d'Electronique et de Microtechnique (CSEM), Neuchâtel, Switzerland
CSEM: The Swiss Research and Development Center, on micro and nanotechnologies
17/1/23

Dr. Maud Vinet
CEA-LETI, Grenoble, France
Quantum Computing Based on Silicon
18/1/23

Δρ. Δημήτρης Κουλεντιανός
Center For Free Electron Laser Science (CFEL) & University of Hamburg, Hamburg, Germany
Πειραματικές μελέτες μοριακών συστημάτων με χρήση ακτινοβολίας συγχρότρου και λέιζερ ελευθέρων ηλεκτρονίων ακτίνων Χ
26/1/23

Prof. Carlo Beenakker
Leiden University, Leiden, The Netherlands
Topological quantum computing with Majorana fermions
8/2/23

Dr. Georges Kotrotsios
Centre Suisse d'Electronique et de Microtechnique (CSEM), Switzerland
Evaluating the economic impact of Research Organizations
20/2/23

Dr. Heike Riel
IBM Fellow, Head Science of Quantum & Information Technology, Lead IBM Research Quantum Europe & Africa
IBM Quantum Computing Roadmap
8/3/23

Prof. Torben R. Jensen
Interdisciplinary Nanoscience Center (iNANO) and Department of Chemistry, University of Aarhus, Denmark
Fast cation conductivity in the solid state – the fundament for development of novel types of batteries
24/3/23

Καθηγ. Σωκράτης Θ. Παντελίδης
Department of Physics and Astronomy and Department of Electrical and Computer Engineering, Vanderbilt University, Nashville, Tennessee 37235, USA
Electron microscopy combined with theory – Exploring new nanoscale frontiers
26/6/23

Lectures at INN

Prof. Giuseppe Barillaro
University of Pisa, Department of Information Engineering, Pisa, Italy
Implantable and bioresorbable chemical sensing systems for in-vivo monitoring of clinical-diagnostic markers 3/7/23

Καθηγ. Ευθύμιος Καξίρας
Department of Physics, Harvard University, Cambridge, MA 02138, USA
Twistronics: a new platform for exploring physics and applications in 2D 11/7/23

Prof. Ibrahim Abdulhalim
Department of Electrooptics and Photonics Engineering and the Ilse Katz Center for Nanoscale Science and Technology, ECE School, Ben Gurion University of the Negev, Beer Sheva 84105, Israel
Miniaturized high-performance photonics devices for sensing, modulation and energy saving 18/7/23

Prof. Giuseppe Barbieri
Institute on Membrane Technology (CNR-ITM), University of Calabria, 87030 Rende CS, Italy
Membrane Assisted Reaction, Separation and Mixing 7/12/23

Αναπλ. καθηγ. Γεώργιος Τσιλομελέκης
Department of Chemical and Biochemical Engineering, Rutgers University, New Jersey, USA
Oxidative Dehydrogenation of Light Alkanes over Metal Oxide Catalysts and the non-trivial role of CO2: A Spectrokinetic Perspective 13/12/23

INN graduate student presentations

Νικήτας Σιάννας
Σιδηροηλεκτρικές τεχνητές ηλεκτρονικές συνάψεις για νευρομορφικούς υπολογιστές

Ipek Moutafis
Recovery and valorization of added value substances from wastewater

Αλέξανδρος Κόντι
Μοντελοποιώντας τη γεωμετρία των νανοδομημένων επιφανειών: Πολυπλοκότητα και χάος 22/3/23

Νίκη Πλακαντωνάκη
Ανάπτυξη νανοδομών άνθρακα για περιβαλλοντικές και ενεργειακές εφαρμογές

Αντελαΐντα Σάχου
Νέες φωτοχημικές πορείες σύνθεσης παραγώγων των χρωστικών BODIPYs μέσω αυτο-οργάνωσης τους σε υδατικά περιβάλλοντα για φωτονικές εφαρμογές 10/5/23

Μιχάλης Βαγενάς
Μετατροπή CO2 σε νανοάνθρακες υψηλής προστιθέμενης αξίας

Λευτέρης Μανουράς
Κατεργασία εμπορικών μεμβρανών με χρήση τεχνολογίας πλάσματος 15/11/23

Έφη-Μαρία Παπία
Στοχαστική γεωμετρία και πορώδη υλικά: Διερευνώντας την ομοιομορφία των πόρων από εικόνες ηλεκτρονικής μικροσκοπίας

Βύρων-Σωτήριος Πετράκης
Σχεδιασμός και χαρακτηρισμός οργανομεταλλικών αυτο-συναρμολογούμενων νανοδομών με δι-ιμίδια περυλενίου 15/12/23

Excellent people & Infrastructures projects

ERC grants

Running ERC project

MIX2FIX

Hybrid, organic-inorganic chalcogenide optoelectronics

Th. Stergiopoulos

NCSR Budget 2.731.750€

New ERC Project (Kick off in first quarter 2024)

TheMa

On-chip energy harvesting and management enabled by thermal engineering of two-dimensional materials.

Alexander El Sahat

NCSR Budget 1.288.750€

Innovative Training Networks (ITN-ETN)

PlaCe-ITN
Pre-modern Plasters and Ceramics

Training the next generation of archaeological scientists: Interdisciplinary studies of pre-modern Plasters and Ceramics from the eastern Mediterranean

P.I.: V. Kilikoglou

NCSR Budget 486.035 €

SMART -X

Study of carrier transport in materials by time resolved spectroscopy with ultrashort soft X-ray light

P.I.: A. Dimoulas

NCSR Budget 243.018 €

Individual Fellowships (IF)

THermIC

Local Thermal and thermoelectroic transport in 2D transition metal dichalcogenide based nanostructures and devices – Thermic

Alexander El Sahat

P.I. A. Dimoulas

NCSR Budget 165.085 €

PARACAT

Paramagnetic Species in Catalysis Research. A Unified Approach Towards Heterogeneous, Homogeneous and Enzyme Catalysis

P.I.: G. Mitrikas

NCSR Budget 18.000 €

Running infrastructure projects

PlasmaForNano

Inorganic nanostructuring to the atomic limit via plasma nanotechnology

P.I.: E. Gogolides

NCSR Budget : 1.1439.424 €

ATT SENSE

Attica Sensor Technology Center

V. Kilikoglou

NCSR Budget : 1.160.000€

New Projects in 2023

EU / HORIZON

SuperClean
Horizon Europe
P.I. E. Gogolides
1/2/2023-31/12/2025
NCSR Budget: 899.875 €

KnowSkite-X
Horizon Europe
P.I. Z. Sideratou
1/1/2023-31/12/2026
NCSR Budget: 509.250 €

SINCERE
National Projects Ε.Σ.Π.Α 2014-2020
P.I. I. Karatasios
1/10/2023-30/09/2026
NCSR Budget: 191.376 €

2D – ENGINE
Horizon Europe
P.I. A. Dimoulas
1/10/2023-30/09/2027
NCSR Budget: 543.875 €

FIXIT
Horizon Europe
P.I. A. Dimoulas
1/11/2023-30/11/2027
NCSR Budget: 425.000 €

LAURICON
Horizon Europe
P.I. I. Bassiakos
1/09/2023-28/02/2026
R Budget: 177.934 €

National Projects

COF4SEA
ESPA / PEP ATTIKIS
P.I. P. Dallas
14/06/2023-31/12/2024
NCSR Budget: 149.517 €

3GPV-INDUSRTY
ESPA
P.I. P. Falaras
01/08/2023-02/12/2024
NCSR Budget: 547.000 €

PeroNANOFOOD
ESPA / ELIDEK
P.I. M. Vasilopoulou
18/12/2023-17/12/2024
NCSR Budget: 80.000 €

COVASTIA
ESPA / ΠΡΑΣΙΝΟ ΤΑΜΕΙΟ
P.I. E. FILIPPAKI
03/04/2023-02/04/2024
NCSR Budget: 200.000 €

Kick off in first quarter of 2024

AEROSOLS
E.E. / HORIZON
P.I. F. Katsaros
1/4/2024 – 31/12/2026
NCSR Budget: 508.750 €

INFRACHIP
E.E. / HORIZON
P.I. P. Dimitrakis
1/1/2024 – 31/12/2027
NCSR Budget: 523.453 €

HEAD
National Projects / ELIDEK
P.I. S. Steriotis
01/02/2024-31/12/2025
NCSR Budget: 191.376 €

TheMa
E.E. / HORIZON ERC
P.I. El Sahat
1/122024 – 31/1/2029
NCSR Budget: 1.288.750 €

RESIN GREEN
E.E. / HORIZON
P.I. P. Argitis
1/1/2024 – 30/6/2027
NCSR Budget: 765.000 €

CONCEPT
E.E. / HORIZON CL4XXX
P.I. A. Dimoulas
1/1/2024 – 31/12/2027
NCSR Budget: 318.625 €

EXERCISE
National Projects / ELIDEK
P.I. E. Gogolides
01/02/2024-31/12/2025
NCSR Budget: 210.000 €

NOUS
E.E. / HORIZON CL4XXX
P.I. P. Dimitrakis
1/1/2024 – 31/12/2026
NCSR Budget: 651.875 €

DIGI4ECO
E.E. / HORIZON Miss-xx
P.I. T. Steriotis
1/3/2024 – 29/2/2028
NCSR Budget: 344.250 €

NuCapCure
E.E. / HORIZON EIC
P.I. K. Stefanopoulos
01/02/2024-31/07/2028
NCSR Budget: 300.093 €

Data4Solar
National Projects / ELIDEK
P.I. D. Davazoglou
01/02/2024-31/12/2025
NCSR Budget: 197.553 €

MultiCool
National Projects / ELIDEK
P.I. N. Kehagias
1/2/2024 – 31/7/2028
NCSR Budget: 300.093 €

Spin- offs

The following is a list of youngest companies that are directly related to INN, and are using partly its facilities for production, or testing, or office space in the Technology Park.

ThetaMetrisis S.A.

ThetaMetrisis S.A. was established in 2008 and was the first spin-off company of the former Institute of Microelectronics (now part of INN). It specializes in non-destructive characterization of coatings in the nano- and micro- scale and biosensors for PoN applications in Health & Food Safety. In 2014, ThetaMetrisis LLC in CA, USA was established, while the company has expanded into the point that of having sales representatives in several European countries and has also penetrated the Asian and Middle-Eastern market with sales representatives all the way to Japan and Korea. In April 2018, the growth of the company led it to its new, larger location.

AISTHISIS Ltd

Aisthisis Technologies Ltd provides intelligent hardware components and solutions on sensing applications bringing to market a novel silicon micromachining technology, SBE (Self-aligning, Binding & Etch-back) that is applied to capacitive, single crystal silicon pressure sensors and switches. Aisthisis also offers services in the field of MEMS development and in particular in MEMS design and process development. The company has been recently expanding in order to include in its products passive wireless RF sensor tags.

Nanometrisis

Nanometrisis is one of the two most recent spin-offs of INN established in 2016. The company creates software tools used for the measurement and quantification of geometric and morphological characteristics of micro and nanostructures during semiconductor manufacturing, or the manufacturing of other nanotechnology products. Nanometrisis software family incorporating state-of-the-art mathematical methodologies inspired by information science and complex theory can characterize the size, topography, roughness and morphology of nanostructures from the analysis of microscopy images.

Nanoplasmas

Nanoplasmas is a company founded in 2016 as spin-off of INN and is the second of the two youngest companies emerging from the institute. The company uses an innovative, patented, plasma-based technology to produce healthcare and diagnostic consumables with enhanced performance. The Nanoplasmas team is highly experienced in surface modifications, plasma processing and device fabrication, and can offer customized solutions for a wide range of requests, such as wetting control, microfluidics fabrication, self-cleaning and antifouling surfaces, and optical properties control

PLINIOS

PLINIOS was founded in 2005 as a spin-off company of INN. Plinios, applying advanced microscopy methods, provides services in the field of evaluation of environmental risks in every kind of facility. The evaluation of these risks is necessary so that the health of the users of the facility will be safeguarded, hazardous substances will be properly managed, compliance with the environmental legislation will be ensured and future investments in that facility will be protected.

Patents in 2023

Compounds for the detection of ligandrol

Emmanouil N. Pitsinos, Yiannis S. Angelis, Michael Petrou, PCT/EP2023/063907, international filing date. Description: The compounds can be used as reference products in the determination of the administration of ligandrol to a subject.

Novel nanocomposites with micro slime layer control properties for fouling release paint applications

Oreozili Sideratou, Fotios Katsaros, Andreas Sapalidis, Sergios Papageorgiou, Zeynep Burcu Baybogan-Isilak, Ali Akcali, European Patent Office, EU Unitary patent number 3170872/07-06-2023 (published in European Patent Bulletin 23/2023).

Description: Innovative nanocomposite 4th generation fouling release paints with micro-slime layer control properties against floral and faunal fouling for application on objects immersed into seawater.

Magnetic Swing Absorption

Dionysios Karousos, Andreas Sapalidis, Goerios Karanikolos, Evangelos Favvas, European Patent Office, number US 2023/0302399 A1 (published in European Patent Bulletin 28/9/2023).

Description: Embodiments include a method of magnetic swing absorption which may include contacting a fluid mixture including one or more gases and a liquid absorbent in a separation chamber, absorbing at least on of said gases using the liquid absorbent, optionally in the presence of a constant inhomogeneous magnetic field.

MagneticBased determination of sorption separation factor for binary gas mixtoures

Dionysios Karousos, Andreas Sapalidis, Goerios Karanikolos, Evangelos Favvas, European Patent Office, number US 2023/0296704 A1 (published in European Patent Bulletin 21/9/2023).

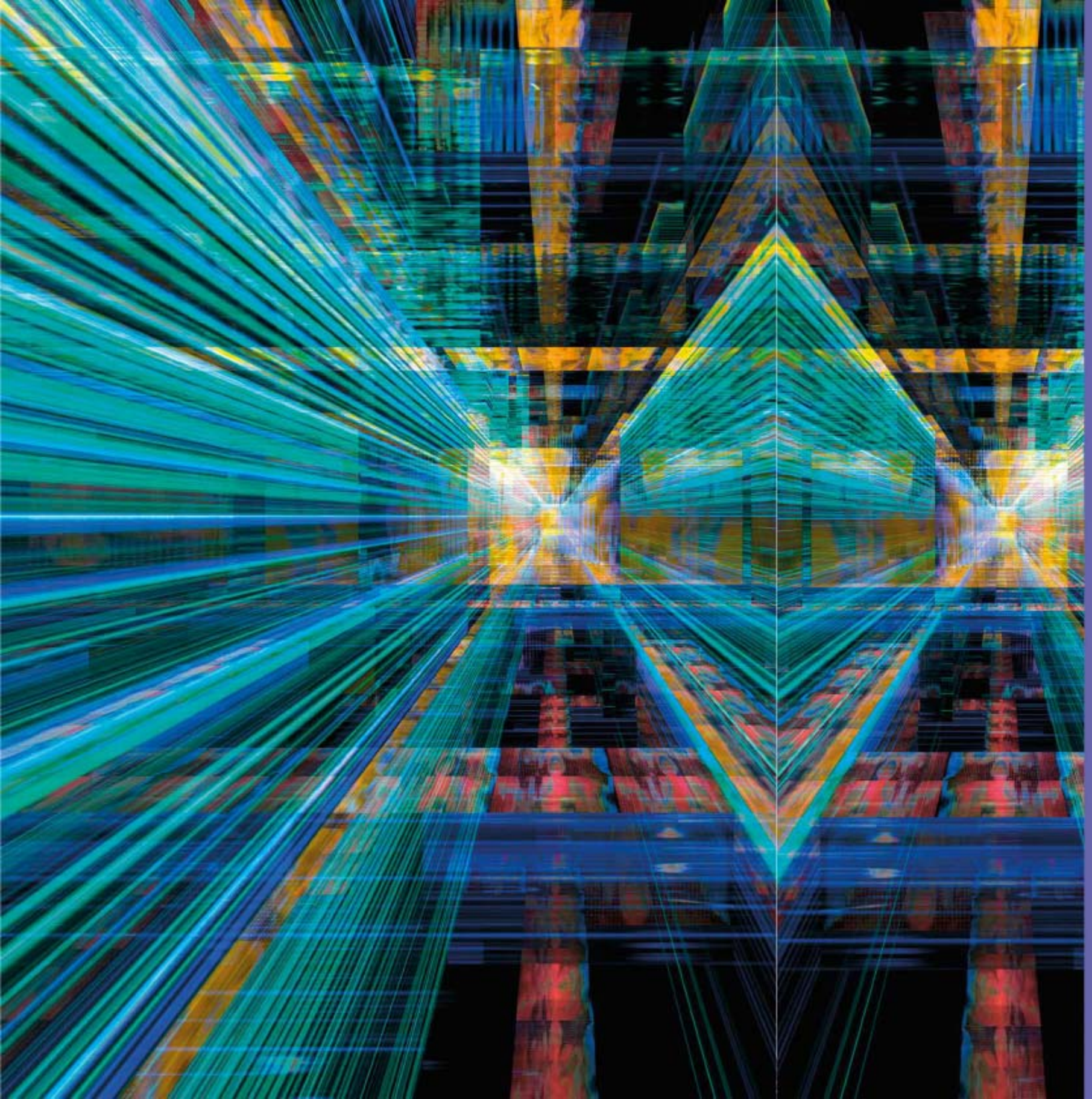
Description: Embodiments include methods (and related systems, devices and apparatuses) for determining a sorption separation factor for a binary gas mixture by applying a magnetic field to at a least a portion of a sorbent disposed in a chamber of a magnetic susceptibility device.

Iminodiacetic Acid Substituted Cyclodextrins as Potentiators Of Beta-Lactam Antibiotics

K. Yannakopoulou, M. Agnes, V. Miriagou, S.-A. Kotsakis, G. Miliotis, European Patent EP3714 904 B1. Filed: 27.3.2019; Granted: 23.8.2023 jointly to NCSR «Demokritos» and Hellenic Pasteur Institute.

Description: Combinatorial therapeutic regimens based on iminodiacetic acid-substituted cyclodextrins are used to treat infections caused by Gram-negative pathogens. The compounds fully restore the activity of β-lactam antibiotics against Gram-negative clinical isolates producing the three main MBL enzymes, both in-vitro and in-vivo and display high bioavailability and a well-tolerated and potent pharmaceutical profile.

Research Highlights addressing societal needs



Digital, Space, Defense & Security

Tunning structural colour by controlling plasmonic metasurfaces properties

Plasmonic colors emerge from resonant interactions between light and metallic nanostructures. As opposed to chemistry-based coloring, nanoscale structural coloring has been proposed to minimize usage of additives and to provide bright non-fading colors. With the development of scalable and low-cost advance nanomanufacturing techniques (exp. nanoimprint lithography), structural colors can open new possibilities in several industrial applications, such as colored plastics, surface decorations, and anti-counterfeiting, providing low cost and easily recyclable products. Our team has demonstrated large area plasmonic colors fabricated by ultraviolet (UV) nanoimprint lithography on a transparent substrates. In search of new low-cost and scalable ways to produce adaptable multi-coloured plasmonic surfaces we explore the possibility of locally tuning the color by changing the effective refractive index of the surrounding nanostructures.



Real Morpho butterfly showing blue colour wings and artificial plasmonic metasurface (5cm x 5cm) showing respectful same blue colour



Dr. Nikolaos Kehagias (Researcher)



Dr. Nikolaos Matthaiakakis (Post-Doctoral Researcher)



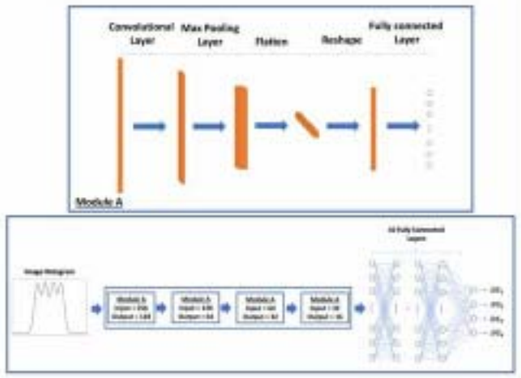
Nafsli Dimogerontaki, (PhD student)



Konstantina Tourlouki (PhD student)

Machine Learning evaluation of microscopy image segmentation methods

Multiphase materials are encountered in several areas of science and technology. Their properties are determined by the fraction of the phases (material compounds) constituting the composite material. Therefore, the quantitative characterization of phase fractions is highly demanded and has been the subject of extensive studies. To this end, a widely used technique is the segmentation of back-scattered electron SEM (BSE-SEM) images given that different phases are depicted with pixel collections of different luminosity. Gaussian mixture models (GMM) are one the most popular and easily implemented methods to segment the BSE-SEM images through the deconvolution of their histograms. However, the accuracy and the limitations of their application have not been fully investigated. Our team designed a neural-network approach to fill this gap and provide a fast tool for the automatic evaluation of the accuracy of GMM predictions for all material phases based on the inspection of the measured SEM image histogram alone. The proposed tool facilitates the decision-making process of an SEM user concerning the optimum choice of a segmentation method.





Nikos Boukos



Vassilis Constantoudis



Michalis Vrigkas

AI vs human artistry with microscopy image metrics

Traditionally, creativity has been seen as the hallmark of human intellect, deeply intertwined with the arts. With the advent of AI, capable of generating artworks, the question arises: can machines match the creative capabilities of humans? Specific mathematical methods, initially tested to understand complex nanomaterial structures in microscopy images, can be harnessed further into analysing a broad range of imagery. This study dives deep into the canvas, by employing a mathematical analysis of paintings across various artistic genres, analyzing them through the lenses of Shannon entropy and complexity. The findings reveal that while AI can mimic general art styles, capturing the diversity of human artists' styles proves more elusive, as highlighted by the metrics' variances. Interestingly, the analysis also revealed that differences can be also found in the color changes regarding pixels of similar luminosity. Overall, this study hopes to provide an approach towards deeper understanding of the prowess of AI models and offer new insights into the ability to distinguish between human created and AI-generated images.



Vassilis Constantoudis

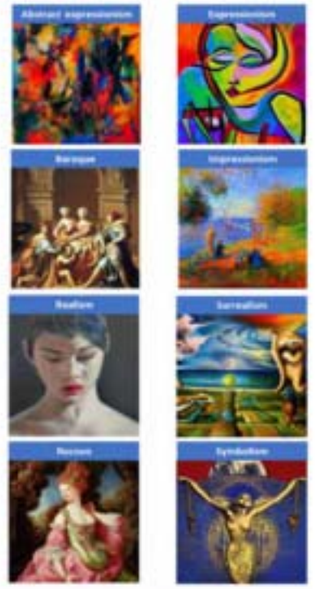


Alexandros Kondi



Efi-Maria Papia

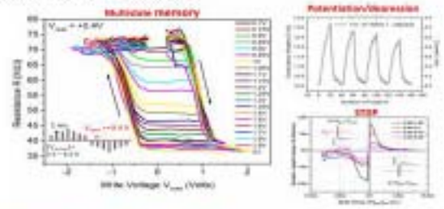
More info:



New ferroelectric field effect electronic synapse for neuromorphic computing

Edge computing in mobile systems with a low power consumption of ~1 mW requires devices with an extremely high energy efficiency of 1000 Terra Operations per Second per Watt (TOPS/W). This could be achieved by emulating the high parallelism and in-memory computing function of the human brain to realize artificial neural networks in hardware in the form of crossbar AI accelerator arrays which perform "multiply-and-accumulate" functions. The memristor is an important device for the storage and update of the synaptic weights leading to analog in-memory computing.

We have demonstrated a new ferroelectric field effect memristor synapse with unprecedented low voltage/low power operation. The device comprises a Si-compatible $Hf_{0.5}Zr_{0.5}O_2$ ferroelectric and a $SrTiO_3$ semiconductor bottom electrode directly integrated with silicon. Due to the combined electronic field effect and ionic redox effect in the semiconductor, the device functions as a programmable resistor with more than 16 stable non-volatile intermediate states (4-bit memory). The device exhibits synaptic plasticity with nearly ideal (linear and symmetric) potentiation and inversion with identical pulses. It also shows biologically plausible synaptic behavior such as pair pulse facilitation and spike timing dependent plasticity operating in the millisecond range at an extremely low voltage below 1V. The estimated energy consumption per programming event is around 8 pJ which is comparable to biological synapses. The devices are suitable for use in large and dense AI accelerator arrays and in future advanced spiking neural networks for unsupervised learning.





Dr. A. Dimoulas



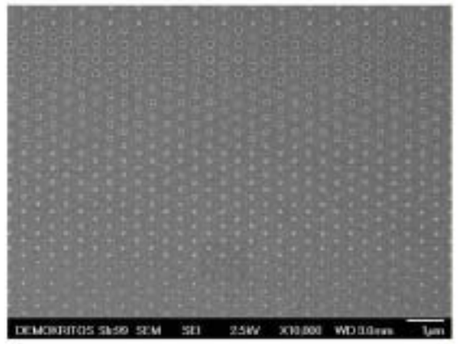
Dr. P. Tsipas

More info:

Resist process engineering and analysis coupled with Electron Beam Lithography

Electrosensitive resists can be precisely exposed and patterned using finely focused high-energy electron beams in a crucial process for the micro/nano-electronics community, known as electron beam lithography (EBL). The physicochemical properties (resolution, sensitivity, contrast, etching rates, process residuals, substrate adhesion etc) typically vary between available resists and, in addition, they can be modulated via controlling processing parameters (thermal tempering / development conditions etc).

Medusa 82 and Medusa 82 UV, two negative tone, inorganic resist formulas rich in Si oxide content, conceived and manufactured by Allresist GmbH, were subjected to exhaustive processing tests at INN's clean room facility using the dedicated 100kV EBL tool installed, for comparative studies and in order to determine best processing conditions for focused EBL applications. Theta-Metrisis (a Demokritos' spin-off company) provided state-of-the-art technological support in the project, offering real-time dissolution monitoring and non-destructive, optical thickness measurements (contrast curves).



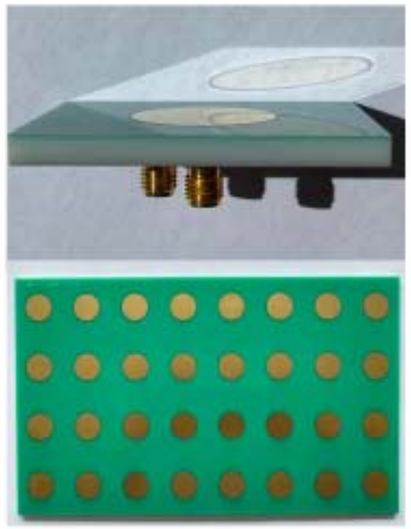
SEM picture of hexagonal dot pattern with increasing dot diameter (minimum critical dimension equal to 20nm).



Dr George Papageorgiou

Multilayer printed antennas and arrays for 5G applications

The development of 5G communications has refocused antenna research in a variety of applicable frequency bands. 5G applications in the 3.5 GHz range emerge as very important for many countries, and motivate the present work. We describe a class of printed patch antennas that involve 3 metal layers all completely integrated within a single dielectric, which are of very high efficiency and significant directivity and gain. The antennas presented have dual linear polarization, and sufficient bandwidth to be suited for sub-6 5G applications, producing advantageous antenna arrays monolithically integrated into a single planar PCB that are thin and lightweight. The feeding mechanism is through an intermediate dedicated metal layer designed to couple the input power to the antenna without a direct metal contact to the radiating patch. The multilayer design allows for monolithic integration of multi-element combiners and phase shifters and results in compact monolithic scanning arrays. Single-element gains reach 7 dBi while 32-element rectangular array gains reach 21 dBi. Theoretical simulations and measurements of fabricated prototypes are in very good agreement and validate the proposed designs.



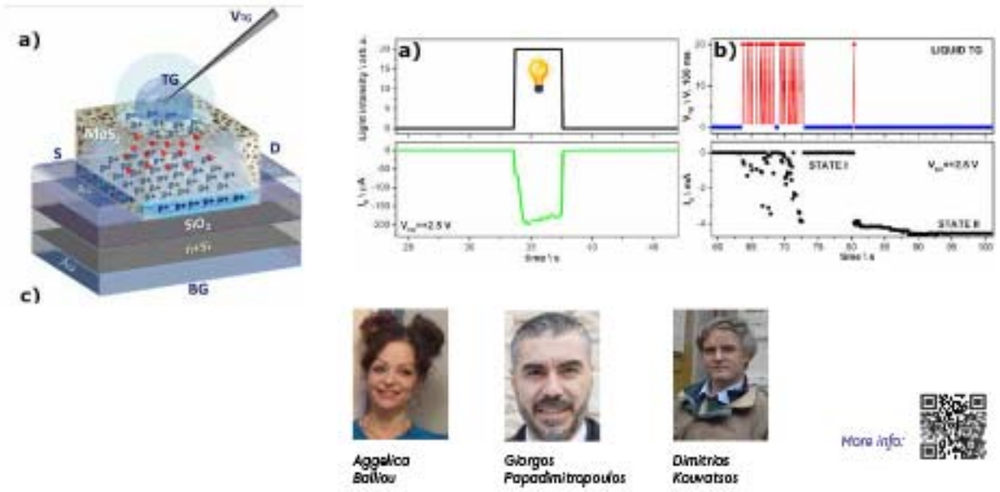


Harry Contopanagos

More info:

Thin Film Devices
TFTs with photoswitching and memory in cheap precursors

Thin film devices in inexpensive precursors at room and low temperatures are essential for electronics on anything. Our research has concerned specialized techniques for the fabrication of thin film transistors (earlier work on sensors), with possible applications in integrated microsystems. Much activity on thin films by mainstream chemical and physical deposition methods is in progress; however, our work is focused on niche methods. It has involved fabrication and characterization of TFTs in MoS_2 thin films deposited at room substrate temperature or spun on various substrates; these procedures are suitable for other precursor films as well. We use our recently developed technique for the fabrication of ionic liquid (CuPc/bu) – solid state mixed channel FETs. This hybrid materials methodology is the first time that liquid phase performance enhancement has been achieved for TFTs in low mobility active films. Besides the massive device improvement earlier obtained, we show that not only photo-enabled switching but also memory functionality are enabled by the hybrid architecture and the CuPc absorbance of UV-visible light.



Aggelica Ballou

Giorgos Papadimitropoulos

Dimitrios Kouvatsos

More info:

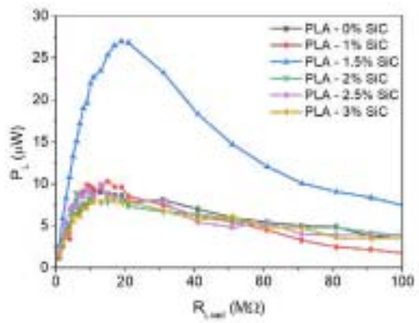


Environment, Energy & Industry

SiC-dopped polylactic acid (PLA) for energy harvesting

The influence of SiC micron-sized particles on the mechanical, electrical, and optical properties of a PLA-SiC composite was investigated for potential application in triboelectric energy harvesting.

The mechanical properties of PLA are enhanced by the inclusion of SiC, depending on the concentration of SiC. In addition, the dielectric constant of the composite material increases as the SiC concentration increases with a maximum at 1.5% SiC where the power output during triboelectric tests reaches about 27μW. The optical properties of the composite are strongly dependent on the concentration of SiC.



Power output vs SiC dopping amount


Dr. Christos Tsamis

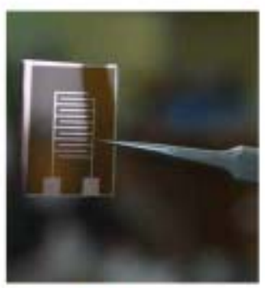

Stephania Skorda

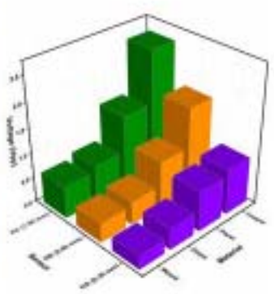

Dr George Vakinis

More info:

Flexible tactile triboelectric sensor

Haptic feedback plays a crucial role, continuously offering individuals vital information about their external surroundings through physical contact. Therefore, rapid advances in human-friendly biomimetic electronics and flexible devices, have allowed the development of advance electronic skins for artificial haptic sensation. In this work, we develop a flexible triboelectric tactile sensor, utilizing the freestanding single-electrode triboelectric nanogenerator principle, realizing concurrent material and texture detection in a single device. Common materials such as wood, paper, copper and glass were used for the identification study along with textured surfaces made of the same materials with microscopic surface features. Simultaneous classification and recognition of materials and textures was performed by a single, 1D convolutional artificial neural network, achieving an average recognition accuracy of 98.4% across all different surfaces.








Dr. Christos Tsamis


Vasiliki Zacharia

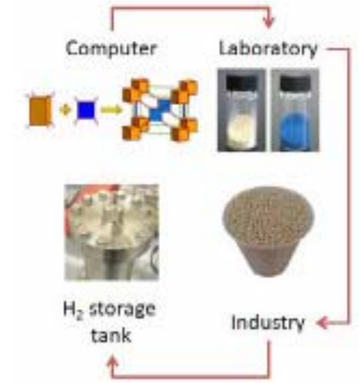

Achilleas Bardakas

Nanoporous Materials for Hydrogen Storage Applications of surfactants' aqueous solutions

Widespread use of hydrogen as an energy carrier is a key priority globally. INN coordinates a European integrated multiscale lab-to-tank approach to develop, validate and demonstrate innovative, low cost, cryo-adsorptive hydrogen storage. It aims at developing monolithic Metal-Organic Framework (MOF) ultra-porous adsorbents with an optimal combination of volumetric and gravimetric hydrogen storage capacity. The targeted materials can store hydrogen efficiently, will be easy and safe to transport, and have a small environmental footprint.

MOFs are light-weight, highly ordered, nanoporous crystalline materials. They are formed by combining inorganic building units and organic linkers. In terms of H_2 storage capacities, MOFs far outperform alternative nanoporous materials due to their tunable ultra-high porosity and functionality.

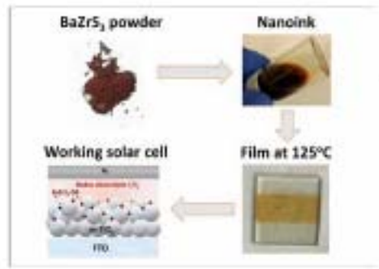
The pertinent activities of INN are expected to contribute to an accelerated deployment of H_2 mobility, while by generating many opportunities of technology transfer to industry, they can also support European autonomy in the strategic value chain of hydrogen. This is a key factor to reach the EU Green Deal objectives and achieve the challenging energy transition as well as climate change targets.



More info:

Chalcogenide Perovskite Solar Cells

Chalcogenide perovskites, such as $BaZrS_3$, manifest as strong candidates to replace toxic metals-containing halide perovskites in optoelectronic applications, but the formation of high-quality films for photovoltaic applications remains a major challenge for now, since very high temperatures are needed to fully crystalize the compound. To circumvent this issue, liquid-phase synthesis, through direct fabrication of perovskite nanocrystals dispersed in an organic solvent or a conversion of a pre-crystalline powder to an ink, has been suggested as a viable strategy for low-temperature processing. However, both cases result in films which cannot be used in the fabrication of solar cells. Our group of "Photovoltaic and Optoelectronic Materials and Devices" lab in INN, adopted a hybrid method using a solid-state synthesis to prepare orthorhombic $BaZrS_3$ powder containing particles of irregular shape and size. Then, the powder was transformed into a very stable ink with adequate concentration using a suitable ligand-coordinating solvent (OA-NMP) system, which could be easily handled in the air. $BaZrS_3$ was infiltrated in mesoporous TiO_2/FTO glass substrates and proof-of-concept photovoltaic devices were fabricated, for the first time in literature, with the combination of a redox electrolyte, reaching a mean PCE of 0.11% and FF of 61%. We believe that this work will pave the way towards the systematic use of $BaZrS_3$, or other similar chalcogenide perovskites, in solar cells and other relevant optoelectronic devices.



More info:

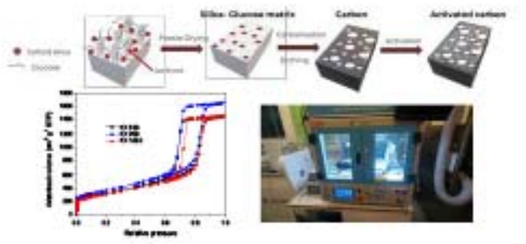

Panagiotis Dallas


Konstantina Gkini


Thomas Stergiopoulos

Rational design of hierarchical porous carbon nanomaterials as electrodes for energy applications

Regarding the synthesis of the electrode materials, hierarchical porous carbos (HPCs) have attracted, recently, much attention as materials for supercapacitors. The hierarchical pores can exhibit the advantages of each pore size with a synergistic effect during the electrochemical charge–discharge process. The macropores can serve as ion-buffering reservoirs, giving a decreased diffusion distance; the mesopores provide the ion-transport pathways with a minimized resistance; and the micropores can enhance the electrical double layer. In this study, ice-templating along with a hard template (colloidal silica) are combined to produce HPCs with desired properties. To enhance the structural characteristics a further step of physical or chemical activation can be considered. Different experimental parameters such the size of the colloidal silica, silica-to-carbon precursor (glucose) mass ratio, and carbonization (pyrolysis) and activation conditions, are optimized. As doping can improve charge mobility on carbon surfaces, methods for nitrogen-doping (n-type) have been applied either during the preparation of the HPCs (in situ approach) by the addition of urea, or by adsorption of ionic liquids (BMIM-based) on the as-prepared HPCs (ex situ approach). The final materials were characterized by a variety of techniques including SEM/TEM, Raman Spectroscopy, liquid nitrogen porosimetry, TGA etc.





Zili Sideratou



Fotis Katsaros



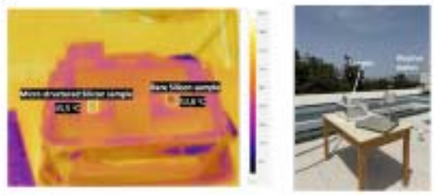
George Romanos

More info:

Enhanced Radiative cooling through transparent micro-structured polymer film fabricated by UV Nanoimprint Lithography

Radiative cooling is a passive cooling technology that lowers the temperature of terestial objects by dissipating heat into outer space. The atmosphere on a cloud free day is trasparent in the main range of wavelgengths 8–13um. This range is called the atmospheric window (AW). Thus, heat in the form of infrared radiation from high temperature terrestial objects escapes towards cold outer space without being absorbed by the atmosphere through the atmospheric window.

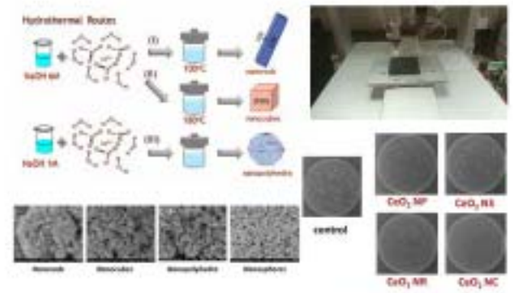
Our team is investigating the rpassive adiative cooling effect of a micro-structured transparent polymer film fabricated by UV-Nanoimprint lithography as promising candidate for effective radiative cooling of solar cells. Real time outdoor temperature measurements were conducted to observe the radiative cooling effect of the micro-grating cooler, as compared to both the unstructured sample and the bare silicone substrate,. The measurements indicate a temperature drop of up to 5 degrees Celsius during mid day hours



(left) IR camera image of structures and unstructured Silicon samples showing a 8 oC difference in temperatures. (right) Experimental set up on INN Building roof top.

Novel nanoceria as antimicrobial coatings

Infectious diseases pose a significant threat to human health and the global economy, accounting for more than 20% of global mortality, while viruses are responsible for about one-third of these deaths. To date, about 200 infectious diseases and about 80% of infectious diseases are transmitted by hands touching contaminated surfaces. Addressing these challenges, the current work is focused on the development of new sustainable antiviral and antimicrobial coatings for textiles and high traffic objects made of plastics and metal, involving bathroom and switches manufacturing industries. In this context, novel active nanomaterials (ANMs) based on cerium oxide were prepared having different sizes, morphologies and exposed crystal facets. Nanoceria can act as an excellent antioxidant agent and protect the healthy cells from oxidative stress by scavenging reactive oxygen species (ROS) or as a pro-oxidant and hence exhibit a strong antibacterial effect. The developed ANMs were characterized by a variety of techniques, including SEM, nitrogen porosimetry, XRD etc., while their antibacterial performance was evaluated according to the standards using Gram-negative E. Coli and Gram-positive S. Aureus bacteria. The developed ANMs were used to develop antimicrobial coatings utilizing an Atmospheric plasma jet treatment on the selected specimens.





Zili Sideratou



Fotis Katsaros

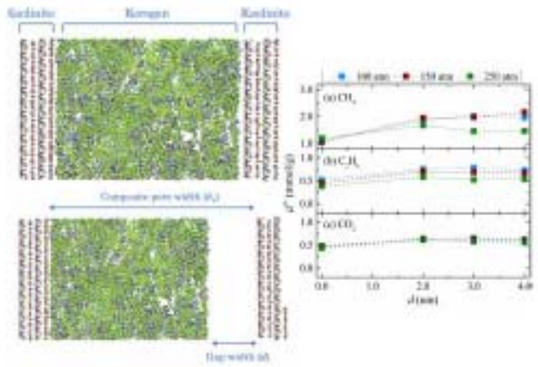


Aggeliki Papavasiliou

More info:

Modeling kerogen pores found in shale formations

Kerogen, a micro-porous amorphous solid, constitutes the primary organic component in potentially lucrative shale formations that host natural gas (aka shale gas). Essentially, it is fossilized organic matter (algal, plankton, pollen, spores, etc.) that has undergone several chemical reactions and changes over millions of years due to burial and exposure to high temperatures and pressures. This degradation process produces the gas in the field, which can also be found within the bulk or adsorb onto the surface of this amorphous organic material. Our team's goal is to gain a deeper understanding of how kerogen porosity characteristics affect the transport properties of the hosted gas, which is crucial for optimizing the extraction process. In this study, we examined how shale gas components and their mixtures behave in hybrid pores made of kerogen and inorganic clay (specifically kaolinite). In this respect, we investigated gas adsorption in the pores, their diffusion, and their preferential distribution. We also examined how these properties change under different conditions and in the presence of void space at the interface between the kerogen and kaolinite regions.





Dr N. Dawass



Dr L.D. Peristeras

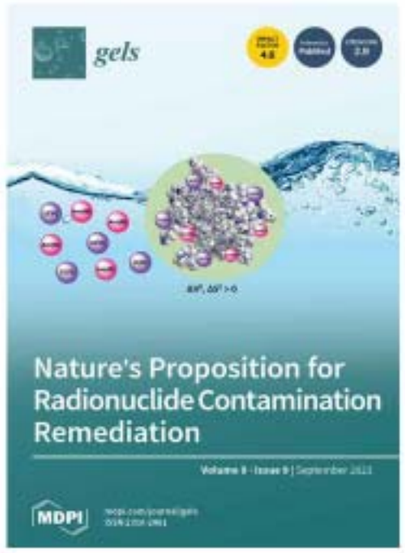


Dr I.G. Economou

More info:

Bioinspired Hybrid Adsorbents Purify Water from Radioactive Elements

Contamination of aqueous resources with radioactive substances is among the critical aspects of environmental pollution. The inspiration from silaffins, the proteins that mediate silica shell formation to diatoms, led to replicating their action with hyperbranched poly(ethylene imine). In this context, two similar methods developed by our group yielded xerogels and nanoparticles with different compositions and properties. Both variants have minimal environmental impact since they do not require organic solvents or high temperatures and do not produce toxic byproducts. Supreme adsorption of americium and uranium ions from ultra-pure water and seawater under various pHs and temperatures was achieved even at ultra-trace levels. Compared to other adsorbents the composites exhibited far higher binding efficiency. Xerogels could remove both actinides even from seawater by almost 90%. The above, along with their simple derivatization to increase the selectivity towards a specific radionuclide and their easy processing to be included in separation technologies, could make these materials attractive candidates for the treatment of radionuclide-contaminated water.




Ioannis Ioannidis

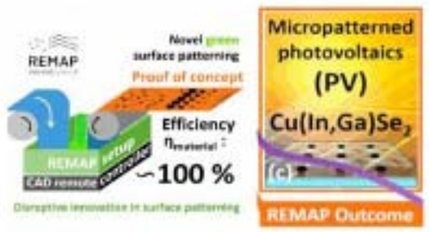

Ioannis Pashalidis


Michael Arkas

More info:

Structuring magnetic fields for green microfabrication

Surface patterning is at the heart of microfabrication that enabled an industrial revolution. In today's microfabrication most of the material and energy, end up into waste streams. REMAP's (Horizon Europe EIC Pathfinder) key to disrupt microfabrication, and provide a green technology, is a novel reusable smart composite fluid containing magnetic nanoparticles that, when placed on the surface to be patterned, can be manipulated remotely by a magnetic controller to form a mask. capable of attaining ca. 100 % material utilization. In cooperation with International Iberian Nanotechnology Laboratory and the University of Genova a first embodiment of the magnetic controller consisting of an array(s) of current lines has been constructed to drive the magnetic particles. Our numerical studies managed to suggest an optimized controller, operating at room temperature, that can create on demand magnetic fields and gradients which in turn can effectively drive the magnetic particles with low energy consumption. In this sense the mask is tunable for specific patterning applications.Our initial goal will be a photovoltaic cell.

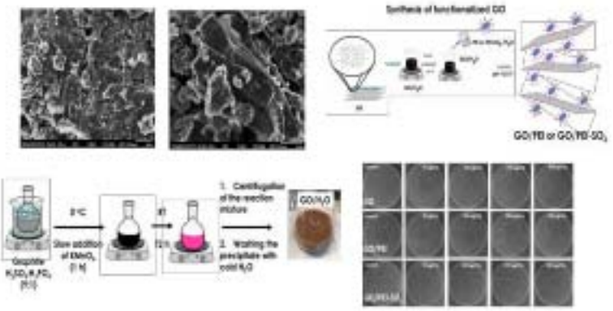



Kalliopi N. Trohidou


Nikolaos Ntallis

More info:

Recycled industrial graphite wastes for the sustainable synthesis of high added value nanomaterials



Waste control and management is one of the great challenges in our modern society. Thus, growing attention is being placed on valorisation of valuable minerals contained within the various industrial waste streams. As natural graphite is considered as Critical Raw Material, the recycling and re-use of graphite wastes from industrial steams is of significant interested. Graphite is a frequently used material in many applications due to its electrical, mechanical and thermal properties. However, graphite dust is produced during the mechanical processing. In general, graphite dust is not hazardous to the environment, but it can lead to health issues. Particularly fine particles can also cause considerable lung damage. In this work, the efforts were focused on the utilising of graphite dust from CARBONTEC moulding process either in fine powder form (<15 μm) or larger residues from machining processes, for the development of advanced nanomaterials for antimicrobial and environmental applications. The first step involves the conversion of graphite dust to highly hydrophilic graphene oxide (GO) by employing an environmental-friendly modified Staudenmaier method, while in a subsequent step hyperbranched polyethyleneimine derivatives are introduced to GO via physical and chemical interaction. The obtained hybrid materials are used either as antimicrobial agents or for the development of membranes for the removal of heavy metals from water streams. The further addition of Fe magnetic nanoparticles on the GO sheets enables their use in batch water purification processes, in which the hybrid nanomaterials can be easily removed and re-used by applying a magnetic field.


Zdi Sideratou

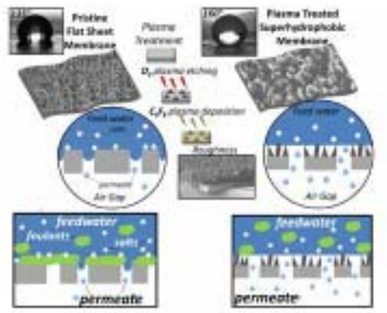

Fotis Katsaros


Mohammed Subrati

More info:

Revolutionizing Membrane Technology for Clean Water Production

In the quest for clean water solutions, our team, in collaboration with the membrane group and European Research centers and companies, have developed a groundbreaking and 'green' method to create superhydrophobic membranes. Our membranes completely repel water and showcase incredible resistance against wetting, scaling, and fouling. By utilizing plasma nanotechnology, we have transformed both initially hydrophobic and initially hydrophilic membranes into superhydrophobic ones. The plasma-treated membranes exhibit remarkable properties, such as durability and stability over prolonged periods, long-hour operations, and against challenging feedwaters such as brines and acids. They can be applied to any membrane distillation mode with consistent performance, resulting in improved clean water production compared to commercial membranes, along with excellent salt rejection.



More info:

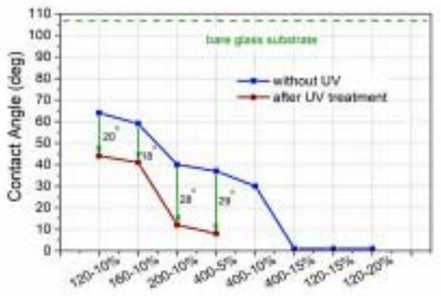

Evangelos Gogolides


Dimosthenis Ioannou


Angelos Zenou

Super-hydrophilic titania coatings for concentrated solar power applications

Superhydrophilic and photocatalytic titania (TiO_2) thin films are widely investigated for self-cleaning glass applications, i.e. titania-coated glass panels used as mirrors in concentrated solar-thermal power (CSP) plants. Among the three possible titania crystal structures – anatase, brookite, and rutile – a material of mostly anatase phase is required for minimizing contact-angle and maximizing the photocatalytic and self-cleaning effects. We have studied ultra-thin (8 to 12 nm thick), optically transparent titania films for CSP applications. We have obtained the desired anatase crystal structure using magnetron sputtering for thin film synthesis, which is a process compatible with industrial large-area and cost-efficient coating technologies. Our main achievement was to develop superhydrophilic (close to zero contact-angle) titania thin films at low deposition temperatures (120°C). This paves the way for developing low thermal budget industrial synthesis processes of the films, thus lowering the manufacturing cost and allowing for their wide commercial application.



Contact angle determined for various 10 nm thick TiO_2 films deposited onto low-Fe extra-clear glass. The numbers on the horizontal axis denote deposition temperature-O_2 fraction. Contact angles have been measured in the as-deposited state (without UV) and after UV treatment.





Konstantinos Giannakopoulos

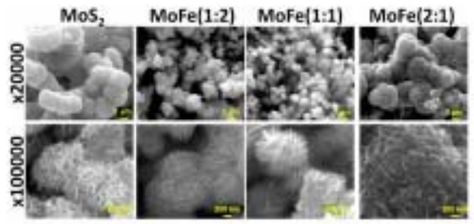


Andreas Kaidatzis

More info:

Novel Bi-Functional MoS_2/α-Fe_2O_3 Nanocomposites for High Photocatalytic Performance

Photocatalytic MoS_2/α-Fe_2O_3 nanocomposites were synthesized, under a two-step hydrothermal route, where the hexagonal molybdenum disulfide flakes were packed in an extended 3D flower-like network and decorated with well-dispersed nanoparticulate α-Fe_2O_3 crystals. The alteration of the precursors' ratio during synthesis influenced the morphology, surface area, and charge transfer resistance of the produced MoFe samples, while the structural and optical properties remained intact. The high purity's and well-crystalized nanocomposites' bi-functional photocatalytic oxidation/reduction performance was evaluated against tetracycline pharmaceutical and Cr^{6+}, achieving 60% and complete removal, respectively, imposing, therefore, the material's superior performance.





Athanasekou Chrysoula

More info:

Pilot operation of innovative Photocatalytic Nanofiltration technology for pollutant removal and water re-use of Agro-industrial effluents

The groups of Dr Polycarpos Falaras and Dr George Romanos at INN developed, fabricated, scaled up and applied in demonstration projects innovative photocatalytic membrane reactors for water purification and reuse. The novel Photo-NF reactor (PNFR) systems integrate synergistically state-of-the-art technologies such as nanofiltration (NF) with photocatalysis, resulting in applicability extension, minimization of the operational cost and limitation of the carbon and environmental footprint.

In the frame of LIFE PureAgroH_2O project a close-to market, patented water purification system with the ability to effectively recycle 15 m^3/day of real agro-wastewater was constructed, installed and tested at ZAGORIN cooperative, Greece.

In parallel, a pre-industrial scale demonstration unit (1,2 m^3/day) was installed by UAL-CIESOL in CITRICOS del Andarax SA industry in Spain, to reinforce the transferability of the new technology.







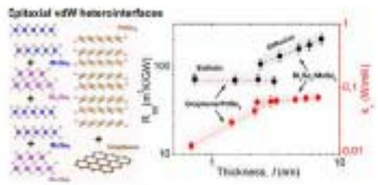
Falaras Romanos

More info:

A European Research Council ERC starting Grant: On-chip energy harvesting and management enabled by Thermal engineering of two-dimensional MAterials

TheMA aims to create a breakthrough in our understanding and ability to control phonon and energy transport at the nanoscale. Its main goal is to create novel 2D semiconductor nanomaterials and heterostructures for thermal management applications and TE devices for power generation beyond current state-of-the-art. Specifically, by using phonon engineering approaches supported by advanced characterization, the project targets the fabrication and on-chip integration of (a) novel engineered transition metal dichalcogenide (TMD) based nanostructures for heat guiding and superior thermal insulation and (b) TE power generators capable of recycling the waste heat from hot spots or environmental interlinks, to deliver sufficient power to sustain low-power electronics. Ultimate goal of the project is to provide innovative solutions for on-chip energy management and energy harvesting for Information and Communication Technologies, the Internet of Things and 2D nanoelectronic devices. The research proposed here will go beyond state-of-the-art providing the in-depth understanding of nanoscale energy dissipation and phonon transport in 2D nanomaterials and lay the foundations for the development of future three-dimensional heterogeneous electronics.







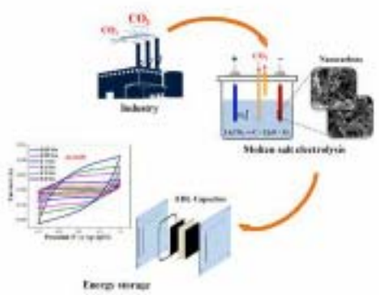
Dr Alexandros El Sachat

More info:

High-added value nanocarbons from greenhouse gases of cement industry

Climate changes due to the increased greenhouse gas emissions, accentuate the issue of CO_2 reduction and its removal from the atmosphere. Electrochemical reduction of CO_2 to solid carbon in molten salts holds the promise of being a cost-effective, commercially viable alternative for mitigating air pollution.

A simple, low cost and scalable approach was developed to produce high added-value, compact and readily-stored form of carbon with potential use in energy storage applications. A molten salt electrochemical system consisting of a eutectic mixture of Li-K carbonates, a galvanized iron (Fe) cathode and a copper (Cu) anode is applied for the conversion of CO_2 to carbon. In brief, activated carbon yielded from molten-salt electrolysis and subsequent activation under CO_2 gas flow at high temperature. The electrochemical performance of the carbon yielded before and after activation was evaluated in sodium sulfate aqueous solution (Na_2SO_4, 0.5M) using a three-electrode configuration with porous carbon, platinum (Pt) sheet and silver/silver chloride (Ag/AgCl) as working, counter and reference electrode, respectively. Electrochemical measurements revealed that the activated porous carbon exhibited remarkable electrochemical performance with capacitance of 577 F/g (at 20 mV/s). The outcome was ascribed to the intrinsic properties including high specific surface area (1024 m^2/g) of carbon produced making it highly attractive as electrode material.





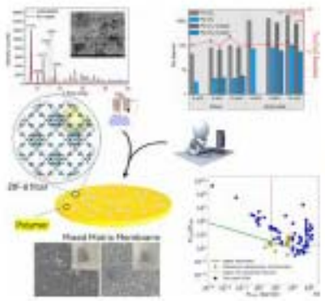
C. Trapalis T. Giannakopoulou N. Todorova N. Plakantonaki

M. Vagenas G. Sideris P. Dallas

More info:

Nanoengineered ZIFs @ membranes for CO_2/CH_4 selectivity

Reducing CO_2 concentration is an urgent environmental issue, making the development of low-cost technologies for efficient CO_2 separation crucial. Membrane-based separation processes are among the most prominent methods. Zeolitic Imidazolate Frameworks (ZIFs) are promising nanoporous materials for creating membranes with exceptional gas separation properties. In collaboration with Dr. P. Krokidas (Computational Intelligence Laboratory, IIT, NCSRD), we demonstrated that molecular-scale modifications to ZIFs variants can significantly enhance the CO_2/CH_4 separation performance of mixed-matrix membranes (MMMs) when used as additives. Initially, molecular simulations predicted the performance of MMMs with ZIF-8 as a filler, which was later experimentally confirmed with ZIF-8 based nanocomposite membranes. Subsequently, new ZIF crystals were computationally designed, and their improved CO_2/CH_4 separation performance of MMMs with the new ZIF variants was predicted. Some of these modified ZIF-based MMMs are expected to exhibit unprecedented CO_2/CH_4 separation performance, which surpasses any reported MMM, highlighting the potential of ZIF nanoengineering in developing highly selective CO_2 membranes. The development of these advanced ZIFs is currently in prog-





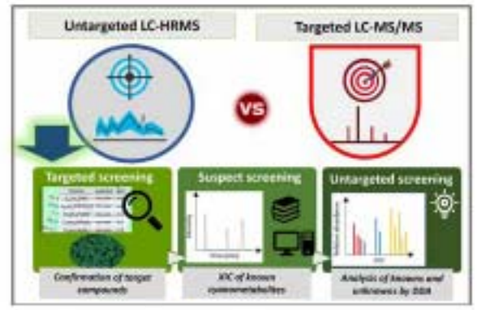
Panagiotis Krokidas Labrini Bountsika

Ioannis Bratsos

More info:

Untargeted and targeted LC-MS and data processing workflow for the comprehensive analysis of oligopeptides from cyanobacteria

Cyanobacteria produce a plethora of structurally diverse bioactive secondary metabolites, including cyanotoxins which pose a serious threat to humans and other living organisms worldwide. Currently, a wide variety of mass spectrometry-based methods for the determination of microcystins (MCs), the most commonly occurring and studied class of cyanotoxins, have been developed and employed for research and monitoring purposes. Our group in collaboration with Italian scientists from the University of Napoli Federico II, has comparatively investigated the qualitative and quantitative MCs profile of cyanobacterial biomass from Lake Kastoria, Greece using targeted and untargeted liquid chromatography–mass spectrometry approaches. Both approaches showed good correlation regarding the total MCs content, while the implemented analytical workflow combining MS spectrometry and a database of cyanometabolites (CyanoMetDB) allowed the annotation of known and discovery of new cyanopeptides. The untargeted strategy proved highly effective for the identification of MCs, microginins, anabaenopeptins, and micropeptins. The systematic interpretation of the acquired fragmentation patterns allowed the elucidation of two new MC structural variants and the proposal of structures for two new microginins and three isomeric micropeptins.





Anastasia Hisiki



Sevasti-Kiriaki Zervou

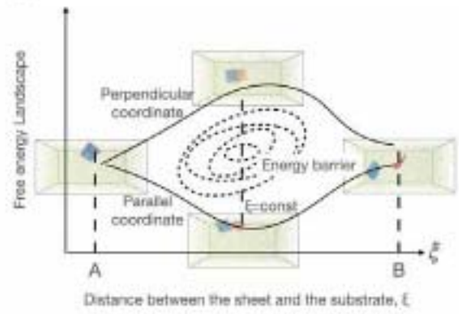


Theodoros M. Triantis

More info:

Graphene Exfoliation Using Solvents: An Umbrella Sampling Study

We conducted molecular dynamics (MD) simulations and umbrella sampling to explore the thermodynamics of peeling a single graphene layer from a graphite-like stack using five solvents: dimethylacetamide (DMA), N-methyl-2-pyrrolidone (NMP), dimethyl sulfoxide (DMSO), cyclohexane (CHX), and water. The graphene was positioned atop three identical layers, with initial simulation setups derived via steered MD along two orientations—parallel and perpendicular to the layers. Our findings indicate consistent wetting behavior across all solvents and demonstrate that exfoliation occurs more efficiently in the parallel direction, aligning with experimental results.



More info:



Anastasios Gkotzias



Cultural Heritage

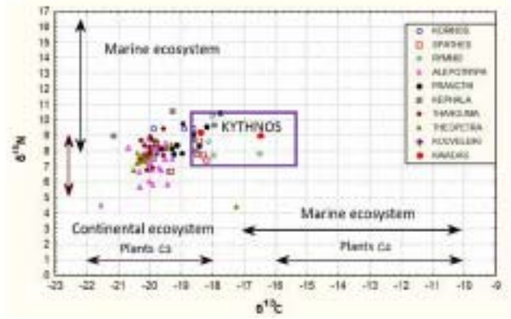
Novel technologies to examine the archaeological treasures of Kythnos island

Bone samples (animal and human) were collected and analyzed in order to implement an archaeoclimatic study, which will be linked to modern climate conditions, and for the reconstruction of the past. To carry out the above analyses, protocols were developed which are following international standards.

The results of the project present isotopic patterns of carbon and oxygen isotopes. δ13C and δ15N, probably indicate a general diet in which most dietary protein came from resident fauna and flora and partly from marine resources. In a C3 diet type, δ13C values would mainly reflect a terrestrial diet, while consumption of marine resources would contribute to elevated levels of C and N isotopes.

The isotopic reconstruction has provided important information regarding the diet of the Kythnos population. As revealed by the isotopic values, low trophic position freshwater input has possibly been detected in the human diet. However, another possibility could be that C4 sources, i.e. millet/corn constituted an important source for the individuals along with C3 items. According to the data, the island's inhabitants had a varied diet including both C3 and C4 terrestrial food sources, and possibly freshwater items.

In addition, in order to digitalise the 3D geospatial platform and the virtual tour application.





Dr Elissavet Dotsika



Petros Koralis

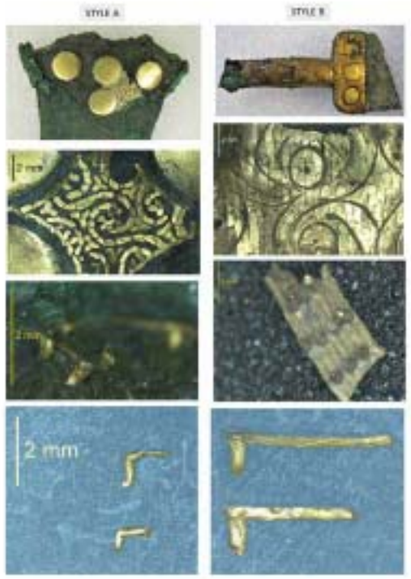
More info:



Mycenaean "gold-embroidery": A combined archaeological, archaeometric and experimental approach

A sophisticated gold-working technique attested in Early Mycenaean Greece (seventeenth-fifteenth centuries BCE) was studied using a combined archaeological, archaeometric and experimental approach. The technique, known as 'gold-embroidery' consisted of the application of hundreds or thousands of tiny L-shaped gold bars (<1 cm long) on the organic hilts and pommels of bronze daggers and swords for decorative purposes. The technique required exceptional skill and was used only for adorning prestigious weapons. It is found in some of the wealthiest tombs of the Aegean Bronze Age, including the Shaft Graves of Mycenae, several tholoi, the Griffin Warrior tomb at Pylos, etc. Emphasis was laid on the experimental reconstruction of the technique which has been based on microscopic observations and data acquired through archaeometric analysis. Our aim was to identify the various stages of production, including how the exceptionally high gold content of the bars was achieved at a time when systematic gold refining was not yet practised in the Aegean.

Study in collaboration with the National Archaeological Museum (Dr Eleni Konstandinidi-Syvridi and Maria Kontaki), Dr Nikolas Papadimitriou and Akis Goumas.



Mycenaean gold-embroidery: Style A and Style B decoration. In Style A, the gold bars were used as decorative elements themselves; they were placed one after another in single, double or triple rows, creating spiraliform patterns on the surface of the handle; in this technique, parts of the organic surface remained uncovered by gold. In Style B, the entire handle was covered with tightly packed gold bars, which created a solid sheathing around the organic material; the gold surface was then smoothed and incised with engraved spirals.



Filippaki Eleni



Yannis Bassiakos

More info:

Age assessment of monumental olive trees from the Ionian islands, Western Greece

Olive tree cultivation dates back to more than 6000 years before current era, to the beginning of the Neolithic period when farming was invented, first around Mesopotamia and later spreading westwards and northwards throughout the Mediterranean and along the Anatolian and Greek coasts. Age assessment of olive trees becomes extremely important for understanding Mediterranean civilizations. The fact that the core region of an olive tree starts decomposing as it gets older presents a serious drawback for direct 14C dating and dendrochronological analyses of olive trees. Generally, olive tree dating is performed using a gross estimation of the dimensions of the corresponding trunks using the local radial growth rate. A plethora of monumental olive trees with trunk perimeters larger than 7 m can have been retrieved, recorded and mapped by the Ionian University, located at the Ionian islands (Corfu, Paxoi, Cephalonia, Ithaca, Lefkada and Zakynthos), in the Western part of Greece. Their corresponding perimeters at human breast height, ranges between 7.5 m and 15 m. Towards an effort to preserve these monumental olive trees, dating was attempted using the following three approaches: (a) calculation of the local radial growth rate from the existing, healthy wood pieces and calculating the number of rings (thus the age) that correspond to the radius of each tree according to the respective perimeter; (b) radiocarbon dating for selected pieces of wood from the trunks and (c) OSL and IRSL dating of the palaeo-sediments either surrounding or beneath the roots of the olive trees. The radial growth rate for these specific monumental trees was calculated within the range 0.8 – 1.2 mm per year, being different from island to island, resulting thus in ages according to the geometric features well above 1000 yr. IRSL and OSL ages agree with those. The maximum ages were yielded in Corfu and Zakynthos, roughly 2200 years before current era. Internal rings were sampled as the oldest preserved ones from the surviving part of the wood for radiocarbon dating. As older wood decomposes fast, the preserved part represents younger dates of tree growth. Hence, the ages that are yielded by 14C are much younger, not exceeding 500 – 600 years.









➢ GARDIKI, Corfu
Perimeter: *11.85 m*
Rad. Growth Age: *1372 ± 124 yrs BCE*
OSL Age: *1266 ± 104 yrs BCE*
IRSL Age: *1311 ± 97 yrs BCE*



➢ ELIA ODYSSEA, Lefkada
Perimeter: *9.90 m*
Rad. Growth Age: *1779 ± 45 yrs BCE*
OSL Age: *1614 ± 61 yrs BCE*
IRSL Age: *1320 ± 172 yrs BCE*



➢ KRANIA, Cephalonia
Perimeter: *11.90 m*
Rad. Growth Age: *1788 ± 79 yrs BCE*
OSL Age: *1544 ± 78 yrs BCE*
IRSL Age: *1602 ± 84 yrs BCE*



Polymeris



Maniatis

More info:

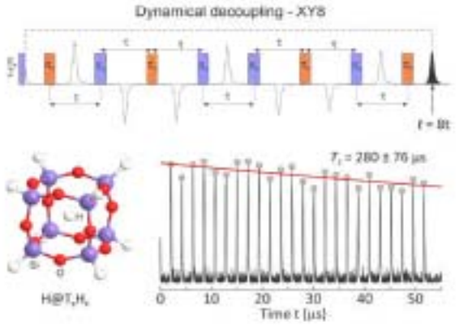


Quantum materials & technologies

Long Electron Spin Coherence Times of Atomic Hydrogen

Encapsulated atomic hydrogen in polyhedral oligomeric silsesquioxane (POSS) cages, H@POSS, is a promising candidate for applications in emerging technologies like spin-based quantum computing (QC). Although this system exhibits one of the largest electron spin-lattice relaxation times of known radicals ($T_1 \approx 1$ min at 10 K), dynamic effects such as methyl rotations result in very short electron spin coherence times T_2 (of the order of 1 μs) at T< 200 K for all POSS derivatives studied so far. As T_2 is the key parameter for QC applications, the potential use of H@POSS as quantum bit (qubit) element has been greatly disregarded up to date due to the obtained short T_2 values.

In this study we employed for the first time advanced EPR methods on the methyl-free derivative $H@T_8H_8$. By applying dynamical decoupling methods an unprecedented level of improvement was achieved with a maximum T_2 = 280 μs. This result demonstrates the great potential of $H@T_8H_8$ in quantum technologies as it can equally compete with endohedral fullerenes in terms of coherence times. (J. Phys. Chem. Lett. 2023, 14, 9590–9595).





George Mitrikas

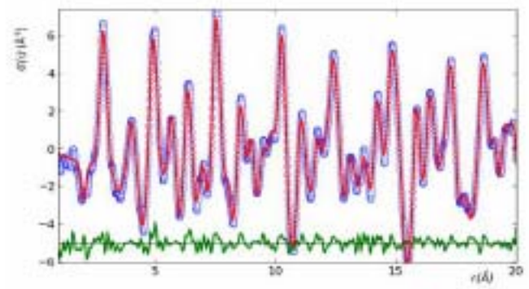
More info:

Local Structure of Quantum Materials by Total Scattering

Quantum materials (QMs) have electronic properties that both can't be explained by classical physics, and that give a unique edge over common materials used in electronics, such as silicon. The edge, in our studies, is strongly correlated electrons that make QMs extra sensitive (and thus extra tunable) to an external control parameter such as temperature.

Strong electron correlations imply a strong coupling between lattice-spin-charge and orbital degrees of freedom leading to complex physical properties and local structure different from the average crystal structure.

Establishing the relationship between local structure and physical properties of QMs is the key requirement to understand their underlying electron-electron correlations and thus tailor their properties. We have investigated the local structure of Ce- and La-based compounds by a combination of synchrotron X-ray and neutron total scattering experiments at Large Scale Research Infrastructures and associated advanced data analysis. Our results pave the way for understanding the structure-property-function relationship in model QMs and thus contribute to the development of the innovative applications such as computing, sensing, energy, medicine.





Evangelia Moschopoulou

More info:

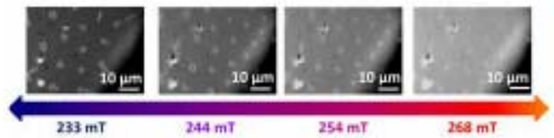
Exploring two (2D) dimensional ferromagnets for spintronics applications

Our research focuses on three different routes regarding novel magnetic materials in spintronics. We investigated exfoliated flakes of the 2D ferromagnet Fe_3GeTe_2. The impact of an oxidized layer on the magnetic domain structure reveals circular double wall (CDW) domains, resembling the topological spin texture of skyrmionium[1]. Through magneto-optical Kerr effect (MOKE) microscopy and micromagnetic simulations, the emergence of robust CDW domains and their transition into Néel-type skyrmions under specific magnetic field protocols is elucidated. This research highlights the potential for controlling magnetic domain behavior, offering promising routes in data storage (racetrack memory devices).

The growth of Bi_2Te_3 topological insulator on $Fe_{5-\delta}GeTe_2$ films[2] significantly enhances saturation magnetization and Curie temperature to a record 570 K, attributed to effective doping and strain-induced stabilization of a high magnetic moment phase. Ferromagnetic resonance measurements indicate a large spin mixing conductance, promising for spin-charge conversion at room temperature.

We have also accomplished controllable high quality Cr_xTe_y epitaxial films[3] with perpendicular magnetic anisotropy and Curie Temperature near room temperature, until very low thicknesses.

More info:





Dr Athanasios Dimoulas

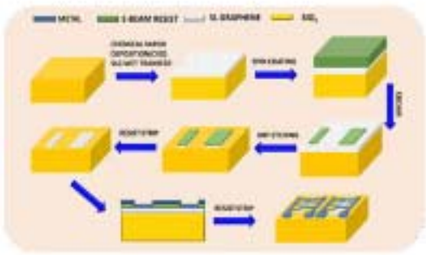


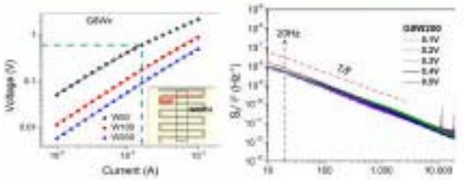
Dr. Polychronis Tsipas
Dr. Eli Georgopoulou-Kotsaki
Aikylas Lintzeris

- Effect of the magnetic field on the stabilized CDW domain lattice by MOKE imaging -

Single Layer Graphene Devices with Interdigitated Electrodes for sensing applications

Single-layer graphene (SLG) is a promising material due to its remarkable thermal, electronic and mechanical properties. In this research work, SLG with interdigitated electrodes (IDE) devices were fabricated because such topologies are suitable for future sensing applications. Specifically, our investigations were focused on the electrical noise properties of these topologies. The first achievement was the optimization of the fabrication processing steps. Following, different SLG IDE topologies were fabricated and tested. The examined topologies had a fixed electrode distance – 8μm – and varied SLG width (50, 100, 200 μm). Current – Voltage and Low Frequency Noise measurements, after further analysis, suggest that the geometric parameters of SLG IDE devices have a crucial impact on device performance.







Panagiotis Dimitrakis



Georgia Samara

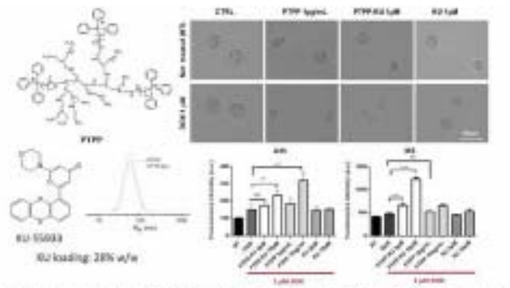
More info:

Health & Agrofood

A Mitochondriotropic Delivery System to Ameliorate Doxorubicin Resistance

Although the anticancer drug doxorubicin (DOX) is widely used in the treatment of breast cancer cells, in particular breast cancer stem cells (BCCs), tumors acquire drug resistance that limits its effectiveness. In particular the enzyme ATM kinase (ATM) repairs DNA damage and therefore favors resistance to DNA-damaging agents such as DOX. Therefore, ATM inhibition has become an attractive therapeutic concept in cancer therapy for the sensitization of cancer cells to chemotherapeutic drugs.

We have previously demonstrated the ability of a functional mitochondriotropic polymeric nanocarrier (PTPP) developed in our lab to preferentially targets BCCs. Herein, we examined the potential of this nano-delivery system to encapsulate the ATM inhibitor KU-55933 (KU) and with in vitro experiments to target and sensitize mammospheres of BCCs, which are considered as a superior model system of cancer tumors than adherent cells, to DOX. It was found that the encapsulation of this ATM inhibitor in the mitochondriotropic nanocarrier has the capacity to suppress doxorubicin resistance in breast cancer mammospheres independently of the cells' p53 status. A notable effect of this combination is a substantial increase in the internalization of doxorubicin, suggesting that this strategy can potently reverse drug resistance in breast cancer stem cells.



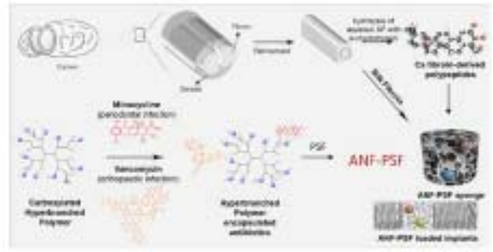
Reduction in mammospheres size by the PTPP encapsulated KU (PTPP–KU) after DOX treatment compared to non-treated cells and doxorubicin internalization compared to non-treated cells in adherent cells (Ads) and in mammospheres (MS).

A. Kaminari
Z. Sideratou
D. Tsiourvas

More info:

Antibiotic-nanofunctionalized peptide-enriched silk fibroin to prevent femoral nonunions in rats

Implant-related infections and infected fractures are significant burdens in orthopedics. Staphylococcus epidermidis is one of the main causes of bone infections related to biofilm formation upon implants. Current antibiotic prophylaxis/therapy is often inadequate to prevent biofilm formation and results in antibiotic resistance. The development of bioactive materials combining antimicrobial and osteoconductive properties offers great potential for the eradication of microorganisms and for the enhancement of bone deposition in the presence of infections. The purpose of this study was to prevent the development of methicillin-resistant S. epidermidis (MRSE)-infected nonunion in a rat model. To this end, a newly developed, by our group, bioactive material, consisting of antibiotic-loaded nanoparticles based on carboxylic acid functionalized hyperbranched aliphatic polyester, were integrated into peptide-enriched silk fibroin sponges with osteoconductive properties (AFN-PSF). These sponges were subsequently placed into non-critical femoral fractures fixed with plates and screws in Wistar rats and infected with MRSE After 8 weeks, bone healing and osteomyelitis were clinically assessed and evaluated by micro-CT, microbiological and histological analyses. The AFN-PSF treated group reached 70% of fracture healing in the absence of signs of osteomyelitis, such as abscesses in the cortical and intraosseous compartments and bone necrosis with sequestra. AFN-PSF sponges have proven effective in preventing the development of infected nonunion in vivo. The proposed nanotechnology for local administration of antibiotics can have a significant impact on patient health in the case of orthopedic infections.

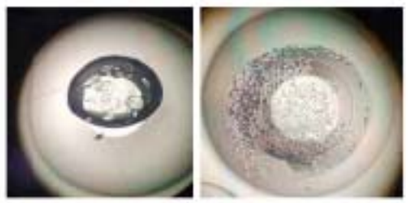


Z.N Sideratou
Dimitris Tsiourvas

More info:

Growing crystals for X-ray free-electron laser crystallography

Proteins are large molecules on which all living matter depends. Finding how each of these molecules is structured is key to understanding the functioning of a living organism in health and disease, and to designing new drugs and vaccines. X-ray crystallography is the dominant method for determining protein structures. A cutting-edge development of that method are X-ray free-electron lasers (XFELs), producing very short and intense beams with which data from tiny crystals are collected. This circumvents the major problem of crystallography, namely the growth of large crystals. Another advantage of XFELs is time resolution, allowing fast enzymatic reactions to be followed in detail. The method requires the growth of millions of very small but high-quality nano/microcrystals, homogeneous in size, quality and crystallographic properties, thus posing a new challenge for crystal growth. A novel theoretical approach was developed and experimentally corroborated, to guide the growth of such crystals. The time needed to reach the desired number density and size of protein crystals was calculated, also accounting for the impact of impurities on microcrystal growth.





Dr. Emmanuel Saridakis



Prof. Naomi E. Chayen

More info:

The Microbial Terroir of the Nemea Zone Agiorgitiko

A combination of classical microbiological analysis and metataxonomics was used for the first time to evaluate the microbial community structure of soil, grapes, and wine from three Agiorgitiko cv. vineyards in the PDO Nemea zone in Greece, with the ultimate goal being to collect pieces of evidence about the microbial terroir of the zone. The classical microbiological analysis highlighted that soil and wine had higher microbial counts than grapes; however, only few significant differences were observed among the three vineyards when comparing samples of the same ecosystem, i.e., soil, grapes, and wine. The metataxonomics analysis revealed that, in general, bacterial communities were more diverse than those of yeasts/fungi, in particular in the case of soil. Furthermore, the geographical region factor was found to significantly influence the microbiota of grapes and wine samples, but not that of soil samples. However, additional experiments are needed and are in progress, including more Agiorgitiko cv. vineyards from the PDO Nemea zone and samplings from different vintages and climate conditions, to assess the hypothesis about a uniform microbial terroir in the zone.



Elissavet Doesika

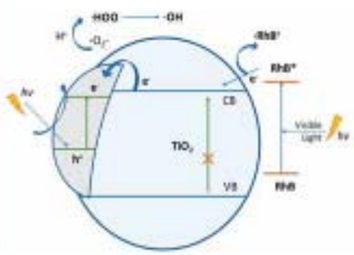


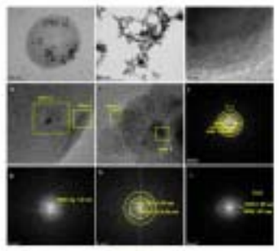
Petros Karalis

More info:

Composite Nanoarchitectonics of Photoactivated Titania-Based Materials with Anticancer Properties

In recent years, researchers have explored the bioactivity of photoinduced titanium dioxide (TiO_2) as a potential alternative therapeutic approach, aiming to reduce the adverse effects associated with conventional cancer treatments. The study focuses on synthesizing titania-based composite materials with potential anticancer properties under visible-light irradiation. TiO_2 nanoparticles modified with silver were embedded in a stimuli-responsive microgel, forming composite particles to support a drug-delivery system using optical fibers for efficient NPs' photoactivation targeting cancer cells. Characterization techniques confirmed successful embedding of Ag-TiO_2 NPs in the microgel. Both Ag-TiO_2 NPs and the composite materials showed high photocatalytic degradation efficiency and significant anticancer potential under visible-light irradiation. The composite material exhibited improved photocatalytic activity compared to Ag-TiO_2 NPs alone due to the structure of microgels. In cell proliferation and cytotoxicity assays, photoactivated composite nanoparticles demonstrated enhanced killing effect on MDA-MB-231 breast cancer cells compared to Ag-TiO_2 NPs alone, while being harmless to MCF-7 and HEK293 cells.







Nikos Boukos



Evangelia Pavlatou

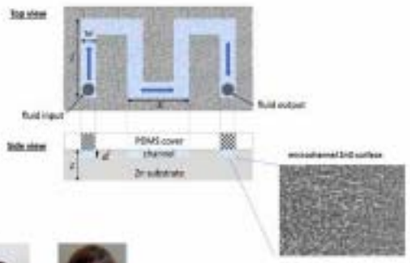


Elias Sakellis

More Info:

Antibacterial ZnO microdevice for bacterial DNA release

In integrated microfluidic systems intended for molecular diagnostics, based on the detection of the genetic material of a pathogen of interest, pathogenic cell lysis is of primary importance to the release of the genetic material. In our work, we explore the antibacterial properties of nanostructured zinc oxide (ZnO) surfaces by incorporating them as walls in a simple-to-fabricate microchannel device. Bacterial cell lysis is demonstrated and quantified in such a device, which functions due to the action of its nanostructured ZnO surfaces in contact with a bacteria-containing fluid. The unprecedented killing efficiency of bacteria in nanostructured ZnO microchannels, effective after a 15 min incubation, paves the way for the implementation of such microchannels in the disinfection of bacteria-containing solutions. In addition, the present microfluidic channel enables, in the dark, efficient release of bacterial DNA for downstream genomic DNA analysis. However, the same device under light can achieve partial inactivation of the released bacterial DNA via reactive oxygen species-mediated oxidative damage, and can find application in cases where the presence of DNA in a sample is not desirable.





Yvonni Mavrogi



Angeliki Tserepi

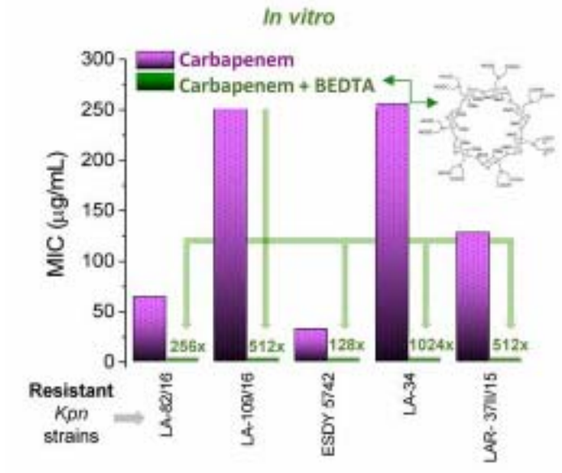
More Info:

Fighting effectively Antimicrobial Resistance

Antimicrobial resistance (AMR) is an urgent global public health threat associated with nearly 5 million deaths in 2019. AMR develops when bacteria become resistant to antibiotics and instead of being killed they continue to multiply, owing to their β-lactamase enzymes that hydrolyze antibiotics such as penicillins, cephalosporins, and carbapenems. Metallo-β-lactamases (MBLs) are bacterial enzymes for which no targeted therapeutic solution is available to date.

We have developed BEDTA, a cyclodextrin derivative, that was studied extensively regarding its structure, physico-chemical properties across the pH range, and capability to bind with the biologically relevant metal ions, Zn^{2+}, Ga^{3+} and radioactive [67Ga] Ga^{3+}. BEDTA inhibited MBL extracts and protected the molecular integrity of a carbapenem in water. When tested against resistant clinical pathogens in vitro, BEDTA achieved potency increase of carbapenem antibiotics up to 1024-fold, rendering each bacterial strain sensitive to the treatment (Carbohydrate Polymers, 2023, 321, 121323).

Part of this work was performed in collaboration with Drs V. Miriagou and G. Miliotis, the Hellenic Pasteur Institute (HPI). A European patent (EP73714904B1) was granted jointly to NCSRD and HPI on this subject in 2023.





K. Yannakopoulou



M. Agnes



V. Miriagou



G. Miliotis

More Info:

Fundamental Research

Unlocking Nature's Power in the Lab: Type II Abyssomicins

Abyssomicins are natural compounds isolated from microorganisms found in the abyss and known for their remarkable medicinal properties, including antibiotic, anticancer, and antiviral activities. These properties make them highly valuable in drug discovery. Our research aimed to synthesize abyssomicins in the lab to understand their potential better and explore their medicinal applications. For instance, abyssomicin C demonstrates potent antibacterial effects against drug-resistant strains, while abyssomicin 2 exhibits promising antiviral activity against HIV. Despite extensive efforts to synthesize abyssomicin C, reproducing abyssomicin 2 and other type II abyssomicins remained challenging.

In 2023, we achieved a significant breakthrough towards type II abyssomicins by successfully synthesizing abyssomicin 2 and neoabyssomicin B. We employed biomimetic synthesis techniques inspired by natural transformations observed in microorganisms to efficiently construct these complex molecules from basic starting materials. This achievement not only provides access to these valuable compounds but also opens avenues for the development of novel medicinal agents. Moving forward, our research focuses on refining synthetic methodologies, investigating structure-activity relationships, and maximizing the therapeutic potential of abyssomicins and their derivatives.





V. Vidali A. S. Foscolos A. Canko

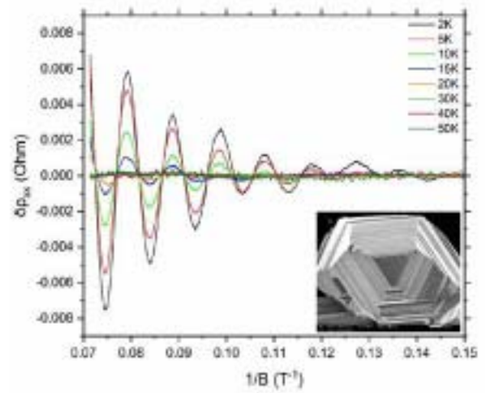
More info:

Topological Insulator Materials and Devices

Among the new materials class of topological insulators (TIs), the chalcogenide semiconductor Bi_2Se_3 is a subject of intense investigations due to its potential integration in room temperature applications such as dissipationless electronics and spintronics.

Bi_2Se_3 has a single Dirac cone at the Γ-point in the first surface Brillouin zone and a direct band gap of 0.3 eV between the valence and the conduction band. Magnetotransport measurements such as magnetoresistance (Rxx), are very important to reveal the exotic topological surface states in TIs.

Prominent two-dimensional (3D) Shubnikov-de Haas oscillations are observed in Bi_2Se_3 single crystals in magnetic fields up to 16 T at temperatures up to 15 K, using a Physical Properties Measurement System (PPMS). The analysis of the SdH oscillations reveals an additional π Berry phase, which is indicative of the presence of two-dimensional (2D) Dirac fermions. This finding suggests the coexistence of 3D bulk transport properties with 2D surface states, characteristic of topological insulators.





Myrto-K Bikouvaraki



Nikolaos Koutsokostas



Thanassis Speliotis

More info:

Development of novel 2D materials following green bottom-up and top-down approaches

In recent years, with the isolation of graphene, two dimensional (2D) materials have attracted significant attention due to their high surface area-to-thickness ratio which maximizes the active site density and resultant properties. They have found applications in many technological fields such as magnetism, energy storage and catalysis. 2D materials are divided in two major categories, the lamellar van der Waals materials, such as graphene and metal chalcogenides, and the very recently discovered non-van der Waals 2D materials, which actually result from chemical bond cutting in traditional 3D structured materials. Among the synthetic methodologies the most common is liquid phase exfoliation, which involves the sonication of layered crystals within appropriate solvents which produces nanosheets of the original crystals. (FIGURE 1 ACCOMPANY)

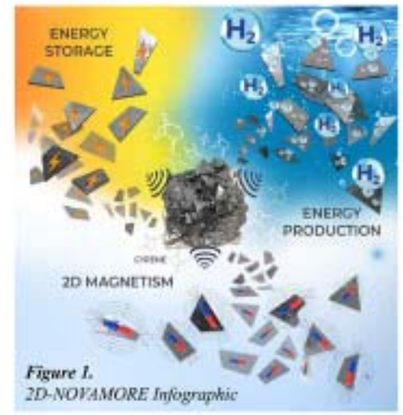
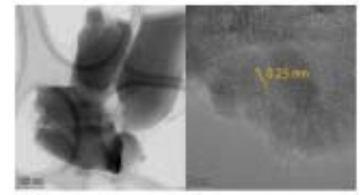


Figure 1.
2D-NOVAMORE Infographic

The research group of Dr. V. Tzitzios, together with international collaborators, following green chemical LPE protocols, have replaced the commonly used toxic carcinogens NMP, DMF, DMSO, using simple water solutions or green organic solvents, like isopropyl alcohol, to synthesize a variety of 2D materials including van der Waals and non-van der Waals analogues such as transition metal borides and oxides. Among these, 2D Ni and Mn borides show interesting electrocatalytic behavior for both Hydrogen and Oxygen Evolution Reactions (HER/OER). In the figure we see representative TEM images of non-van der Waals α-Fe_2O_3 2D hematene nanosheets (as the planar 0.23 nm d-spacing corresponds to the (113) lattice of hematite.) and magnetene, the magnetite, Fe_3O_4, 2D. (FIGURE 2 ACCOMPANY)





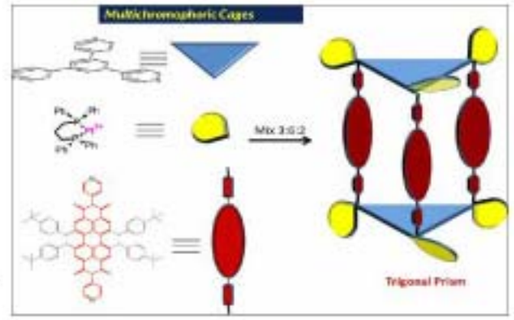
Dr. Vasileios Tzitzios

More info:

The art of building geometries with precise topology using subcomponents Self-assembly

The group focuses on the design and supramolecular synthesis – via various self-assembly protocols – of cleverly engineered self-assembled molecular systems capable of harvesting light for tuning and tailoring the properties of advanced photonic nanomaterials. More specifically, we are interested in constructing stiff and compact chromophoric arrays in a topologically well-defined way through programmable self-assembly for performing specific light functions e.g., accumulation and tuning in fluorescence, charge transfer (CT), electronic energy transfer (EET), EET based sensing systems, solar energy conversion etc.

The above design could make the structural basis for maximizing chromophore communication through donor – acceptor electronic energy / electron transfer phenomena for multifunctional applications.





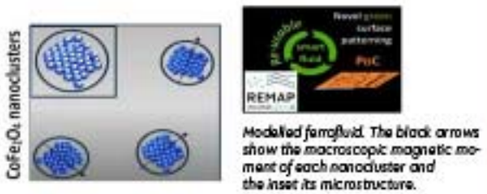
G. Pistolis

More info:

Magnetic Field Driven Cluster Formation in Ferrofluids

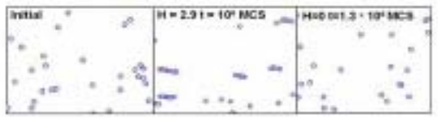
The ability to control remotely the cluster formation process in ferrofluids using magnetic fields opens new perspectives for advanced biomedical-technological applications. We investigate the optimum conditions for cluster formation in a ferrofluid under the field application for its use in microfabrication. The conditions of cluster dissociation process are also studied in order to suggest a green surface patterning method by creating reusable masks.

We model the cluster creation of magnetic nanoclusters in the fluid using the Diffusion Limited Cluster Aggregation method. We study $CoFe_2O_4$ nanoclusters of diameter 60 nm in water produced in CNR and Genova. Each nanocluster is composed of iso-oriented exchanged coupled nanoparticles of ~7nm diameter and it is covered with an Oleic acid (OA) shell. Our simulations demonstrate that the high magnetic moment and anisotropy of the nanoclusters play important role in the formation of clusters in the ferrofluid in the presence of the field and that steric interaction from the OA coating contributes to the cluster dissociation process when the magnetic field (H) is switched off.



Modelled ferrofluid. The black arrows show the macroscopic magnetic moment of each nanocluster and the inset its microstructure.

Snapshots of the $CoFe_2O_4$ nanoclusters configurations in the fluid: (left) initial, (middle) after the application of the field, (right) after the field was off. Time t (in Monte Carlo steps(MCS)).





K. Trohidou

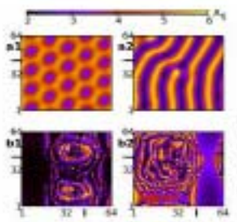


M. Vasilakaki

More Info:

From intriguing Turing patterns to spectacular chimera states

Oscillating reactions, also known as chemical clocks, have been studied intensively in the past, with notable examples being the Belousov–Zhabotinsky reaction (1958) and the CIMA reaction (1990). They are characterized by periodical color changing or periodic gas emissions, and this periodic activity was earlier considered a contradiction to common sense. The explanation of the mechanisms behind the unexpected concentration oscillations was proposed in the 1970s and relies on the nonlinear nature of the interactions between the species giving rise to oscillatory dynamics and to spectacular Turing patterns when spatial diffusion is taken into account (as demonstrated by Alan Turing in his 1952 seminal paper). We quest the existence of a different unexpected spatiotemporal effect, the chimera states, which are mainly observed in nonlinear reactive dynamics at intermediate coupling ranges, whereas the Turing patterns emerge at the limit of local diffusive coupling. To that purpose, we study the generic Brusselator model, which has been extensively used as a kinetically and thermodynamically consistent model for reaction-induced oscillations. For this model, we show, in a unifying description, that by appropriate choice of the parameter values and coupling ranges, we can pass from impressive spatial Turing patterns to spectacular oscillating spatiotemporal chimera states.



a1) & a2) Typical spatial Turing patterns in 2D

b1) and b2) Spatiotemporal chimera patterns in 2D



Astero Provata



Konstas Anesiadis



Ioanna Hizanidis

More Info:

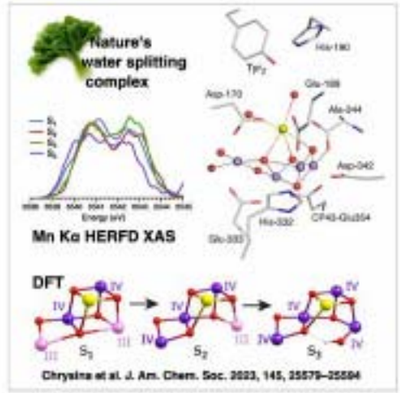
From photoinduced biological water oxidation to molecular magnets

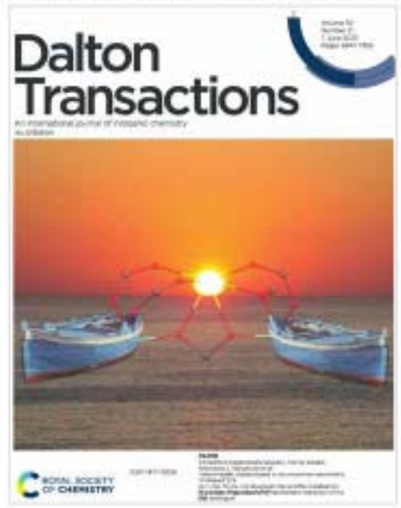
Polynuclear Metal Clusters (PMCs) are found in biological systems catalyzing important reactions. PMCs can be prepared by synthetic methods and several applications have been proposed. Such moieties constitute the subject of intense research from our group.

Photosystem II of plants, algae and cyanobacteria catalyzes water splitting, empowered by sunlight. The active site for this reaction is the PMC Mn_4CaO_5 complex which is embedded in Photosystem II, binds two water molecules and cycles through five oxidation states S_{0-4}. After four electron and four proton removal steps, O_2 is formed.

For the first time, Mn Kα High Energy Resolution Fluorescence-Detected X-ray absorption spectroscopy was employed on Photosystem II to acquire well-resolved spectra of the pre-edge region that can be correlated to TD-DFT calculated spectra and give the geometric and electronic description of all S-states.

The results support Mn-based oxidation in all S-transitions and exclude the early O-bond formation in the S_3 state. In the field of Molecular Magnetism, heterometallic 3d/4f PMCs are systematically studied as potential candidates for applications such as magnetic storage, magnetic cooling, and quantum computing devices. We studied a family of such clusters based on an uncommon asymmetric "V shaped" $[Fe^{3+}(\mu\text{-OR})Ln^{3+}(\mu\text{-OR})_2Fe^{3+}]^{6+}$ (Ln = Gd, Tb, Dy, Ho). By application of static and dynamic magnetic susceptibility measurements and Mössbauer Spectroscopy we investigated the magnetic interactions between the 4f and 3d metallic ions in these clusters. Slow magnetic relaxation was observed for the Dy analogue.







Yannis Sanakis



Michael Pissas

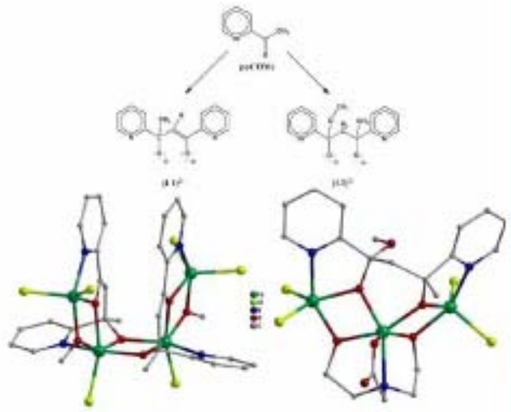


Maria Chrysina

More Info:

Structural and Physical Properties of Iron(III) Complexes with New Ligands Formed In-situ

The research of Crystallography and Coordination Chemistry Materials (CCCM) Group focuses in the design, synthesis, magnetic and spectroscopic characterization of coordination compounds, their thorough and in-depth crystal structure-physical properties study and understanding, in order to achieve high quality results. Along these lines compounds $[Fe_6Cl_6(OMe)_2(L1)_2]$ (**1**) and $[Fe_3Cl_4(bicine)(L2)]$ (**2**) were obtained. The ligands $(L1)^{2-}$ and $(L2)^{2-}$ are formed only in-situ and in the presence of Fe^{III} ions via aldol-type reactions of the methyl-2-pyridyl ketone (pyCOMe). Both complexes contain Fe^{III} ions with octahedral and square pyramidal geometries which can be distinguished by Mössbauer spectroscopy. Below 80 K, the Mössbauer spectra of **2** indicate the onset of relaxation effects. At 1.5 K the spectrum of **2** consists of magnetic sextets. An in-depth theoretical study shows that the difference in the effective hyperfine magnetic fields of the two square pyramidal sites stems from the differences in the internal magnetic fields $B_{0,1}$ and $B_{0,3}$ and not from possible differentiation of the exchange coupling constants. Mössbauer hyperfine parameters, isomer shift, δ, (for **1** and **2**) and internal hyperfine field, B_0 and the theoretical analysis indicate that the Fe^{III} sites in the square pyramidal environment of the present structures present a more covalent character. Magnetic studies indicate antiferromagnetic interactions leading to an S = 0 ground state in **1** and to an S = 5/2 ground state in **2**, consistent with Electron Paramagnetic Resonance spectroscopy. This study shows that pyCOMe is an excellent pro-ligand which can be activated under various reaction conditions, in the presence of metal ions and combinations of them, in order to afford new types of ligands and complexes with novel metal topologies and physical properties.



More Info:



Psychari Vassiliki



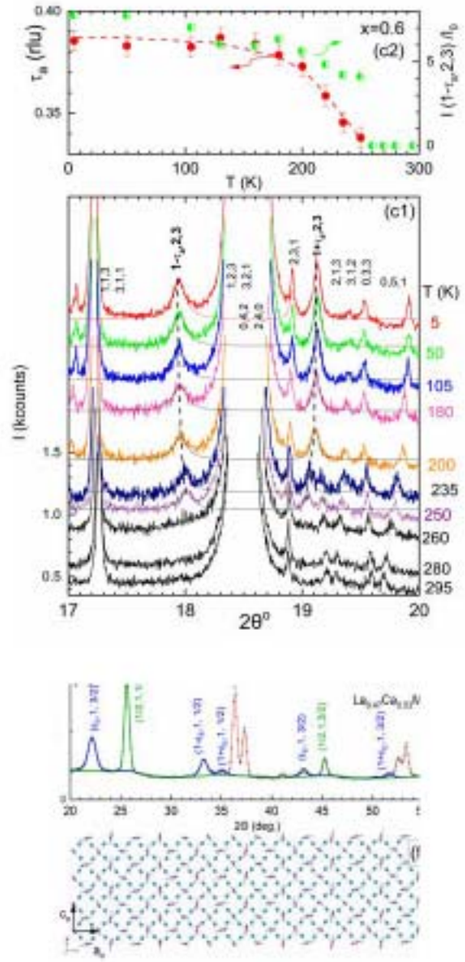
Raptopoulou Catherine



Yannis Sanakis

Mixed orbital states and modulated crystal and magnetic structures in $La_{1-x}Ca_xMnO_3$ deduced from synchrotron X-ray and neutron diffraction data.

Several important phenomena, including ferromagnetic magnetoresistance effects, charge, and orbital-ordered states, have been observed in the model doped $La_{1-x}Ca_xMnO_3$ manganese perovskite. We have studied the crystal structure in a series of compounds with 0.5< x≤0.6 using ultrahigh-resolution synchrotron X-ray (see figs. C1&c2) and neutron (see figs. e&f) diffraction data in high-quality polycrystalline samples. The experimental results reveal that all compounds undergo a structural transition at $T<T_{CO}(x)$~200–220 K with the concomitant emergence of superlattice Bragg peaks, which can be indexed assuming a superstructure with a modulation propagation vector, τ. At the base temperature of 5 K, the modulation vector of the superstructure $\tau=[\tau_a,0,0]$ is parallel to the a-axis, with τ_a varying linearly with x, as τ_a~1-x. A sinusoidal modulated structure has been proposed to interpret the neutron diffraction data. This result may be linked to a mixed orbital state of the manganese ions. Our findings may be useful in understanding phenomena related to spin, charge, and orbital ordering more deeply, as well as symmetry breaking and emergent order in quantum states [1,2].





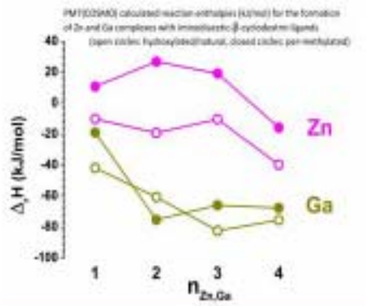
Michael Pissas

More Info:

Theoretical Calculations on Metal Complexes with Cyclodextrin-iminodiacetate Ligands

The resistance of bacteria to widely used antibiotics has been associated, among others, with the presence of Zn^{2+} cations in the active center of metallo-β-lactamases (MBLs), enzymes that hydrolyze β-lactam antibiotics. Since synthetic derivatives of cyclodextrins with iminodiacetate groups possess the ability to bind metal ions, they can effectively lead to MBL deactivation by sequestering Zn^{2+} cations. In addition, formation of stable complexes with radioactive Ga^{3+} cations enables the examination of biodistribution and pharmacokinetics of these ligands towards future applications.

In this collaborative research with the group of Dr. Yannakopoulou, semiempirical PM7 calculations in simulated water medium were performed to reveal structural and thermochemical aspects of the coordination complexes of iminodiacetic-substituted derivatives of natural and methylated cyclodextrins with Zn^{2+} and Ga^{3+} cations. It was found that each derivative can bind stably (exothermicaly) up to four metal ions, facilitated by conformational changes of the substituents and the cyclodextrin macrocycle. These results assist in the rationalization of the corresponding experimental findings and provide details of complexes formation.




Yannis G. Lazarou


Marco Agnes


Konstantina Yannakopoulou

More Info:

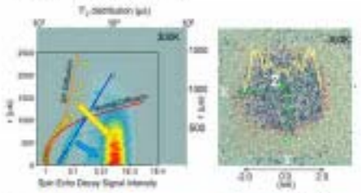
Diffusion NMR studies of nanoconfined Ionic Liquids

Room temperature ionic liquids (RTILs) are organic salts which are liquid at ambient temperatures owing to the large asymmetric organic cations underlying their chemical structure.

By adjusting the cation-anion combination, the physical properties of RTILs can be conveniently tailored; moreover they can be further improved by incorporating RTILs into solid (nano)porous materials, widening the range of their potential applications from energy storage and production devices to gas absorption systems.

Experimental elucidation of the effect of confinement on the dynamic properties of ILs is crucial for a deeper understanding of their microfluidic properties.

In this work, 1H NMR diffusion experiments were conducted to investigate molecular dynamics in the liquid state high-temperature regime of the RTIL [BMIM]+[TCM]- entrapped into MCM-41 and SBA-15 silica materials. By combining MD simulations with a new time-resolved diffusion NMR method developed in our lab, we showed that the RTIL exhibits an intricate dynamic ordering and stratified diffusion close to single file diffusion within the narrow MCM-41 nanopores, whereas almost normal diffusion was detected in the wider SBA-15.




Dr. Michael Fardis


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