Information Book

MATERIALS & ENERGY

ICOME'22

ICOME'22: Int. Conf. On Materials and Energy
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ICOME'22

ICOME22 – INTERNATIONAL ATTENDEES

CONTENTS

WELCOME

After the success of the International Conference on Materials & Energy (ICOME'15) in the nice Mediterranean city Martil - Tetouan in Morocco, followed by the edition of 2016 in the beautiful Atlantic city of La Rochelle in France, the edition 2017 in the amazing Eastern part of China at Tianjin, ICOME'18 in the sunny coastal city Donostia-San Sebastian located at the North of Spain, ICOME'19 in the sweet city of Hammamet in Tunisia and back to France ICOME'21 in a very successful online edition.

This edition 2022 was scheduled in Azerbaijan, in the magnificent port city of Baku. The organizers choose this place to be onsite to renew the links developed within the ICOME community who suffered of the Pandemic situation during two editions 20 & 21.

The ICOME'22 Conference is an excellent meeting devoted to cutting-edge research that meets the scientific needs of university researchers, industrials and professionals in order to explore new horizons of knowledge on various subjects related to the fields of interconnection between materials and energy. This edition is coupled to the International Conference of Thermal Engineering, ICTEA serie's chaired by Professor Ziad Saghir fron Toronto.

The presidents of the ICOME series: Prof. R. Bennacer (Univ. Paris Saclay / ENS-Paris-Saclay) and Prof. M. El-Ganaoui (University of Lorraine / IUT Longwy), thanks warmly Profs Yusif Abdullayev and Elchin Suleymanov from Baku Engineering University for their effort to host us with ICTEA. Welcome the participants and hope that everyone will find in this event subjects of interest, and a great pleasure in exchanging with the materials, thermal and energy communities.

XOŞ GƏLMİŞSİNİZ

Aralıq dənizinin sahilində yerləşən və Mərakeşin gözəl şəhərlərindən biri olan Tetuan şəhərində təşkil edilmiş "Materiallar və Enerji" adlı beynəlxalq konfransın (ICOME'15) müvəffəqiyyətindən sonra, konfrans ardıcıl olaraq 2016-ci ildə Atlantik okeanın sahil şəhərlərindən biri olan heyrətamiz La Rochelledə, 2017-ci ildə Şərqi Çinin füsünkar Tianjin şəhərində, 2018-ci ildə İspaniyanım şimal hissəsində yerləşən günəşli sahil şəhərlərindən biri olan Donastia-San Sebatianda (ICOME'18), 2019-cu ildə Tunisin valehedici şəhəri Hammametdə (ICOME'19) və 2021-ci ildə yenidən Fransada onlayn şəkildə keşirilmişdir.

2022-ci ildə baş tutması planlaşdırılan konfransın Azərbaycanın ecazkar liman şəhəri olan Bakıda keçirilməsi nəzərdə tutulmuşdur. Təşkilatçılar 20 və 21-ci il nəşrləri zamanı Pandemiyadan dolayı əziyyət çəkən ICOME kollektivi daxilində, inkişaf etdirilən əlaqələri yeniləmək məqsədi ilə baş tutacaq növbəti konfrans üçün Bakını seçdilər.

ICOME'22 Konfransı Materiallar və Enerji arasındakı qarşılıqlı əlaqə sahələri ilə bağlı olan müxtəlif mövzulara dair yeni perspektivləri kəşf etmək məqsədi ilə universitet tədqiqatçılarının, sənayeçilərin və peşəkarların elmi ehtiyaclarına cavab verən qabaqcıl tədqiqatlara həsr olunmuş bir elmi konfransdır. ICOME'22 konfransı Torontodan professor Ziad Saghirin sədrliyi ilə ICTEA seriyasının Beynəlxalq İstilik Mühəndisliyi Konfransı ilə birləşdirilmişdir.

ICOME konfransının prezidentləri: Prof. R. Bennacer (Paris-Saclay Universiteti / ENS-Paris-Saclay) və Prof. M. El-Ganaoui (Lotaringiya Universiteti / IUT Longwy).

Professor Yusif Abdullayev və Elçin Süleymanova ICTEA ilə əməkdaşlığımız çərçivəsində baş tutacaq bu konfransın Bakı Mühəndislik Universitetində keçirilməsində bizə göstərmiş olduqları dəstəkdən dolayı onlara öz minnətdarlığımızı bildiririk. Konfrans iştirakçılarını salamlayırıq və ümid edirik ki, hər kəs bu tədbirdə maraqlı mövzularla tanış olacaq və materiallar, istilik və enerji ilə bağlı elmi tədqiqatlarla məşğul olan tədqiqatçılarla elmi biliklərin mübadiləsindən böyük zövq alacaqlar.

FOREWORD

The global health crisis of COVID 19 has shown more than ever that the eyes of the citizens are turned towards science in order to bring very quickly palliative and then decisive solutions to the pandemic. In such situation threatening the human species, the prerogative of Science would like researchers to work together in a spirit of sharing information, methods and discoveries, simply working for the sustainability of Man and life in general when it is threatened. Although the situation prevented any face-to-face meeting, the exchanges continued.

Indeed, the evolution of knowledge during the last two centuries allows today, thanks to the development of virtual interfaces and to the progress of the algorithmic, to transport sound and visual information which tend to generalize to the sensory. No one knows the limit of this exercise. In an increasingly reliable, stable and fast way, this connection made possible the continuity of pedagogical transmission and scientific research. This is another demonstration that the knowledge produced, accumulated and preserved is today a kind of lifeline-saving arch for doctors and patients, litigators and judges, teachers and students, professors and doctoral students, to continue to advise, assist, dialogue, transmit and create the knowledge of tomorrow. In this sense, the high places of knowledge that are the Universities, the Academies of Sciences, the Schools have largely fulfilled their saving missions towards the whole humanity.

In mathematics, if the extraction of the square root of a number became a child's play with the advent of calculators, its extraction with a sheet of paper, a pencil and the four elementary operations was previously, an exercise that could be long. Similarly, for prehistoric man, bringing a quantity of water to boil without having a metal container despite the domination of fire was in the same order of challenge as extracting the root of a number without a calculator.

At first, computers worked with lamps, today's computers (for all purposes) are based on the use of transistors industrialized since 1950 and their design is closely linked to the advent of rare earths and soon quantum. By chance, Moore's law (doubling every eighteen months of the density of transistors in processors) sees its predictions come true in the challenge of materials. This law is accompanied in a global context by another law called Dennard's law (increase in computing power at constant energy), which opens the challenge of energy efficiency. Without these two competitions between materials and energy (involving many scientific disciplines), the reader is free to imagine what his daily, life would have been like during the lockdowns that have disrupted the existence of the world's citizens since the end of 2019.

In this spirit, the ICOME (International Conference of Materials & Energy) aims to bring annually an updated and balanced picture of advances in the fields of materials and energy and

to address significant progress in both fundamental and applied research as well as in societal areas.

This virtuous circle has punctuated the history of humanity by taking advantage of all the advances in knowledge as a natural laboratory or as a crucible providing innovations allowing experimental physics and numerical mathematics to continue their breakthroughs. Among these breakthroughs, we will particularly note those in optoelectronics, laser physics or high-performance computing.

The ICOME 2020 edition was supposed to take place in Metz, in Lorraine, and address advances in the fields of materials and energy. This edition was to take place under the auspices and legacy of the mathematician Henri Poincaré (Nancy) and the poet Paul Verlaine (Metz), symbolizing science and society. This conference returns after an international tour in Africa and Asia, especially after the success of the 2019 edition in Tunisia. ICOME is also a bridge between the two shores of the Mediterranean, the crucible of a civilization that has largely influenced in its own way the course of the history of materials and energy.

The edition of ICOME has been postponed to June 2021 and again the health conditions do not allow a face-to-face event, the committee opted to maintain an online edition as a new postponement would be unfavorable to the various strong links created all these years.

The 2022 edition pursue on the spirit of regaining a presential exchange and we shoos the City of Baku, Azarbaijan following the invitation of our friend Prof. Ziad Saghir to join ICEA event that he is sharing.

We are particularly grateful to the international speakers who were willing to come in 2020 and who reiterated their solidarity with this online edition of 2021 and attend on 2022. Our gratitude also goes to the chairs of sessions and round tables. All authors and contributors have coped and maintained their interest in the event, we hope to live up to their expectations.

Usually, the conference is coupled with a thematic school for PhD students and newly-qualified doctors. It is a privileged place of exchange between juniors and seniors who take advantage of the event's atmosphere to benefit from the seniors' advice and experience. Only face-to-face exchanges can ensure and fully consolidate the benefits of the seniors' values. The committee has chosen to reschedule the theme school for a more important face-to-face event during the fall of 2022 to guarantee the benefice for important community of Phd Students.

During this edition of ICOME'22, participants are invited to three days of intense activity, through twelve (8) plenary lectures given by renowned scientists.

The series of lectures on materials and energy promotes initiatives and values science as a vector of accumulation of human progress, cultural exchange, economy of mind, sharing and

investment in intelligence, strength of argument, guarantee of respect for opinions, initiator of creativity, support for the quest for truth... In this sense, the reference to the universal scientist Averroès born in Cordoba, Spain in 1126 and died in Marrakech, Morocco in 1198, through the prize bearing his name reinforces this vision of a man who places truth beyond the beliefs and allegiances of his time, intelligence beyond temporal interest and societal use.

"Knowledge acquired in a foreign country can be a homeland and ignorance can be an exile lived in one's own country"
Averroès (1126-1198).

The organizers of the ICOME 22 edition wish everyone a fruitful event where young researchers can deepen their knowledge both onsite and online while waiting for better days.

The organizers would like to thank the entities that supported the event and in particular the laboratories and institutes of the University of Lorraine that encouraged and supported the holding of this edition in Lorraine and accompanied the ICOME series since its creation.

Prof. M. El-Ganaoui, Chair ICOME Serie's, University of Lorraine.

Prof. R. Bennacer, Honorary Chair ICOME Serie's, Université Paris-saclay.

ICOME Series Chairs

Prof. M. El-GANAOUI: *is a full professor at the University of Lorraine and researcher in the Jacques Villermaux Federation for mechanics, energy and processes (FR 28 63/LERMAB). He is heading the research in energy in the Henri Poincaré Institute of Technology in Longwy. Previously, he was an associate professor in the University of Limoges and the SPCTS UMR 6638 CNRS laboratory where he was responsible for the Physics Department (2004-2010) and the international cooperation service (2006- 2010) in the Faculty of science and technology. His research aims to understand heat and mass transfers through modeling and numerical simulation with a specific activity in the field of the solid -liquid-vapor phase change. Applications concern materials and energy and benefit to energy systems including phenomena for sustainable building (Eco-materials). He teaches the mechanics of continuous media, heat transfers, and numerical methods. He was advisor of more than 25 Phd Thesis with strong international interaction noticeably in the Euro-Mediterranean context. He participated/managed the PAI Australia, Canada, Maghreb (Tassili, Utique, Volubilis), China (Xugangqi). El Ganaoui has participated in the Edition of more than 10 special issues and conference proceedings, co-authored over than 200 publications in journals (rank A) and participated in more than 100 international conferences including ten he co-organized. He is member of many international scientific societies in mechanics and heat transfers.*

Prof. Dr. Ing. R. BENNACER: *is an Engineer in Mechanical field (1989), and he got his PhD thesis at Pierre et Marie Curie University (Paris 6) in 1993. He worked as lecturer in the University Paris XI (1993/94), became an associate professor at Cergy Pontoise University in 1994 and full Professor in 2008. He moved as senior Professor to the prestigious school Ecole Normale Superieure (Paris-Saclay) since 2010. He becomes in 2017 an Exceptional National Class Professor. He is also adjunced professor at Tianjin Uni. Of comm. (China) and UMB Univ. He assumed several responsibilities, director of the LEEVAM research team (2003-2007), Licence degrees (2008-2010), Aggregation title (2010-2011), Master research degree (2011 2013), Transfer and Environmental Research Unit (CNRS LMT-Lab) (since July 2012), dean of Civil/Environmental department (Oct. 2012/Sep. 2016) and since 2019 Coordinate International Affairs Related To Ph.D Univ. Paris-Saclay. His present research activity is within the LMT laboratory where he manages Transfer and Environmental Research Unit. His Research field covers wide spectrum and several domains. It covers the building material for energy applications or on durability aspect, renewable and energy system. The expertise covers the direct numerical simulation including CFD coupling on multi-scales. The previous approach is consolidated by analytical or reduction approach in order to identify the instabilities and global behavior bifurcation and similarity controlling parameters in multiphysics situations. He published around 10 book chapters and more than 150 referenced international journals (Rank A).*

SHARING CODES WITH ICTEA (INT. CONFERENCE OF THERMAL ENGINEERING)

Ziad Saghir, Professor,
Ryerson University, Toronto, Canada
ICTEA serie's Chair

Prof M. Ziad Saghir is a Professor at Ryerson University and Canada's most experienced reduced-gravity researcher. He is Canada's top performer at leveraging departmental and provincial research funds with national (NSERC, CSA) and international funding agencies to pursue Canadian space science objectives onboard the International Space Station (ISS). His talent as a space scientist and university educator is consistently requested by the international space physical science mission community. He leads a group of very strong graduate students and post-docs that come from academia and industry, with interest in and application to deep hydrocarbon reservoirs. His innovation is recognized internationally through consistent invitations from European researchers that identify him as applying the maximum knowledge gained from long-duration gravity-driven phenomena in fluid physics to industrial processes. He has been PI or Co-I of Foton-M2 and M3 SCCO recoverable satellite missions (2007), the ISS SODI-IVIDIL (2009) and DSC (2010) missions, the ISS SODI-DCMIX mission (2011-15), and was the national coordinator of the CSA discipline working group on the role of gravity in metals and alloys. Canada's contribution to the SODI-DCMIX mission is to clarify the role of gravity on the movement of hydrocarbons across temperature gradients-important knowledge for Canada's deep oil reservoir sector (Hybernia Oil field and Northern exploration of oil reservoir deposits). Over the past decade, Prof. Saghir has been working in collaboration with TOTAL and researchers in France to apply innovation to benefit Canada's competitiveness in hydrocarbon extraction from oil reservoirs, a top priority of the Federal Government. He has published over 200 scientific journal paper related to energy. He is currently the chair of the International conference on Thermal Engineering (www.ictea.ca).

SCIENTIFIC HOSTING IN AZARBAIJAN

Department of Chemical Engineering

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Yusif Abdullayev earns his Ph.D. from ANAS, Institute of Petrochemical Processes, Baku, Azerbaijan. He did postdoctoral researches at Middle East Technical University, Turkey (2011/12, Scientific and Technological Research Council of Turkey, 2216- Research fellowship), Emory University (2013, NSF grant), University at Buffalo (2015/16, Fulbright Visiting Scholar) USA. He is currently working as the chair of the Chemical Engineering Department at Baku Engineering University. His research focus is mainly related to computational and experimental studies on identifying boundaries between catalytic and solvation effects of ionic liquids in organic

synthesis, application of ionic liquid as a 'green' catalyst to convert biomass into 5-HMF. He patented electrochemical carbon dioxide conversion to value-added organic chemicals based on transition metal electrocatalysts (PCT Int. Appl. (2020), WO 2020008267 A2 20200109) and US (U.S. Pat. Appl. Publ. (2020), US 20200010964 A1 20200109).

INT. SCIENTIFIC COMMITTEE

Timchenko V.	*NSW University*	*Australia*
Uzunova M.	*ECAM-EPMI University*	*France*
Vieira G.M.R.	*CEFET/RJ*	*Brazil*
Yuen R.	*City University of Hong Kong*	*China*
Zhu Ji-Hong	*Northwestern Polytech. University*	*China*

ICOME SCIENTIFIC SECRETARY & WEBMASTER

Dr. Souad MORSLI: *Assistant Professor at University of Lorraine, UL-ENIM -Metz Previously Associate Professor in Sciences and Technology of Oran Mohamed Boudiaf / USTOMB. Department of Marine Engineering. Her research interests focus on the field of heat & mass transfer, aeration dynamics, and energy optimizations.*

Dr. Salma KOUZI: *after a master degree, she is a PhD student (cosupervising) at Abdelmalek Essaadi University and University of Lorraine. Here research work deals with biobased materials in international context.*

Dr. Karim RAGUI: *After being Associate Professor at Houari Boumediene University of Science and Technology (USTHB) he joint the Academy of Science University (Beijin/China). His research interests focus on the field of heat & mass transfer, Supercritical fluids, porous matrix, nanotechnology, pollutants spreading, energy optimizations. He is an Editor-in-Board and Guess Editor in several international journals.*

ICOME 22 TECHNICAL SC.COMMITTEE

Warm thanks to the reviewers, the administration staff, and the students, as well, for their devotion, allowing the organization success of the present event (see the website for the list) http://www.icome.ecam-epmi.fr/committees/Operational.html

KEYNOTE / INVITED LECTURER

Topic : Energy from Materials: Strategies.

By: Prof. Biagio MORRONE, University of Campania "L. Vanvitelli" Italy.

Prof. Biagio MORRONE: *Born in 1967 in Italy, received his Master Degree in Mechanical Engineering in 1992, University of Naples Federico II, earned his Ph.D. in 1995, University of Naples Federico II, with a thesis on numerical and experimental natural convection in channels. 1994, Visiting Ph.D. student at Idaho State University, USA, on numerical analysis of the electronic components cooling and analytical solutions of heat transfer in solid. 1998-2002 junior researcher and 2002-up to now associate professor of Applied Thermodynamics and Energy Management at the University of Campania. Member of the College of Doctorate in "Mathematics, Physics and Engineering applications" teaching courses on "Numerical Methods in Physics and Engineering" at the University of Campania. Visiting researcher in India in 2018, visiting professor in France Cergy-ICAM EPMI 2019 leading researcher of scientific projects to produce bio-hydrogen and bio-methane from animal manure and organic fraction of municipal solid waste; leading researcher of scientific projects on Ground Energy Pile Heat Pumps; researcher for several projects in Energy recovery from Biomass; Invited speaker at several conferences on the use of bio-hydrogen in Internal Combustion Engines and Biomass to Energy conversion; co-author of more than 60 scientific publications on international journals, many others presented at international and national conferences and several book chapters; main research topics are: biomass-to-energy conversion, recovery of materials from biomass treatments, alternative fuels for internal combustion engines, heat exchangers, Organic Rankine Cycles, ground coupled heat pumps, numerical heat transfer.*

Topic : Design of nanomaterials for hydrogen production and storage: Modeling and Simulation.

By: Prof. Abdelilah BENYOUSSEF, Academy of Science, Morroco.

For hydrogen to be a clean energy vector, it must be produced from renewable energies by processes that do not release greenhouse gases. These processes include: - electrolysis by photovoltaic, by thermal solar concentrating (CSP) and by wind turbine-Thermolysis and thermochemistry by concentrated solar energy - or photo-electrolysis by photovoltaic and solar thermal with concentration. Photocatalysis is one of the most promising processes for the hydrogen production from renewable energies. The main process in solid state hydrogen storage is the interaction between the hydrogen and the surface of the storage medium. Because of their enormous surface area, nanostructured materials can enhance the efficiency of this process and hence improve the storage capabilities. Various efforts have been made to enhance the hydrogen storage properties. In this presentation, particular attention will be paid to the design of new nanomaterials for the two applications mentioned above; hydrogen production and storage.

Prof. Abdelilah BENYOUSSEF: *Received his "Doctorat d'état" degree from the Paris-Sud University in 1983. He is a permanent member of the Moroccan Hassan II Academy of Science and Technology. His main interest topics are Ab initio calculation and Monte carlo method in modeling and simulation of new materials for renewable energy; Magnetism and phase transition in condensed matter; complex systems and critical self-organization in statistical physics. He is a co-author of more than 400 research publications and book chapters and about 100 conference presentations including numerous invited papers and talks. He has co-chaired or co-organized several international conferences. He holds a number of patents and supervised 40 postgraduate research candidates.*

Topic : Application of AI and machine learning for quality control of BIM : Review.

By: Prof. A. David BASSIR, Belfort-Montbéliard University.

Quality control is very important aspect in Building Information Modeling (BIM) workflows. Whatever stage of the lifecycle it is important to get and to follow building indicators. In the BIM it is very data consuming field and analysis of these data require advance numerical tool tools from image processing to big data analysis. Artificial intelligent (AI) and Machine Learning (ML) had proven their efficiency to deal with automate processes and extract useful sources of data in different industries. In addition to the indicators tracking, AI and ML can make a good prediction about when and where to provide maintenance and/or quality control. In this article, a review of the AI and ML application in BIM with a focus on quality control aspect will be presented. Further suggestions and challenges will be also discussed.

Prof. A. David BASSIR: *Professor at the French University of Technology and Senior Researcher at ENS-Université Paris-Saclay. He holds MSc and PhD in structural optimization from University of Franche-Comte. His administrative positions and duties included Dean at University Institutes of Technology, University of Lorraine, Consul of Science and Technology at the French Embassy in China, General Director of Research at the ESTP-ENSAM (Paris), Space Craft engineer at GECI Technology in different Space Agencies such as Arianespace (France) and (Astrium Group) and more. Prof. Bassir was an invited visiting professor in leading universities, including TUDelft, Shanghai Jiaotong, Northwestern Polytechnical, University of Oviedo, MIT Boston and Chinese Academy of Sciences. He published over 120 papers in journals, books and conference proceedings on various subjects of Composites materials, Parameter identification, Additive manufacturing, Structural Optimization and Multiscale modelling and analysis. He serves as member of various expert committees in many international organizations and highly estimated scientific societies. Since 2012, he is the founder and the president of the Sino-French Association for Sciences and Technology.*

Topic : Photonics for Life.

By : Prof. Jean-Michel NUNZI , Queen's University, Canada.

Canada Research Chair, Queen's University, Canada.

Technology was often a drive for scientific development. However, besides what science can do for technologies several questions remain quite open, like do evolution, intelligence and the origins of life belong to what Physics can deal with? How may this happen? Self-organization naturally provides materials that can manipulate light and light-matter interactions in a manner that allows building new nano-photonic devices. With that inspiration, we show how light can naturally induce chiral structures [1], or help us design new light harvesting devices like near-IR photodetector using the rectification effect induced by dipole orientation in a thin film [2]. 'New' materials like two-dimensional transition metal di-chalcogenides also provide an interesting route to highly efficient light matter interaction processes [3]. We currently design device structures that allow the fabrication of hot electron-based photodetectors, which are highly sensitive to the NIR range, sensitive to polarization, as well as easy and cost-effective to fabricate. They are highly demanded devices for machine vision and recognition. In a preliminary step towards what we dream of to achieve globe cooling, we also extend our approach to self-organizing structures that permit radiation control from buildings and structures, in order to provide passive cooling or heating solutions under zero energy consumption.

[1] Mazaheri, L.; Lebel, O.; Nunzi, J.M. Transfer of chirality from light to a Disperse Red-1 molecular glass surface, Opt. Lett. 42 (2017) 4845.
[2] Mirzaee, S.M.A.; Lebel, O.; Nunzi, J.M. A simple unbiased hot-electron polarization-sensitive near-infrared photo-detector. ACS Appl. Mater. Inter. 10 (2018) 11862.
[3] Wang, L.; Zhang, S.; McEvoy, N.; Sun, Y.Y.; Huang, J.; Xie, Y.; Dong, N.; Zhang, X.; Kislyakov, I.M.; Nunzi, J.M.; Zhang, L.; Wang, J. Nonlinear Optical Signatures of Transition from Semiconductor to Semimetal in PtSe2. Laser & Photon. Rev. 13 (2019) 1900052.

Prof. Jean-Michel NUNZI: *graduated from l'Ecole de Physique et Chime, Paris in 1982. He joined l'Ecole Polytechnique for a PhD on the nonlinear optics of surface plasma waves (plasmons). He was then hired as full-time Researcher in Organic Photonics at the Atomic Energy Commission (Saclay) in 1984. He joined the Department of Physics at the University of Angers as Professor in 2000, where he built the Plastic Solar Cells Technology Research Team. He moved to Queen's University as Tier 1 Canada Research Chair in Chiral Photonics in 2006 and in Photonics for Life since 2013. He studies Self-organization, Organic and nano-Photonics, including the Chemistry, Instrumentation, Processing and Physics of nanomaterials and devices as well as their use for energy and sustainable development. His Google H-factor is 53.*

Pr. Ali ZAOUI

Université de Lille

Topic : Predicting new compounds using high-throughput ab initio computation.

By: Prof. Ali ZAOUI, Lille University, France.

In this talk I will give, first, an overview on some recent studies related to semiconductors in the bulk, doped, alloys and superlattices cases. It will be presented for different structures and phases under pressure and temperature effects. In addition, electronic and optical properties of the considered prototype materials will be presented and discussed. Detailed analysis will be given at the nanoscale level from first-principles calculations based on density functional theory. In the second part of my talk I will present some recent results related to surface morphology of carbonates, as well as their behaviors under water and pressure effects. The hydrous phases are of considerable interest for their role as precursors to stable carbonate minerals. I will present detailed recent results concerning structural and energetic stability of dry and hydrous surfaces of calcium carbonate polymorphs using two recently developed force-fields. Finally I will show and discuss the computed morphology pictures obtained from MD simulation and compared to observed SEM images. Besides, further recent studies will be shown regarding the interface between clay and carbonate surfaces under anisotropic constrains as well as shear stress. Various mechanical properties will be presented with and without the presence of water, under nuclear radioactive storage conditions. The third and last part of my talk will be devoted to the application of evolutionary algorithm and density functional theory. I will show the investigation of the thermodynamic, mechanical, dynamical and optical properties of some binary and ternary compounds. I will, in particular highlights in the case of alloys the prevailing role of chemical and stress effects behind the giant optical band-gap bowing.

Prof. Ali ZAOUI : *Full professor (Polytech'Lille / University of Lille) since February 2005. He is actually professor of Exceptional Class 2. In September 1999 he was employed as a research associate at the INFM (National Institute of Matter Physics), Italy. He then jointed the Max Planck Institute of Stuttgart, in Germany. His research has been mainly dedicated to the modeling and simulation methods based on first-principles, molecular dynamics and Monte Carlo. They cover a wide range of materials and fields of research including Semiconductors, metals, geo-materials, water, interaction water and soil, environment, nano-composites, surfaces, interfaces. He has published over 200 papers in international journals and has supervised around 30 PhD students. In addition, he is director of the international master program nanoscience and nanotechnology for civil engineering at Polytech'Lille (http://master-nngc.univ-lille1.fr), and he is member of the national committee of universities in France. Since January 2020, he is Director of the regional laboratory of civil engineering and geo-environment, LGCgE (more than 220 people) in the north of France. (https://www.lgcge.fr).*

Topic : Predictive Unlocking the Low-Dimensional Nanocarbon Allotropes Functionality at the Ion-Assisted Pulse-Plasma Deposition.

By: Prof. Alexander LUKIN, Western-Caucasus Research Center, Tuapse, Russian Federation.

Low-dimensional nanocarbon allotropes represent promising nanoscale building blocks as they possess unique structural, chemical and physical properties that are of great interest for the high-end applications in the emerging field of nanotechnology. The "holy grail" of one-dimensional carbon allotropes, an ideal one-dimensional form of carbon, named as a carbine, represents an infinitely long linear chain of carbon atoms. The growth of the macroscopic crystals of carbyne is inhibited by the instability and high reactivity of this allotropic form of carbon. Relatively recently, were found new route to compensate for the above disadvantage by encapsulating oriented linear chains of carbon atoms - the monatomic carbon filaments into the matrice of amorphous carbon, creating bends and controlling the end groups in the process of ion-assisted pulse-plasma growth. Such kind of carbon nanostructured meta materials were named as an 2D-ordered linear-chain carbon, that represents a two-dimensionally packed hexagonal array of carbon chains held by the Van der Waals forces with the inter chain spacing approximately being between (4.8-5.03) angstroms. The outstanding nano-architecture, physical and chemical properties, determined by the unique combination of electronic bond structures between the boundary nano-allotropes in this nano-matrice, provide a huge application potential and versatility of these carbon nanomaterials. Application of the 2D-ordered linear-chain carbon opens possibilities for enhancing the functional properties of a number of nanomaterials and to unlock their full potential for practical applications in advanced nanotechnologies and high-end devices.

Improving the technological capabilities of growing and precision programming of the properties of the low dimensional carbon allotropes as well as carbyne-enriched nanomaterials allows create new versions of the multifunctional hybrid nanomaterials with a set of new unique properties and, thereby, reveal fundamentally new opportunities practical use of these nanomaterials.

Nowadays, the research on materials science is rapidly entering a phase of data-driven age. For predictive grows the 2D-ordered linear-chain carbon-based functionalizing nano-matrixes with a unique set of programmable nanoarchitecture and properties, by using the results of experimental testing, we propose apply a new paradigm in Materials Science – a science based on data and deep informatics of nanomaterials. In this area, the experimental data is a new resource, and knowledge is extracted from datasets of materials.

We propose fine tuning the vibrational signature, functionality and nano-architecture of the 2D-ordered linear-chain carbon-based nano-matrices by using the surface acoustic waves (SAW)-assisted precision micro/nano manipulation by the pulse-plasma grows zone combined with the data-driven carbon nanomaterials genome approach, which is a deep materials informatics-based tool-kit, belonging to the fourth scientific paradigm. The use of SAW tool-kit makes it possible to precisely manipulate by bond breaking and formation during the ion-assisted pulse-plasma growth and, accordingly, by sp-phases transformations in the nano-matrice growth zone. The possibility of programmable Chladni patterns excitation at the nanoscale is a key approach for controlling the nano-architecture and properties of growing 2D-ordered linear-chain carbon-based nano-matrices. Since the required combination of sp-phases in the composition of the nano-matrices being grown can be provided in a narrow range of technological growth parameters, the selection and exact provision of which is a difficult task,

the use of SAW tool-kit opens new possibilities for precision tuning of parameters in the nano-matrice growth zone for providing the required combination of the sp-phases.
The proposed data-driven carbon nanomaterials genome approach establishes linkages between key modes and parameters of ion-assisted pulse-plasma growing of the functionalizing nano-matrices and their resulting nanoarchitecture and physicochemical properties through a set of multifactorial computational models, developed with use extensive experimental data for a selected set of key descriptors or fingerprints.
Development of the data-driven carbon nanomaterials genome approach is an effective catalyst for the creation of new modifications of multifunctional carbon nanomaterials with a set of new unique properties, the discovery of new application areas of the multifunctional carbon-based nanomaterials as well as for intensification of the development of promising high-tech devices.
***Prof. Alexander LUKIN:** Got a M.S. degree (Rocket Propulsion Engineer) from Izhevsk State Technical University with the Diploma of Excellence (1985) and Ph.D. degree (Phys. & Math.) from the Physics-Technical Institute of the Ural Branch of the Russian Academy of Sciences (1993). Dr. Lukin was involved in critically-important research programs associated with the development of the solid propulsion systems that support the upper stages of intercontinental ballistic rockets. Dr. Lukin is Associate Fellow and Lifetime Member of the American Institute of Aeronautics and Astronautics (AIAA), International Member of the AIAA Solid Rockets Technical Committee (SRTC); Member of the AIAA United Nations Committee On Peaceful Uses of Outer Space (UN-COPUOS) Working Group (WG); Member of the International Advisory Committee of the State Key Laboratory for Modification of Chemical Fibers and Polymer Materials (SKLFPM) in Donghua University, Shanghai, China; Professor-Advisor of the Shaanxi Research Institute of Applied Physics-Chemistry, China; Academic Consultant of the North-Western Polytechnic University, China; Member of the National Graphene Association (NGA). Dr Alexander Lukin is Expert of the Russian Academy of Sciences, Expert of the Expertise Councils of the Russian Science Foundation, Expert of Federal Register of Experts of the Ministry of Education and Science of the Russian Federation in the area of Space and Transport Systems, Honorary Fellow and Chair of the Research Sub-committee of the Academic Council of the Australian Institute of High Energetic Materials (Sippy Downs, Australia). More details is available at the following reference: http://www.wcrc.ru/Lukin-CV-2022.pdf*
Dr. Lukin's areas of research interest are in aerospace propulsion; energetic materials; carbon-based nanomaterials; deep materials informatics; ion-assisted pulsed-plasma deposition; self-organizing of the micro/nano-scale structures; plasma-acoustic coupling mechanism; nanoclusters; cymatics; micro/nano-pattern formation; advanced propulsion materials; ignition and combustion of propellants for space and rocket propulsion; unstable and abnormal combustion of the energetic materials; microscale combustion mechanisms; functional nanomaterials; advanced plasma technology application.

Topic : Wildfire physics and modelling.

By: ***Prof. Sofiane MERADJI, Aix-Marseille University (AMU), France.***
Prof. Dominique MORVAN, Aix-Marseille University (AMU), France.
Prof. Gilbert ACCARY, Lebanese University, France.

This work reports on the modeling and 3D numerical simulations of wildfire propagation. The mathematical model is based on a multiphase formulation and a homogenization approach that consists in averaging the conservation equations (mass, momentum, energy) governing the evolution of variables representing the state of the vegetation/atmosphere system, within a control volume containing both the solid-vegetation phase and the surrounding gas phase. The relationship between the rate of spread (ROS) and the wind velocity is revisited, through the role played by the two forces governing the trajectory of the flame front and the plume, namely the ratio between the buoyancy of the plume and the inertia due to wind. The ratio between these two forces is introduced, through the Byram's convective number. The existence of two regimes of propagation of surface fires (wind-driven fire vs plume-dominated fire) and the relative importance of the two modes of heat transfer (by convection and radiation) on the propagation of a fire front are discussed.

Prof Dominique MORVAN*: Searcher at CNRS from 1985 to 2000, Professor in Mechanical Engineering at Aix-Marseille University (AMU) since 2000. Scientific background: Mechanical engineering, Fluid Mechanics, Biomechanics, Heat and Mass transfer, Computational Fluid Mechanics, Turbulence, Wildfire modelling. Director of the Department of Mechanical Engineering (AMU) from 2014 to 2020, Associate editor of the International Journal of Wildland Fire.*

Prof Sofiane MERADJI: *Holder of a PhD in Computational Fluid Mechanics, obtained at the University of Aix-Marseille II in 1999, I started my research activity around the theme of forest fires, in 2006, during the European project FIRE PARADOX. Since 2010, I am a Research Engineer in Scientific Computing at the University of Toulon, in a laboratory of Applied Mathematics and Computer Science. My research focuses on the fire physics and tools development on HPC architectures.*

Prof Gilbert ACCARY: *BE in Mechanical Engineering from the Lebanese University in 2001, PhD in fluid mechanics for Aix-Marseille University (France) in 2005. Full Professor at the Lebanese University-Faculty of Engineering since 2014, where he teaches fluid mechanics, gas dynamics, heat transfer, and CFD. His main current research fields are the physics-based modeling of wildfire spread and the water desalination processes.*

Topic : RES Heat-Renewable Energy System for Residential Building Heating and Electricity Production.

By: Prof. Paweł OCLON, Cracow University, Poland.

Co-Author: Piotr Cisek, Ph.D., Cracow University, Poland.

Prof Paweł Ocłoń: *Full Professor at the Cracow University of Technology, Department of Energy. He received his Ph.D. (2014) and DSc (2017) in Energy Engineering from Cracow University of Technology. His research focuses on numerical modelling; process optimization; renewable energy sources.*

Piotr Cisek: *is an Assistant Professor at the Cracow University of Technology, Department of Energy. He received his Ph.D. (2017) in Energy Engineering from Cracow University of Technology. His research focuses on heat storage, computational heat transfer, renewable energy sources, as well as green hydrogen production, storage, and utilization.*

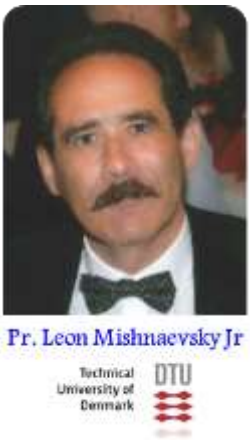
Topic : Surface Enhanced Visible Absorption of Dye Molecules in the Near-Field of Gold Nano-Antennas.

By : Pr. Zouheir SEKKAT, Mohamed V University, Morocco.

rof. Zouheir SEKKAT: *Full professor of the Department of Chemistry, of the Faculty of Sciences, of Mohammed V University in Rabat, Rabat, Morocco, and Director of the Optics & Photonics Centre, Moroccan Foundation for Advanced Science & Innovation & Research, MAScIR, of the University Mohammed VI Polytechnic, Morocco, and Cross-appointed full professor of Osaka University, Japan. Sekkat's research interests, are in the fields of Photonics and Nanotechnology, including green photonics, i.e. renewable energies, and agro-photonics, by remote sensing, and bio-photonics, for medical diagnostics and therapy, and smart materials for, for example, future materials for direct conversion of light energy into mechanical energy. These research and development area are supported by expertise in Nonlinear Optics, Photochemistry, Photoreactive polymers, Plasmonics and Near-field Nano Optics and Spectroscopy, Waveguide Optics, Holography, 3D Nano-printing, and Photovoltaics, as well as other experties. In 2006, he received the Elsevier prize for the most cited paper in Morocco. He has authored and co-authored more than 170 international publications, with 4714 citations and h-index of 37 (ISI), and 6 patents and book chapters and edited a book. In 2010, he received a distinction prize from the Ministry of education of Morocco, and in 2006, he was appointed as a corresponding member of the Hassan II Academy of Sciences and Technology, and he is currently Expert of this academy. In 2019 he was elected to the rank of fellow of the African Academy of Sciences, and SPIE in 2020 and OSA in 2021.*

Topic : Novel materials and computational modelling for the development of wind energy.

By : Prof. Leon MISHNAEVSKY Jr, Technical University of Denmark.



The intensive development of renewable energy in general, and wind energy, in particular, is expected in next years and decades. Wind turbines became larger and larger over last decades, with blades reaching hundred meters. The requirements toward wind turbine materials are extraordinary high, in particular, for wind turbine blades. A wind turbine is expected to serve for 25-30 years. With view on the extraordinary durability and reliability requirements toward wind turbine blades, and high maintenance costs, the wind turbine materials should demonstrate extraordinary strength and fatigue resistance, combined with low weight. Contemporary materials science aspects related to the development and expansion of wind energy are discussed in this presentation. Possibilities of development of structural composites from bio-based elements, recyclable polymers and thermoplastics, which have the same strength as the usual fiber glass epoxy, are discussed in this presentation.

***Prof. Leon Mishnaevsky Jr.:** Senior Scientist at the Technical University of Denmark. Author of textbooks "Computational Mesomechanics of Composites" and " Micromechanics and Nanosimulation of Metals and Composites". Coordinator of Innovation Foundation project "DURALEDGE/ Durable leading edges for high tip speed wind turbine blades", Danida Foundation project "Maintenance and repair strategies for wind energy development", US-Danish collaborative network "Structural health monitoring of wind turbine blades", and others. Habilitation (Dr. Habil. Mechanics) from TU Darmstadt. former visiting professor at Rutgers University/USA, CUMTB Beijing, and ENSAM France.*

Topic : Development of Industrial Engineerin-Academical Research.

By : Chakib BOJJI, ENSET - Rabat, Morocco.

Pr. Hélène AGEORGES

Université de Limoges

Topic : Towards the control of porosity formation in materials obtained by thermal spraying: an asset to predict their properties.

By: Prof. A. Hélène AGEORGES, University of Limoges, France.

The control of the porosity formation in the materials made by thermal spraying is of great interest to predict their properties. Understand the mechanisms to limit or to increase porosity could expand their applications. For example, highly porous ceramic materials can be employed for thermal insulating applications in the aerospace field. Porous particles can be used in medical industry to introduce into them drugs for a controlled and prolonged release directly on the affected site to improve the efficacy of medical treatments. In another side, dense coatings can increase mechanical properties and the corrosion resistance. It has been established that the porosity formation and distribution in the final material depend on the relationship between the initial particle size distribution used and the thermal spraying parameters such as the power of the source, the gases used and the spray distance. In order to increase the porosity in coatings or in particles, a pore former can be added which it be eliminated during or after the elaboration.

Prof. A. Hélène AGEORGES: *Associate Professor at the University of Limoges, in the topics such as Renewable Energy, Energy Efficiency, Sustainable Development, Thermal Spraying. Head of Bachelor Program of Renewable Energy. Head of the Master Program of Energy Efficiency and Sustainable Development (Dual Diploma University of Limoges / University of Mascareignes in Mauritius. Researcher in Surface Engineering by Thermal Spray Technologies at the Institute of research for ceramics (IRCER), Limoges, France. Her research topics focus on advanced properties of coatings through the use of new materials and innovative processes in fields such as high wear resistance, low friction coefficient, thermal insulation, high temperature protective coatings (thermal and environmental barrier coatings), bioactivity (implant coatings), photocatalysis to meet the requirements of various specific applications. She studies nano and micro-structured coating effects, tribology, wear mechanisms, porosity formation, activity of bioglasses. She contributes to the development of new easy and quick methods of mechanical property measurements for industry. Dr. Ageorges also had contributions to the manufacturing of feedstock powders for thermal spray coatings: cermets, composites for industrial applications and bioactive glasses for biomedical use. She holds a PhD in plasma process engineering from the University of Toulouse, France.*

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Baku local time	09:00 10:00	10:00 10:30	10:30 11:00	11:00 11:30	11:45 12:45	13:20 14:20	14:25 14:55	15:00 15:30	15:30 15:40	15:45 16:15	16:25 17:25	17:30 18:00	18:00 18:15	18:15
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ICOME22 Awards

Best Presentation Award

The ICOME event want to reward involvement, merit and professionalism of young scientist students. An award of better presentation (Phd) will be provided for each sessions and consist on the ICOME medal and free fees for the next ICOME edition.

On 2021 Wolfram Mathematica award involvement and merit of young scientist students doing research using theoretical/Mathematical approach. Priority is given to student using Symbolic computing.

Averroes Award

The new edition of the Averroes[1] prize will take place at this conference, and aims to highlight a scientist or a decision maker who contributed significantly to the development and vitality of international scientific partnership with results, training of young researchers going to scribing the action in a permanent way.

"Ignorance leads to fear, fear leads to hatred and hatred leads to violence. That is the equation"

(Averroes, 1126-1198)

[1] Averroes (Ibn Rochd) European intellectual, born in Spain, died in Morocco, both a philosopher, a theologian, a lawyer, a mathematician and a 12th century Andalusian doctor

AVERROES PRIZES

2020/2021: Geoffrey LEVERMORE, Emeritus Professor, UK.

Geoffrey LEVERMORE: *Prof. Geoffrey LEVERMORE : Emeritus Professor of the Built Environment. Author of about 130 refereed journal papers, 44 invited papers and lectures and 25 book chapters and books. He was an investigator on grants worth £14.53m, 17 with UK Research Councils worth £12.75m, PI on 12 worth £2.27m. Chair of the Task Group and editor of CIBSE Guide A Environmental Design, Chapter A2 External Design Data 1999, 2006 and 2013. In 2007 he was one of the Lead Authors of the Intergovernmental Panel on Climate Change (IPCC) awarded the Nobel Peace Prize with Al Gore. From 2002 to 2009 he was Co-ordinator of Working Commission W108: 'Impact of climate change on the built environment' of the CIB. In 2010 he was awarded a CIBSE Silver Medal. He is still researching part-time, analysing climate change, the urban heat island and building energy use. He has published 22 papers since 2011. He has given seven Keynote Speeches to conferences in Turkey, Dubai, France and China since 2017 and is a member of the Daikin European Konwakai which recently met in Japan.*

2019: Abdelilah BENYOUSSEF, member of the Moroccan Academy of Science and Technology (Hassan II)

Abdelilah BENYOUSSEF: *received his (Doctorat d'état) degree from the Paris-Sud University in 1983. He is a permanent member of the Moroccan Hassan II Academy of*

Science and Technology, since 2006. He is associate professor in the materials and nanomaterials center of the Moroccan Foundation for Advanced Science, Innovation and Research. He is National coordinator of the Competences Pole of Condensed Matter and Systems Modeling. He is also an editor in chief of the Moroccan Journal of Condensed Matter. He is President of the Moroccan Society of Statistical Physics and Condensed Matter. He has been visiting professor in many centers, laboratories and Universities. The main interest topics of Abdelilah Benyoussef are Ab initio calculation and Monte carlo method in modeling and simulation of new materials for renewable energy; Magnetism and phase transition in condensed matter; complex systems and critical self-organization in statistical physics. He is a co-author of more than 400 research publications and book chapters and about 100 conference presentations including numerous invited papers and talks.

2018: *Sassi BEN NASRALLAH, Presidential award in 2003*

Born in 1955, Sassi Ben Nasrallah is a doctor in physical sciences. He joined higher education as an assistant professor at ENIS and then as a lecturer and was then promoted to the post of Professor of Higher Education at ENIM. He has contributed a lot to teaching, especially research, since in 1999 he created the Laboratory of Thermal and Energetic Systems, which is one of the most renowned laboratories both nationally and internationally. He is the author of more than 300 scientific articles in major journals, and he supervised several PhD students. Sassi Ben Nasrallah won a presidential award in 2003. The professor has also led several research projects as well as scientific meetings. He has been a professor in both Tunisian and French universities, and is well known for his studies at the Central School of Paris, IMFT Toulouse, Mine's School of Nantes and many others. Sassi Ben Nasrallah founded and chaired the Tunisian Energy Association (ATE). The Ministry of Higher Education announced, on June 30 2017, the death of Sassi Ben Nasrallah, professor of higher education at the National School of Engineering of Monastir.

2017: Abdul Majeed MOHAMAD, Education Excellence awards

Abdul Majeed Mohamad *Professor in Eastern Mediterranean University, Cyprus (1993-1999). Since 2000 he is Prof. of thermofluid in Dept. of Mechanical Engineering, University of Calgary, Canada. Dr. Mohamad held few admin positions, director of graduate studies, acting director for Centre for Environmental Engineering Centre for Research and Education. Dr. Mohamad has been invited by many institutes around the world (France, Germany, China, USA, Poland, Saudi Arabia, Canada, Portugal, Morocco, Tunisia, Turkey, Indonesia, and Ecuador), as invited Professor and lecturer. He is one of the highly cited researches. Dr. Mohamad elected Fellow Member of American Society of Mechanical Engineer (ASME).Scientific council member of International Centre for Heat and Mass Transfer. He has been awarded Research Excellence and Graduate Teaching Excellence awards from University of Calgary, Dept. of Mechanical Engineering, Canada.*

2016: Michel COMBARNOUS, French Academy of Sciences

Michel Combarnous, *Professor "Emeritus" at the University of Bordeaux, has been associate professor at the University of Gabès (Tunisia) (2006-2011). A specialist in fluid mechanics and energetics, he was encharged of the Department « Engineering Sciences » at CNRS (1980-1985). He is a founding member of « Académie des Technologies », and Corresponding Member of the Academy of Sciences, since 1978 (www.academie-sciences.fr). Prof. Combarnous has accomplished a huge cooperative work involving north-south Mediterranean cooperation*

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