International Summer School on Advanced Materials for Energy

ISSAME

Université du Littoral Côte d'Opale

Saint-Omer, France

December 13–14, 2021

ISSAME Chairs

Dr. Dharmendra SINGH
Dr. Amina TACHAFINE

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The First edition of International Summer School on Advanced Materials for Energy

ISSAME

Saint-Omer- France

December 13-14, 2021

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Dynamics and Structure of Molecular Materials Unit
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ISSAME Venue: **Amphithéatre, IUT du Littoral-Côte d'Opale, Avenue Descartes 62219 Longuenesse, France**

Le mot du Président de la Communauté d'agglomération du Pays de Saint-Omer

Les élus de la Communauté d'agglomération du Pays de Saint-Omer sont très heureux d'accueillir le colloque international sur les matériaux et applications diélectriques ainsi que l'école doctorale les 13 et 14 décembre prochain.

Tant ce colloque que l'école doctorale sont une première et permettront de réunir compétences et expertises autour d'une thématique particulièrement d'actualité.

Depuis 2016, le territoire du Pays de Saint-Omer a engagé un partenariat étroit avec l'Université Littoral Côte d'Opale afin de favoriser le développement de nouvelles formations mais aussi les travaux de recherches menés par les différents laboratoires et en particulier le LISIC (Laboratoire d'informatique, Signal et Image de la Côte d'Opale) que l'UDSMM (Unité de Dynamique et Structure des Matériaux Moléculaires).

Plus que jamais dans une société en profonde transformation, la recherche a toute sa place et prend une importance toute particulière pour aider à la transition digitale, environnementale, sociétale et l'innovation sous toutes ses formes et ses applications dans le monde économique.

La Communauté d'agglomération tient à féliciter les organisateurs de ce colloque et a souhaité apporter son soutien à cette initiative totalement en phase avec la stratégie du territoire.

C'est le triptyque collectivité / monde économique / formation-recherche qui constitue le socle indispensable d'une stratégie de développement économique d'un territoire, l'organisation de ce colloque y apporte naturellement sa contribution.

Avec tous mes vœux de réussite et de succès.

Joël DUQUENOY
Président
Communauté d'agglomération
du Pays de Saint-Omer

Preface

The **International Summer School on Advanced Materials for Energy (ISSAME)** is intended for young scientists and PhD students interested in Materials Science for energy.

The scope of this Summer School is to familiarize students with the state of the art in advanced materials for energy.

ISSAME is focused on theoretical and experimental aspects of synthesis and characterization of advanced materials for energy, i.e. materials that meet a strong societal demand for the conversion and storage of electrical energy as well as energy savings. The school aims to present an overview of the latest developments in the theory of these advanced materials, their modelling, processing, characterisation and applications.

It will cover topics like Electronic and Optical Materials, Polymers and Composites, oxides, semiconducting, metallic and organic materials, materials for supercapacitors, fuel cells and batteries, photovoltaic devices and related technologies.

Lectures in these areas will be given by high-level researchers. So, participants will have the opportunity to discuss their own research work and exchange with the scientists involved in this area.

A.Pr. SINGH Dharmendra and TACHAFINE Amina, Chairs of ISSAME 2021

University of Littoral-Côte d'Opale, Calais, France

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https://isydma6.univ-littoral.fr/pre-conference-site/

CET	Monday, 13/12/2021
8.30-9.00	Registration
9.00-9.30	Opening Ceremony of ISSAME 2021
9.30-10.00	Welcome Reception
	Chair: Prof. Stéphane LONGUEMART
10.00-10.45	**Lecture 1: Prof. Jeroen BEECKMAN** *Ferroelectric thin films for electro-optic modulators, piezoelectric actuation and nonlinear optical conversion*
10.45-11.30	**Lecture 2: Prof. Vincent LADMIRAL** (online) *Macromolecular engineering of electroactive fluoropolymers*
11.30-12.15	**Lecture 3: Prof. Suleyman ER** (online) *Automating the virtual discovery of molecules for energy storage*
12.15-13.15	**Lunch Break**
	Chair: Dr. Michael DEPRIESTER
13.15-14.00	**Lecture 4: Prof. Ingo DIERKING** (online) *Polymer stabilisation of liquid crystal structures and phases and their application in smart windows*
14.00-14.45	**Lecture 5: Prof. Azeez Abdullah BARZINJY** *Green Synthesis of Nanoparticles: From Preparation to Applications*
14.45-15.30	**Lecture 6: Prof. Frédéric SAUVAGE** (online) *Transparent and Colorless Dye-Sensitized Solar Cells*
15.30-16.00	**Coffee Break**
16.00-17.00	**Round Table Discussion** *Chair Person : Prof. Jeroen BEECKMAN*
17.30-19.30	**St. Omer Visit** *(Théâtre de Saint Omer / La Maison du Marais)*
19.30-21.30	**Gala Dinner (at Château de Tilques)** *Address : 12 Rue du Château, 62500 Tilques*

CET	Tuesday, 14/12/2021
	Chair: Prof. Johan LAUWAERT
9.00-9.45	**Lecture 7: Matthieu BECUWE** *Organic, hybrid and polymer materials for energy*
9.45-10.30	**Lecture 8: Prof. Yogendra Kumar MISHRA** (online) *Tetrapods based Smart Materials for Advanced Technologies*
10.30-10.45	**Coffee Break**
10.45-11.30	**Lecture 9: Prof. Luciano DE SIO** (online) *Green nanoscale biophotonics: from real-time biosensing to photo-thermal therapy*
11.30-12.15	**Lecture 10: Prof. Michael DEPRIESTER** *Thermoelectric materials: Principle, characterization and modern applications*
12.15-13.00	**Lecture 11: Prof. Stéphane LONGUEMART** *Refrigeration using electrocaloric effect*
13.00-14.00	**Lunch Break**
	Chair: Prof. Ashok VASEASHTA
14.00-14.45	**Lecture 12: Prof. Johan LAUWAERT** *Solar cell simulations via SCAPS*
14.45-15.30	**Lecture 13: Prof. Mamatha NAGARAJ** (online) *Liquid crystals for organic electronic devices*
15.30-16.15	**Lecture 14: Prof. Mustapha JOUIAD** *Towards nanomaterials engineering for solar energy harvesting and conversion*
16.15-16.30	**Coffee Break**
16.30-17.15	**Lecture 15: Dr. Deepak Pratap SINGH** (online) *Electrochemistry in energy storage and conversion*
17.15-18.00	**Lecture 16: Prof. Mustapha MABROUKI** *Detection of the photoacoustic signal by an unconventional technique*
18.00-19.00 19.00	**Round Table Discussion** *Chair Person : Prof. Mustapha JOUIAD* **Closing Ceremony & Return to Calais**

Green Synthesis of Nanoparticles: From Preparation to Applications

Azeez Abdullah Barzinjy[1,2*]
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Abstract

Nanotechnology is an emerging field of science. The base of nanotechnology is nanoparticles. The size of nanoparticles ranges from 1 to 100 nm. The nanoparticles are classified into different classes such as inorganic nanoparticles, organic nanoparticles, ceramic nanoparticles and carbon base nanoparticles. The inorganic nanoparticles are further classified into metal nanoparticles and metal oxide nanoparticles. Similarly, carbon base nanoparticles classified into Fullerene, Carbon nanotubes, Graphene, Carbon nanofiber and carbon black. Nanoparticles are also classified on the basis of dimension such as zero-dimension, one-dimension, two-dimension and three-dimension nanoparticles. The nanoparticles are synthesized by using two approaches like top-down approach and bottom-up approach. Since the main methods for producing nanoparticles are chemical and physical methods which are often expensive and potentially harmful to both the environment and the user. So, we did our best in our researches to synthesize metallic nanoparticles using plant extracts and stay away from expensive and toxic chemicals at the same time. Therefore, it is with great pride that our research group is considered a pioneer in the region, and many high quality research articles have been published by our group highlighting the necessary needs of the community [1-22] regarding green synthesis nanomaterials. After synthesizing different types of nanoparticles, using easy, one-pot, inexpensive and green process, from locally grown plant extracts, different characterization techniques have been used to investigate structure, size, morphology, thermal behavior, surface area, surface charge, chemical composition and optical properties of the nanoparticles. After synthesizing and characterization process, the green synthesized nanoparticles were employed in thin film application, gas-sensing, enhancing solar panel efficiency, wastewater treatment, catalytic application, harvesting sunlight for solar thermal generation and many other applications.

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Prof. Matthieu BECUWE

Laboratoire de Réactivité et Chimie des Solides (LRCS), Université de Picardie Jules Verne (UPJV)
Amiens

France

Ferroelectric thin films for electro-optic modulators, piezoelectric actuation and nonlinear optical conversion

Abstract:
Preferentially oriented ferroelectric thin films with high quality can be deposited on almost any substrate when using a suitable lanthanide based thin intermediate layer. The films are deposited using a chemical solution deposition method, developed at Ghent University. Both lead zirconate titanate (PZT) and barium titanate (BTO) deposited with this process show excellent oriented growth. Such thin films are interesting for a number of applications because they exhibit strong electro-optic coefficients, piezoelectric coefficients and a strong second order nonlinear susceptibility. Measurement of the electro-optic coefficients reveal that PZT layers can be poled once and retain their high electro-optic coefficient, which means that no constant DC voltage is required for electro-optic modulation. PZT based electro-optic modulators have been integrated onto a SiN photonic platform and high-speed electro-optic modulators have been demonstrated with a bandwidth of up to 30 GHz. Similar modulation of waveguides is also possible by using the piezoelectric effect. Surface acoustic waves are generated inside the PZT thin film and are used to modulate an optical signal through the acousto-optic effect. Finally, it has also been demonstrated that the PZT thin films exhibit a very strong second order susceptibility of 128 pm/V. The sign of the susceptibility can be changed by applying DC voltages which opens up the possibility of quasi-phase matching.

Prof. Jeroen BEECKMAN

Electronics and Information Systems Department
Faculty of Engineering and Architecture, Ghent University, Ghent, Belgium

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Prof. Luciano De Sio

Department of Sciences and Biotechnology Medical-Surgical**, Sapienza University of Rome, Italy**

Green nanoscale biophotonics: from real-time biosensing to photo-thermal therapy

Short Abstract: Nanotechnology and nanomaterials play a crucial role in modern and cross-disciplinary science thanks to the capability to monitor and manipulate biomaterials at the nanoscale. In this framework, gold nanoparticles have gained significant attention thanks to their unique thermo-optical and spectroscopic properties. In this talk, I present and discuss the latest achievements in plasmonic-assisted biomedical applications. From environmental biosensing to cancer therapy, a new generation of "green" and biophotonic applications are reported and discussed.

Thermoelectric materials: Principle, characterization and modern applications

Michael DEPRIESTER

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Abstract

Due to concerns over resource conservation and climate change, the world is looking for alternatives to fossil fuels. Among technical solutions, thermoelectric devices allow the conversion of waste heat energy into electricity. Its physical principles are known since the 19th century, but first energy applications date from the middle of the 20th century. These converters were during a long time restrained to some niche markets, especially spatial applications for their high reliability with no moving parts. A too low transformation yield has prevented its large-scale deployment. Since the end of the 20th, this field has regained momentum when it was predicted that nanostructures could enhance the conversion efficiency [1, 2].

Thermoelectric researchers are focus on a main objective: increasing the figure of merit directly related to the energy conversion efficiency. The dimensionless figure of merit is given by [3]:

$$ZT = \frac{\sigma\, S^2}{\kappa} T,$$

where the transport parameters σ, S and κ are respectively the electrical conductivity, the Seebeck coefficient and the total thermal conductivity. T is the averaged working temperature alongside the device into consideration. Improving a thermoelectric material consists of increasing σ, S and decreasing κ. However, these transport parameters are physically interrelated, consequently fostering one parameter is usually detrimental to the other ones. In this talk, we will focus on the different strategies applied to lower the thermal conductivity without impacting negatively (too much) the two other transport parameters [3].

Material performances can be assessed from their figure of merit values. So, measuring properly the transport parameters values entering the definition of ZT and estimating their associated uncertainties is of main importance. Potentialities of some techniques used to characterize the transport properties of thermoelectric materials will be discussed. Finally, some modern applications of thermoelectric materials will be presented.

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Ingo Dierking

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Polymer stabilization of liquid crystal structures and phases

Polymer stabilized liquid crystals are formed by subjecting a small amount of bifunctional photoreactive monomers, uniformly dissolved with a photo-initiator in a liquid crystal host, to UV irradiation. The formed polymer network templates the liquid crystal director field in which it was formed, thus stabilizing the structure. The effect of stabilization depends largely on the monomer concentration, the solubility limit of the monomer in the liquid crystal, but also on applied conditions during network formation, such as temperature, time of irradiation, UV intensity and dose. Polymer modified liquid crystals in general are promising materials for a range of electro-optic and photonic applications, for example paper-like reflective displays with flexible substrates, privacy windows or foils, self-healing ferroelectric liquid crystal devices, Kerr effect based fast switching Blue Phase displays, or smart windows, reflecting light in the visible or the IR region.

We will discuss polymer stabilization for several different liquid crystal phases and structures, demonstrating the imaging of director fields via topological defects. We will further show the formation of helical polymer networks, which are used in reflective displays, privacy windows and smart windows for energy saving. Plywood structures are demonstrated resulting from twist grain boundary phases, which are similar to biological systems. At last, we will discuss the performance and principles of polymer stabilised Blue Phases for novel, fast switching display applications in devices without orientation layers.

It is concluded that polymer modified liquid crystals do not only show potential for fundament research, but also open the door to a wealth of applications ranging from electro-optic devices to photonics, from optical to energy saving technologies.

Automating the virtual discovery of molecules for energy storage

Süleyman Er [1,2*]

[1] DIFFER - Dutch Institute for Fundamental Energy Research, De Zaale 20, 5612 AJ Eindhoven, The Netherlands

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Abstract:

The further development of existing chemical compounds or the discovery of completely new ones are frequently required for achieving breakthrough advancements. Therefore, the research on the intriguing chemistries of compounds is central to the innovation cycle of new technologies, such as the research on clean energy storage systems. Redox flow batteries are a type of rechargeable batteries where chemical energy is provided by two chemical components, called electrolytes, which are dissolved in liquids that are pumped through the system on separate sides of a membrane. A central issue for developing all-organic redox flow batteries for intermittent renewable electricity storage is the discovery of electrolytes that would satisfy multiple criteria of synthesizability, suitable redox potentials, rapid kinetics, solubility, stability, and safety. An overarching challenge is the speedy identification of useful compounds in an almost infinite chemical space. In this regard, high-throughput computational screening, which relies on robust quantum chemistry methods while utilizing agile software tools on powerful computers, is an insuperable method. In parallel, machine learning methods excel in making fast predictions of material properties and finding insights when they learn from high-quality and large-quantity experimental and computational data. In this course, I will present how computational chemistry and machine learning can be effectively used for the discovery of new electrolytes for energy storage in redox flow batteries. Additionally, I will discuss our efforts on using a combination of physics-based computation, machine learning, and automated vendor search on a systematically generated library of molecules, as well as on the full cell electrochemical characterizations of purchasable and safe compounds from the virtual library. This work therefore is an exemplary application of the high-throughput computational screening guided experiments on a focused chemical space of candidate energy storage materials.

Prof. Mustapha JOUIAD

Laboratoire de Physique de la Matière Condensée (LPMC), Université de Picardie Jules Verne (UPJV), Amiens**, France**

Towards nanomaterials engineering for solar energy harvesting and conversion

Abstract: The inherent increasing demand in clean energy solutions and new technologies has prompted scientists to custom the materials design and properties for targeted application. Most of the emerging materials such as 0D, 1D and 2D materials that demonstrate promising properties, are complex with more and more reduced dimensions. Special fabrication techniques as well as advanced multiscale characterization in conjunction with modelling, have emerged to make the processing of these materials possible and easily tuneable to meet the targeted application. In this talk, examples of nanoengineered materials exhibiting high optical performances that can serve as high-yield photocatalysts for solar energy harvesting will be tackled with special emphasis to the physics underlaying their performances.

Macromolecular engineering of electroactive fluoropolymers

Vincent LADMIRAL

ICGM, Univ Montpellier, CNRS, ENSCM, Montpellier, FRANCE

Abstract

Fluoropolymers are an important class of polymers endowed with remarkable properties (ferro- and piezoelectricity).[1] The development of efficient Reversible Deactivation Radical Polymerization (RDRP) techniques for VDF (and TrFE) has not been as fast or intense as that of other vinyl monomers. Until recently, only Iodine Transfer Polymerization was able to afford some degree of control on the polymerization of VDF. This talk will provide a detailed account of the recent advances made in the RDRP of VDF and TrFE using RAFT[2,3] and CMRP[4] techniques. The monomers were homopolymerized in the presence of *O*-ethyl-*S*-(1-methoxycarbonyl)ethyldithiocarbonate and tert-amyl peroxy-2-ethylhexanoate as xanthate chain transfer agent and initiator respectively in dimethyl carbonate at 74 °C. Due to reverse addition these polymerizations lead to two different dormant species: the regularly and inversely terminated PVDF and PTrFE chains. Due to the much lower reactivity of the dormant chains resulting from a head-to-head addition these dormant species accumulate very fast in the reaction medium until they constitute 100% of the xanthate-terminated chains. After this point, the RAFT equilibrium slows down and the control of the polymerization is severely degraded.[5] In addition, both polymerization are severely affected by hydrogen abstraction leading to H-terminated dead-chain. In the case of VDF, a head-to-head addition is always followed by a tail-to-tail addition. In contrast, our NMR study revealed tail-to-head additions (reverse propagation) in the case of TrFE. In spite of the aforementioned loss of control, macromolecular engineering remained possible and relatively well-defined fluoropolymer-based architectures were synthesized. However, a better controlled homopolymerization of VDF was observed when Cobalt-Mediated Radical Polymerization was used.[6]

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Prof. Johan Lauwaert

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Solar cell simulations via SCAPS.

Advanced semiconductor materials for energy will assist the road to photovoltaics without the use of scarce or toxic material. These novel materials are in the ideal way combined as a junction to form a solar cell. For such a layered structure with many possible mechanisms that have impact on the performance an adequate numerical model is necessary. Therefore computer modelling is essential for our understanding and the corresponding progress of these solar cell technologies. Consequently, SCAPS and other simulation packages for thin film solar cells are very successful. In this lecture an introduction will be given on the use of SCAPS as a modelling tool for solar cells and the conventional characterization techniques for photovoltaics.

Prof. Stéphane LONGUEMART

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Refrigeration using electrocaloric effect

Abstract : Due to the increasing energy demand and the related environmental issues, a large amount of research works is carried out for allowing the exploitation of particular physical phenomena for cooling applications, in replacement of refrigerant fluid based devices. Solid state cooling technologies using caloric materials have attracted recently a large interest. The exploitation of the magnetocaloric effect is probably one of the most known and studied so far, but other phenomena like elastocaloric or electrocaloric effect are nowadays considered for building more efficient and respectful refrigeration devices. In this talk, the electrocaloric effect in polar materials and the available methods to characterize it will be presented. In the second part, focus will be made on the development of electrocaloric based refrigeration devices and the issues to tackle before envisaging commercial applications.

Detection of the photoacoustic signal by an unconventional technique

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Photoacoustic (or optoacoustic[1,2]) refers to the generation of mechanical waves in an object illuminated by electromagnetic radiation. The first to report the existence of such a phenomenon was Alexander Graham Bell in 1880[3], who discovered that sound waves could emanate from objects illuminated by sunlight.

Little progress was made before the 1970s because of the lack of a usable light source and it was only with the rise of the laser that the photoacoustic effect came out of the shadows[3]. From then on, scientists saw its interest, in particular for biophysics and even medicine.

On the other hand, the discovery of atomic force microscopy (AFM) [4] was followed by a significant interest in the study of the physical, chemical and mechanical properties of materials.

Initially AFM designed for imaging with atomic and molecular resolution has now been combined with other techniques to give rise to other applications such as (PFM) pulsed forced microscopy) [5], (CFM) chemical force microscopy (chemical force microscopy) for the determination of functional groups[6], as well as magnetic force microscopy to image magnetic dissipation[7], and again near-field optical microscope (SNOM) scanning for imaging local optical properties[8,9]. Note also the acoustic force microscopy imaging (SAFM) [10,11,12] which makes it possible to analyze the propagation of the transverse acoustic wave with a submicron resolution as well as the UFM ultrasonic force microscopy [13] in the determination and measurement recently the contact stiffness of a thin film on a silicon substrate[14]. Studies combining SPM in general and acoustic waves[15] directly have made it possible to locally measure the viscoelasticity of samples beyond the surface. Specifically those who combined STM measurements and the effect of laser light on the tip (expansion heating) and its impact on the measured STM signal. Finally the work done by U. Rabe and al [16] modifying the classic AFM to image a silicon surface and using an acoustic excitation generated by a transducer. This work allowed them to achieve lateral resolutions of the order of 100 nm for an excitation frequency of 20MHz..

The interest of this course is focused on the detection of acoustic and thermal waves and more precisely the detection of manometric deformations within a solid by combining the two techniques presented previously, namely AFM and photoacoustic. The latter is based on the effect linked to the conversion of light energy into thermal energy during a non-radiative de-excitation of the sample and identifiable by pressure oscillations[17] and which provides information on the properties of non-destructive materials. . Note that this technique remains limited by the need to use a closed cell for the detection of the photoacoustic signal. This coupling of AFM and pulsed PA in our case made it possible to take measurements in air with a much wider temporal resolution

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Tetrapods based Smart Materials for Advanced Technologies

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Considering the size dependent utilization complexities of nanoscopic dimensions towards real applications, the focus of nanomaterials community is merging to three-dimensional (3D) form of materials which are built out interconnected nanostructures. This talk will briefly introduce the importance of complex shaped nanostructures towards smart 3D nanomaterials structuring. A simple flame based single step approach was developed for synthesizing zinc oxide tetrapods which demonstrated many applications in different technologies. These tetrapods have been used as building blocks to construct highly porous interconnected 3D nanonetworks in form of flexible ceramics which offer further new application avenues. Additionally, these 3D networks have been utilized as sacrificial templates to develop hollow tetrapodal 3D networks from almost any desired material, carbons, nitrides, oxides, polymers, hydrogels, etc. The sacrificial template-based strategy offers new and unique opportunities in the direction of 3D nanomaterials engineering and accordingly advanced technological applications. Some examples of 3D nanomaterials engineering will be demonstrated alongwith their applications [1-10]. The scopes of 3D nanostructuring based smart materials in sensing, electronics, optoelectronics, energy, and biomedical engineering will be briefly highlighted in the talk.

Keywords: *Smart materials, Tetrapods, Hybrid nanomaterials, Advanced Technologies*

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Liquid crystals for organic electronic devices

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Liquid crystals are a class of materials that elegantly combine characteristics of the conventional solid and isotropic liquid. The most familiar application of liquid crystals is the liquid crystal displays or LCDs. Liquid crystals are also promising for organic electronic devices. Compared to their inorganic counterparts, liquid crystals can enable lower-cost, tuneable, biodegradable, lighter, thinner and flexible organic devices. In this presentation, an outline of some of the amazing complex molecular and supramolecular self-assembled structures formed by liquid crystals will be discussed. The current status of research and applications of liquid crystals in organic transistors and solar cells, the promises and challenges will be presented.

Electrochemistry in energy storage and conversion

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Abstract:

For centuries, the electrochemistry has been an integral part of our societal and industrial progress. Its application ranges from traditional electroplating for corrosion protection to the state of art sensors for health care and chemical industry, as well as for the energy storage/conversion to efficiently utilize the renewable energy production. Today, as we are marching towards realizing an emission free and clean energy society, the electrochemical methods are going to lay the foundation for this endeavor and create a new energy economy. This lecture will focus on energy storage in batteries, their application, current trends, challenges and potential remedies. Working principals of various battery chemistry and concept will be presented and compared with other electrochemical devices/methods for electric mobility and storage application.

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