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General informations

The OAJ Materials and Devices is a journal created at the end oy 2016, devoted to all aspects of materials and related devices. It is Open Access and free of charges for authors.

Our aim was to create a high quality journal, with a strict peer-review process, and complying with the transparency rules edicted by the DOAJ, COPE,...

Materials and Devices publishes several types of articles :

- A : regular papers, that should present the results of original research, not published or submitted somewhere else.
- L : short papers, presenting original results, written as letters, focusing on one or few particular aspects, representing a very significant progress, for rapid publication.
- R : review papers, that presents a summary of results published in literature, on fields covered by the journal.
- T : technical papers, on the development of laboratory techniques and aparatus relevant to studies on materials and related devices. Such papers will present the details of a given technique, and an example of application in real condition, they may also take the form of overviews or reviews. In one of these last cases, the word « review » or « overview » will appear explicitly in the title of the article.
- Ur : Unexpected and « negative » results, the journal accepts papers describing unexpected results, or results considered as negative, provided that the original ground arguments are sound, and that a reasonable interpretation can be proposed. Typical examples are : a synthesis process that is generally successful, which aborts in given cases, or give different unexpected but interesting results, results contradicting a theory or a model, etc. The idea to publish such papers is mainly to save time to the scientific community by giving information that is generally not available, except as private communications between researchers.
- Opinion articles, the journal accepts submissions of this type of papers in which authors express, expose, and motivate their opinion, suggestions, proposals, analyzes, on general, philosophical, political aspects, policies related to researches on Materials and on Devices, on all subjects from the production of the scientific results, to the publication and use of those results. See details in the journal's site.
- Comments: short articles allowing to discuss specific points of an article that preferentially has been published in the OAJ Materials and Devices, and that is of particular importance for the readership of the journal. They should not attack the article, but provide a scientific, objective view or commentary, or complementary informations in a respectuous style.
- Conf: conference papers : OAJ Materials and Devices may also publish conference proceedings and conference papers in special volumes. Organizers of conference interested should contact the journal in advance to know details.

(Updated on june, 21st, 2019)

Aims and scope of the journal

The topics covered by the journal are wide, it aims at publishing papers on :

- all aspects related to materials, namely according to their chemical formula (oxides, fluorides, carbon compounds, …, organic, inorganic), to their physical properties (conductors, super-conductors, semi-conductors, insulators, dielectrics,...), to their nature (crystalline or amorphous materials, liquid crystals, modulated systems, aperiodic materials, nanomaterials and nanostructured materials)… or environmental type (ecomaterials), or according to some specific applications. Papers on biomaterials, geomaterials, archeomaterials or on studies of ancient materials are also welcome. A particular attention is also paid on environmental studies related with materials. Authors are also encouraged to submit papers on theoretical studies applied to materials, including pure mathematical approaches, physical approaches, models, numerical simulations, etc.

- devices in a wide sense. Concerning Devices, the scope is restricted to those integrating given materials (for instance memories based on some specific magnetic materials) or those related to materials in their study or use (for instance specific instruments in materials science, devices of interest for the use of particular materials,...) . Papers on all types of such devices are welcome.

Policy of the journal

Materials and Devices is an **Open Access (*)** journal which publishes original, and peer-reviewed papers accessible only via internet, freely for all. Your published article can be freely downloaded, and self archiving of your paper is allowed!

We apply « *the principles of transparency and best practice in scholarly publishing* » as defined by the Committee on Publication Ethics (COPE), the Directory of Open Access Journals (DOAJ), and the Open Access Scholarly Publishers Organization (OASPA). The journal is now indexed by the DOAJ and listed by this organization.

Evaluation – peer-reviewing : After reception, the paper is sent to reviewers for evaluation. In case of negative or divergent opinions of reviewers, the editor-in-chief sends the paper to another reviewer and then gives a final decision based on all reports. Reviewers are asked to reply within three weeks to warranty a fast publication process.

International editorial board – list of members

Orientation of the journal, choice of reviewers, special issues, editorial policy, etc, are discussed by the international editorial board.

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People interested in this project are welcome ! Contact us to submit your proposals, ideas, suggestions, or to get involved in some actions !

Materials and Devices (ISSN 2495-3911) is a relatively new journal, and as such, is not yet indexed. However in future we shall consider as a priority task, to reach a significant impact factor for this journal.

جامعة مولاي إسماعيل
UNIVERSITÉ MOULAY ISMAÏL

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Laboratory of Advanced Materials Studies and Applications (LEM2A)
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Forewords

The International Conference on Advanced Materials, Microscopy and Energy (ICAMME'19) was held in Faculty of Sciences University Moulay Ismail Meknes-Morocco from April 17 to 19, 2019. This event has included different kinds of presentations given by researchers and experts from the national and international scientific community, including keynote speakers, special sessions, posters and tutorials. It has covered a wide spectrum of topics.

A specialized spring school was held from April 15 to 16, 2019 before the Conference. The lectures during this school have covered fundamental and applied aspects related to Advanced Materials and Advanced Microscopy and spectroscopy techniques. The lecturers were international experts in these areas. The school was intended in order of priority to PhD students, Masters 2, Engineers and researchers.

ICAMME'19 was an ideal platform for all International and National Scientists, Professors, Students, and Industrials. There were feature talks by eminent personalities from academics and industries on recent advances in field of Materials Science, Microscopy, Engineering, Technology and Energy. It has known more than 150 participants around the globe with thought Keynote lectures, Oral Presentations and Poster Presentations. This was an excellent opportunity for the delegates from Universities and Institutes to interact with the world class Scientists.

The conference **ICAMME'19,** over three days, has permitted:

1. to round up specialists in the advanced materials research field (theoretical and experimental),
2. to discover the scientific community and research in the Moulay Ismail University,
3. to review to the younger generation today, through various scientific presentations, the evolution of the advanced materials, and the revolution in nanotechnology and their applications in renewable energy.

We thank the members of the Scientific Committee and all the invited speakers.

We recall that the financial support of the conference was provided largely by:

1. The Moulay Ismail University
2. The Laboratory of Advanced Materials Studies and Applications (LEM2A)

We are sure that everyone has found in this meeting an important topical interest, a great pleasure on exchanging with the inter-Mediterranean scientific community.

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ID: 270039

Seeing, analyzing and measuring in the nano-world with a Scanning Transmission Electron Microscope (STEM)

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Abstract: In electron microscopy, the information results from the interaction mechanisms between the primary beam of electrons and the material under study. Consequently, all recent efforts and successes to improve the instrumentation and simultaneously record the relevant signals and to develop the required software for data processing and for theoretical simulation, have radically extended the domains of application for the newly designed instruments into the nano-world, as well in materials as in life sciences. The demonstrated breakthroughs in electron optics, such as the design, the practical realization and the use of correctors, filters and monochromators together with the permanent progress in detector efficiency, have pushed forward the performance limits, in terms of spatial resolution in imaging (sub-Å), as well as for energy resolution (down to the 10 meV) in electron energy-loss spectroscopy (EELS). The STEM approach is well adapted to a thorough exploration, pixel after pixel, of the response of the specimen, in particular at the (sub)-nm level, Spectrum-imaging modes deliver atomically-resolved structural maps through a set of angular detectors (HAADF, MAADF, ABF) in combination with elemental maps provided either by the core-loss EELS and/or the EDX signals. The improved energy resolution in EELS gives access to fine details in the electronic states which can be related to bonding, transfer of charge or environment variations at the unit-cell level. In the near-IR/visible/UV spectral domain, EELS can now be recorded together with the optical emission spectrum (Cathodo-Luminescence), thus combining the advantages of the ultimate resolution in space (electron spectroscopy) and in energy or wave-length (photon spectroscopy). A detailed comparison between absorption and emission spectroscopy mapping is thus possible at a resolution not attainable with optical techniques.

As a consequence, nano-objects of natural or artificial origin, can now be fully characterized individually. This will be demonstrated on several families of nanostructures such as: (i) 2D nanomaterials (C, BN), - either as graphene-type sheaths or single-walled nanotubes -, or nanostructured oxide compounds, where the atomic structure, the identity and bonding type of dopants and the photon emission properties of defects can be probed with these techniques; (ii) the optical properties of individual nanoparticles with varying shape, size, substrate and interactions, where surface plasmon modes (at typical energies down to 1eV and below) in metallic ones and surface phonon modes (at typical energies in the tens to hundreds of meV) in insulating ones, are mapped together with their associated electro-magnetic field configurations. Furthermore, the combination of both spectroscopies – EELS and CL – is also quite instrumental in the study of optically emitting nanostructures, such as quantum dots or fluorescent nanoparticles.

This multi-signal approach in the STEM constitutes the first step for designing and using the next generation of instrument dedicated to nanophysics, incorporating for instance time-resolution with pulsed electron guns or control of the environmental parameters at the specimen level (temperature, gas or liquid cell, laser beam illumination) in a dedicated nanolaboratory.

Keywords: scanning transmission electron microscopy, nanoanalysis, atomic scale characterization, plasmon and phonon maps, individual defects and nanostructures

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ID: 270051

Deforming minirals and rocks: from the atoms to plate tectonics and the the rheology of the mantle

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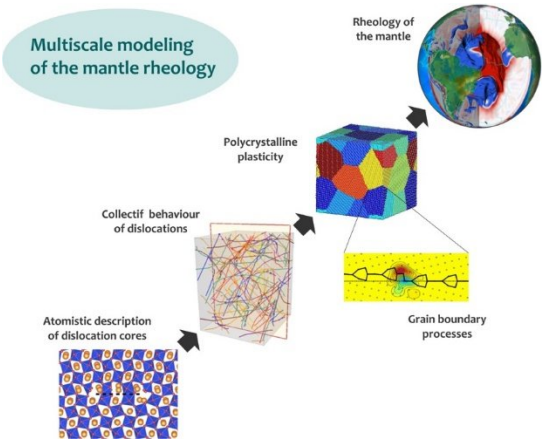
Abstract: The Earth is still a hot planet; 98% of its volume is at temperature in excess 1000°C. This internal heat is evacuated to the surface through large scale convection cells which stir the mantle. Cold, dense subducting plates sink in the mantle whereas plumes from deep regions, possibly the core mantle boundary, bring heat and matter to the surface. Since the mantle is made of solids rocks, these movements result from plastic deformation. It is thus at the microscopic scale of crystal defects that the origin of these large-scale phenomena must be searched. A further difficulty comes from the extreme conditions of the Earth's interior. At the core mantle boundary (ca. 2900 km depth), the temperature is close to 3500°C and, more importantly, the pressure reaches 135 GPa. Moreover, the strain-rate is extremely small which precludes to be reproduced in laboratory experiments.

For these reasons, we have developed an alternative approach of the rheology of mantle minerals based on multiscale numerical modelling. This approach links our understanding of elementary mechanisms at the microscopic scale with the deformation behavior observed at the macroscopic scale, such as flow laws. First, dislocations are modelled at the atomic scale with a particular attention to the core structure of screw dislocations which often govern mobility. The thermally activated mechanisms of dislocation motion are then modelled to yield velocity laws of individual defects. The next step aims at describing the collective behavior of dislocations to provide constitutive equations. The main results of this approach applied to the most common phases of the Earth's mantle are presented.



We show that pressure has a very important effect on dislocation glide which can be strongly inhibited in some silicates. We propose in such cases that an alternative mechanism, pure climb creep, allows deformation to proceed under mantle conditions. We suggest that pure climb creep may represent a major deformation mode for the convection of planetary interiors.

ID: 270037

Deep brain electrical stimulation for neurological and psychiatric disorders

Abdelhamid BENAZZOUZ

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Abstract: Biotechnology faces a variety of challenges in the development of innovative therapeutic and diagnostic products for use in patients. Another challenge is to understand the pathophysiology of neurodegenerative diseases to develop new pharmacological and/or neurosurgical approaches to treat patients in order to reverse the symptoms or to stop the evolution of the diseases. One of the debilitating brain pathologies is Parkinson's disease (PD) representing the second most common neurodegenerative disorder after Alzheimer disease. PD is characterized by the manifestation of motor symptoms, which are mainly attributed to the degeneration of dopamine neurons in the pars compacta of substantia nigra. Based on advancements in the understanding of the pathophysiology of the disease, especially in animal models, the subthalamic nucleus (STN) has been, a small deep brain structure involved in motor functions, pointed as a major target for deep brain stimulation (DBS) in the treatment of motor symptoms. First, we developed this approach in a non-human primate model of PD and then successfully transferred to parkinsonian patients. The success and benefit of stimulation is due to the precise stereotaxic targeting of the subthalamic nucleus for optimal electrode implantation. Precise targeting is based on the use of good-quality MRI for the visualization of brain structures, electrophysiological recordings of neuronal activities and stimulation tests to evaluate online the beneficial and side effects of stimulation. STN DBS is an established neurosurgical intervention, considered as the gold strandard in the therapy of PD, providing a more constant and predictable benefit than pharmacological treatments. STN DBS is an excellent exemplary case from "bench to bedside", which demonstrated the decisive role played by the non-human primate model in the discovery of this neurosurgical therapy. The benefits of STN DBS include spectacular improvement in motor performance, decreased motor fluctuations and bradykinesia, tremor reduction and a reduction in dopaminergic drug requirements and dyskinesias. However, the mechanisms of action underlying its therapeutic effectiveness are complex and still under debate. Majority of electrophysiological studies, including ours, have shown an inhibition of the neuronal activity during DBS of the target nuclei in rodents, MPTP non-human primates as well as in patients. In conclusion, STN DBS is a safe therapy and the rate of serious psychiatric complications and other side effects is very low. For this reason, DBS of other brain nuclei are used for other neurological and psychiatric pathologies, such as Dystonia, essential tremor, obsessive compulsive disorders…

Keywords: Deep Brain Stimulation, Subthalamic Nucleus, Parkinson's Disease, Psychiatric Disorders, Animal Models.

ID: 270044

Organic–inorganic nanohybrid materials: Self-assembling and properties

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Abstract: Over the past decade, significant effort has been directed towards the elucidation of synthesis/structure/function correlations to guide the development of synthetic strategies for controlling the composition, size and shape of nanomaterials. In this context, organic–inorganic nanohybrids incorporating bridged silsesquioxanes have been of particular interest, due to their versatility and the structural control that can be achieved through independent modulation of the properties of the organic bridge and inorganic moieties. Such strategies have also been applied to the production of thin films on a variety of substrates, driven by the continuing need to develop new and enhanced materials with nanostructures engineered over multiple length scales for applications in electronics, optics, sensing, ferromagnetics, shape-selective membranes, etc.

In this talk, I will first describe the mechanisms that control the evolution of the organized solid from energy efficient sol−gel processing: self-assembly, hydrolysis, polycondensation of precursor molecules, and nucleation and growth of the hybrid solid in solution. The preparation of thin films will be then given [1,2]. The influence of key chemical (particularly pH and ageing time) and physical parameters (spinning speed) on the morphology of the resulting coatings will be depicted, and a model describing the structural evolutions of the coatings will be presented as a general approach for producing self-structured coatings under far-from-equilibrium conditions [3]. Finally I will present application of these nanomaterials in the domain of transparent luminescent solar concentrators [4].

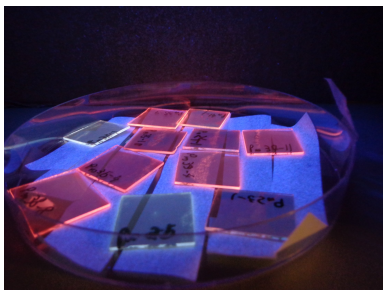
References:

[1] Langmuir 2013, 29, 5581−5588

[2] Physical Chemistry Chemical Physics 2019 accepted DOI: 10.1039/C8CP06625F

[3] Physical Chemistry Chemical Physics 2016 18, 7946

[4] ACS Appl. Mater. Interfaces 2015 7(16), 8770 -8778



ID: 270047

Modulating single-walled carbon nanotube opto-electronic properties by dye confinement

Laurent ALVAREZ

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Abstract: Dye encapsulation into host single-walled carbon nanotubes is an elegant way to create hybrid nano-systems with tunable opto-electronic properties [1]. To this aim, different kinds of molecules (either electron donor or acceptor, absorbing either in the blue or the red visible range) are encapsulated into metallic or semiconducting nanotubes displaying different diameters. Up to now, we have mainly studied encapsulated quaterthiophene derivatives (4T), tetracyanoquinodimethane (TCNQ) and phthalocyanine (MPc) molecules. In this work, we discuss the supramolecular organization of dyes inside the nanotube, the optical properties and the charge transfer for some of our hybrid systems. For instance, using Raman spectroscopy, a significant electron transfer is reported with 4T, whose magnitude strongly depends on the nanotube diameter, and on the metallic or semiconducting character. Experiments also suggest a photo-activated electron transfer for small diameter (~9 Å) semiconducting and metallic tubes. Confinement of electron donor (4T) (respectively electron acceptor (TCNQ)) into small diameter tubes leads to a red shift (blue shift) of the optical absorption energy and an increase (decrease) of the photoluminescence intensities, evidenced by the photoluminescence excitation maps.

[1] A. Salvati, A. Belhboub, Alvarez, R. Leparc, S. Rols, P. Hermet,B. Jousselme, K. Suenaga, A. Rahmani, J-L.Bantignies, OAJ Materials and Devices, Vol 2, #1, p 18 (2017) – DOI: 10.23647/ca.md20170407

ID: 270040

Structure refinement using precession electron diffraction tomography and dynamical diffraction applied to mineral geo-thermometers

Damien JACOB

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Abstract: A recently developed method using Precession Electron Diffraction Tomography (PEDT) and dynamical calculations of diffracted intensities allows the solution and refinement of structures with high accuracy based on data obtained at the nanoscale in a Transmission Electron Microscope (TEM) [1, 2]. The method has been applied with success to many organic and inorganic structures, thus including electron beam sensitive materials [3].

More specifically, structure refinement can be used for the quantification of cation partitioning on specific crystallographic sites of know structures. This is applied in order to retrieving the time-temperature formation conditions of mineralogical samples such as pyroxenes or spinels appearing as inclusions in various igneous or metamorphic rocks. In many cases, those specific grains are located in a complex environment made of intricate phases at a sub-micron scale, which precludes the use of X-ray Diffraction with a micrometre probe size. Targeted structures can thus only be extracted using a focused ion-beam (FIB) microscope and studied as thin foils in a TEM.

In this paper we present results demonstrating the validity of this approach applied on pyroxene (Mg,Fe)SiO3 and spinel (Mg,Fe)3O4 structures with various compositions and thermal histories. As standards for this preliminary methodological study, the samples of interest have been synthetized in laboratory and heat-treated under controlled atmosphere. TEM sample preparation was achieved using either simple mechanical crushing or ion-milling in a FIB. We will discussed the influence of the thinning process, refinement method and parameters on the reliability of the results as compared to those obtained at a larger scale using X-ray diffraction on the same samples.

Keywords: *TEM, PEDT, dynamical refinement, minerals, geo-thermometer.*

References:

[1] Palatinus *et al.* (2015), Acta Cryst. A, 71(2), 1-10.

[2] Palatinus *et al.* (2015), Acta Cryst. B, 71(6), 740-751.

[3] Palatinus *et al.* (2017), Science, 355(6321), 166-169.

ID: 270043

Higher performance PMNT based wearable piezoelectric energy harvester

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Abstract: With developing wearable and portable electronic devices, the piezoelectric energy harvesters draw much attentions to convert the mechanical energy from body movements into electrical energy, extending the battery life or realizing the self-powered electronic devices. Several key issues are discussed in this talk on the impedance match of mechanic vibration source, electric impedance match of load output, and flexible performance of piezoelectric vibrators.

After optimized the piezoelectric, dielectric, and elastic performances of PIN-PMN-PT and PMN-PT single crystals and their composites, the high performances of piezoelectric energy harvester were designed and fabricated. The macro-flexible piezoelectric energy harvester and cantilever-based rigid resonant piezoelectric energy harvester have fabricated with higher performances. An array-type MF-PEH with the structure of ABS flexible substrate/PI flexible circuit board/PIMNT wafer array was designed and fabricated by using bulk piezoelectric PIMNT single crystal. When bended to a radius is 5.04 cm (the calculated average strain induced in the PIMNT is 0.225%), the device can generate an open circuit voltage of 23.2 V and short-circuit current of 105 mA. The maximum instantaneous output power of the device reaches as high as 0.25 mW, which is 50% higher than the best reported PMN-PT nano generators.

A plastic-composite-plastic (PCP structure) sandwich structure MF-PEH was designed and prepared by using a PIMNT single crystal/epoxy 2-2 composite, which greatly improved the flexibility of the MF-PEH while maintaining excellent output performance. The bendable radius of this MF-PEH can be less than1.05 cm, which is 1/5 of the previous array-type MF-PEH. Under a bending radius of 1.05 cm and 4.2 Hz excitation frequency, the open circuit voltage and short circuit current of the device reach 12.9 V and 29 mA respectively, with a maximum instantaneous power density of 0.28 mW/cm3 at a matching impedance of 400 kΩ, which is comparable to that of the array-type MF-PEH.

ID: 270038

Event of the Modern Electronic Era With Perovskite Structure Materials

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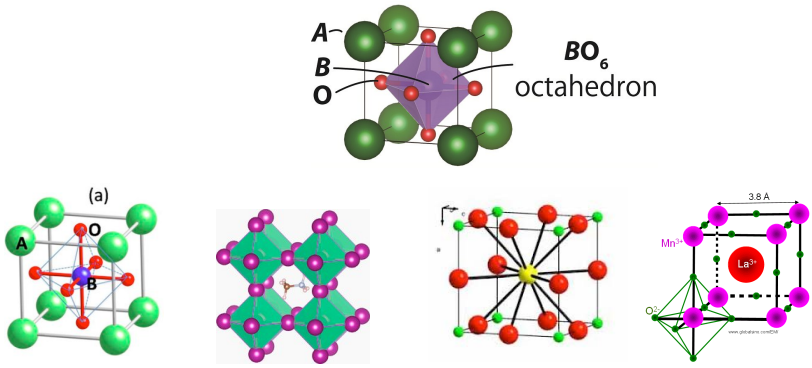
Abstract: The Perovskite structure was identified from CaTiO3 mineral collected in Oural Mountains. Fig.1 represents various views of the crystal lattice with the general formula ABX3 and ABO3 for oxide perovskites. The network could be related to the rock salt structure where A and O sites are reputed equivalent and where appropriate octahedral vacancies are created. The basic unit cell is desperately simple…!, while the explanation of the non linear physical behaviour (relaxor behaviour, piezoelectric properties, etc.) becomes very quickly highly complex in perovskite solid solutions. The role of lead in the high performance of Pb-based perovskites is central in current scientific discussions. In the present lecture we will extend such analysis.



(a) (b) A=organic cation (c) (d) A=inorganic ion

Fig.1.- 3D View of the unit cell of the Perovskite ABX3.

The crystal chemistry of BaTiO3 and related solid solutions has allowed elaborating the first electronic miniaturised devices in the history of modern electronic technology. The first modern electronic era started by the elaboration of miniaturised capacitors made from modified barium titanate materials.

It is also very surprising to notice that the Perovskite structure has a great impact factor on huge domains of human activities (present and more to come!): i) dielectrics with MLCC technology, ii) piezoelectrics with actuators applications, etc., iii) solar energy conversion, iv) etc.

It is indeed worth to mention that all fundamental research conducted on perovskites (structure dynamics, etc.) are also of importance for geophysical simulation as the high pressure perovskite MgSiO3 (brigmanite) constitutes the principal mineral phase of the Earth's lower mantle.

ID: 270053

Oxide ion conductors for solid oxide cells

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Abstract: Oxide ion conductors are the main components of Solid Oxide Fuel Cells (SOFC) and Solid Oxide Electrolyser Cells (SOEC). Both applications rely on a dense electrolyte ceramic separating two compartments, one containing air and the other the fuel, usually hydrogen. To allow the oxygen transfer, porous electrodes have to be added on both sides of the electrolyte. Whereas the electrolyte must be a pure oxide ion conductor to avoid short circuit, the electrode materials must exhibit mixed ionic electronic conductivity. Despite years of research, yttria stabilized zirconia (YSZ) remains the best electrolyte material but its low ionic conductivity results in operation temperatures higher than 700 C. To decrease these operating conditions, doped ceria has been studied but su ers of a risk of reduction of cerium IV into cerium III. Among oxide ion conductors, bismuth based materials display the best ionic conductivity. They are unfortunately not stable under hydrogen atmosphere. However, as shown by the group of Wachsman [1] from the University of Maryland, a combination of these two materials could oer operation temperatures as low as 350°C. However, to come to the market, there is still a need to find high performance cathode materials able to operate at such reduced temperature.

After a review on both SOC electrolyte and electrode materials, the main techniques of characterisation of these materials will be introduced with a focus on the research currently carried out at UCCS.

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ID: 270042

Additive manufacturing : scientific, economic and educational opportunities

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Abstract: Additive Manufacturing (AM) has a wide array of applications, such as creating custom medical devices, aerospace components, and artwork. The potential uses continuing to grow, it's important that this type of manufacturing can keep up with the demand. However, analyzing and optimizing this complex process can be difficult. What can engineers do to overcome this challenge? Additive manufacturing is a bit like sewing or weaving. In both processes, a heterogeneous finished product is created by controlling how different raw materials are consolidated. In weaving, the materials are usually thread and yarn; however, additive manufacturing can use many materials, including polymers, metal alloys, ceramics, biological materials and composites. Combining the right materials, optimizing geometry of the part (inner filling and outer geometry), finding the right deposition path are some keys for creating an ideal finished product. This wide range of materials means that additive manufacturing can be used to design a large amount of unique objects across many industries. For instance, by using the right materials and transformation conditions, engineers can make objects that withstand or adapt to severe environmental conditions. Such objects could even adapt to certain temperatures or chemical conditions by changing their shape or releasing chemical species (like drugs) that are trapped in a matrix. A transformation over time would add another dimension to the printed part, resulting in "4D printing". Incorporating electronics devices, controlling the local material anisotropy during growing and bio-printing are the next challenges in 3d printing. The many opportunities that come with additive manufacturing make it "an unavoidable manufacturing process," as it "offers new opportunities to develop optimized structures with advanced materials." However, before engineers can create these structures, they have to improve the additive manufacturing process. Computational multiphysics and physical analysis can be combined to optimize both the process and the product performance. AM is multiphysics and multiscale transformation processes and then offer complex engineering challenges. The use of high technology and optimization of product performance are usual goals for engineers. AM which merge traditional engineering and digital engineering has then its full place in higher education. Finally, the cost of developing 3D printing solutions for education are low, the training process for the use and development of the digital channel is affordable, AM is then an educational opportunity. Examples of 3D-printing of novel composites based on silica particles, graphene and photopolymers will be presented.

Keywords: Additive manufacturing, multiphysics, multiscale, Physical analysis.

ID: 270045

Haadf and abf-stem study of new promising Ruddlesden–Popper member component for it-sofc

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Abstract. Rare-earth containing layered perovskite-related oxides, especially An+1BnO3n+1 Ruddlesden-Popper homologous series1,2, are nowadays attracting much interest as promising components, mainly cathodes, for intermediate temperature solid oxide fuel cells (IT-SOCF). The excellent chemical and thermal stability of transition metal perovskite related oxides that belong to the Ruddlesden–Popper (R–P) homologous series with the general formula $A_{n+1}B_nO_{3n+1}$ $((ABO_3)_nAO)$ (A=Rare and/or alkaline earth elements and B= transition metal), in which the multiple perovskite layers that are n octahedra thick alternating with single AO rock salt layers, make them very attractive materials. Electronic conduction may occur in perovskite-like blocks, built up from corner-sharing BO_6 octahedra, where B-cations occupying the center of the polyhedra can present multiple non-localized oxidation states. Besides, AO rock-salt layers may present anionic vacancies and/or interstitial oxygen ions, both defects resulting in ionic conduction. In this communication, the a new members3,4 with n=1, 2 and ∞ of Ruddlesden–Popper series, has been prepared and a detailed structural characterization has been carried out by High Resolution Transmission Electron Microscopy (HRTEM) by using a JEOL JEM-3000F electron microscope and Scanning Transmission Electron Microscopy (STEM) performed on a JEOL JEM-ARM200cF microscope (Cold Field Emission Gun).

Keywords: Rare-earth, IT-SOCF, Electron Microscopy, HAADF and ABF-STEM.

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ID: 270056

Gaseous Scanning Electron Microscopy (GSEM): Perspectives For Gaseous Transmission Electron Microscopy (GTEM)

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Abstract. Conventional Electron Microscopy (CEM) is one of the most important techniques used to observe materials at nanoscale. The high-vacuum specimen chamber in the CEM and the size of the interaction volume is the consequence of the elastic and inelastic collisions between the incident electrons and the atoms of the surface of the specimen. The principal recognized artifact is the degradation of the X-ray spatial resolution delineated by this interaction volume in particular, the resultant X-rays emission volume. The size of the interaction and emission volume depends strongly on the intrinsic properties of material itself as the density, the atomic number, the excitation energy and the energy of the incident electron beam. This phenomenon gives rise to artifacts during analysis by the energy dispersive spectrometry (EDS) for example, especially if the material is inhomogeneous, or at the interface of two different adjacent materials.

Because imaging and the nano-microanalysis of hydrated and insulating materials using electron beam probe methods (Conventional S(T)EM, Auger Electron Microscopy,...) are very limited by the necessity to keep the sample under high vacuum and the presence of the charge effect, with GSEM it is possible to overcome these difficulties. But all these phenomena can be changed if the high-vacuum in specimen chamber in the CEM is changed by a gaseous environment. For example, the volume of interaction do not depends on the energy of the incident electron beam only but is depending on the interaction between the energy of the incident electron beam and the gaseous environment also. In this case the interface between two materials must be reconsidered. In this conference, experimental and theoretical aspects of GSEM will be discussed and the interface changes between two dielectric materials silica and polymer will be illustrated as examples. In addition some perspectives of Gaseous Transmission Electron Microscopy (GTEM) will be presented.

Keywords: Interfaces, Silica, Polymers, GSEM, GTEM, Gases.

ID: 270048

Pickering emulsions : From experiment to theory

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Abstract. Pickering emulsions are dispersions of a liquid in another unlike one, huile-in- water or water-in-oil, for example. The droplets of the dispersed liquid are stabilized by a strong adsorption of nanoparticles on their surfaces, which have no particular preference for the two phases. These kinds of emulsions are more stable than those with surfactants. Also, one can use diblock polymers where the attached chains have opposite preferences for the two liquids. Beside their stabilizer feature, Pickering emulsions are recently used to synthesize new advanced materials by polymerization. In this conference, we talk about new findings dealt with Pickering emulsions from experimental and theoretical point of view.

Ref.: S El-Moudny, M. Benhamou, M Badia, M Ossmani,OAJ Materials and Devices, 2018, 3 (1) p2404 (2018). ⟨10.23647/ca.md20182404⟩

Keywords: Pickering emulsions, Stabilization, Nanoparticles, Experiment, Theory

ID: 270036

Nonresonant polarized Raman spectra calculations of doped single wall carbon nanotubes

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Abstract. Several spectroscopic technics are commonly used for the characterization of carbon nanotube and graphene samples. In particular, Raman spectroscopy is widely used by experimentalists [(1)] as a fast and nondestructive method to identify the type of nanotubes and to study their vibrational properties and their electronic structures. In this study, Raman spectra of doped single-walled carbon nanotubes (SWCNTs) are calculated by using the spectral moment's method [(2)] in the framework of the bond polarizability model. The effects of the nanotube diameter, chirality and doping concentration on the Raman active modes were all examined. Results reveal that the tangential Raman band G of SWCNTs show strong dependence on the concentration of doping atoms/molecules, its defects, and the TMs adsorbed. The dependence of the calculated frequency and intensity of Raman modes on the nanotube diameter and the dopant concentration ratio is analyzed.

The obtained results are compared with the experimental data reported in the literature [(see 3)].

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ID: 270050

Regenerative biomaterial matrices for traumatic spinal cord injury repair

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Abstract: Human traumatic spinal cord injury (SCI) has significant social consequences and can lead to life-long disability; loss of motor and sensory functions. This is due to the limited ability of the adult human central nervous system for self-repair after injury, in contrast to peripheral nervous system. Barriers to regeneration include impaired revascularization at the lesion site, establishment of an astrocyte glia and fibrous scar that releases inhibitory molecules in addition to those contained within myelin debris, and cystic cavity formation. In addition, ischemia and persistent inflammation resulting from blood spinal cord barrier breakdown, lead to secondary damage through neurodegenerative lesions that extend caudal and rostral from the initial impact, aggravating the neurological deficits.

Few, if any effective treatments exist for patients suffering from spinal cord trauma. Nevertheless, fundamental research has made considerable progress, including development of strategies to overcome the hurdles that impede recovery from SCI within animal models (mainly rodent). These strategies have brought important insights into neuro-restoration.

New hope for SCI treatment appears to arise not least thanks to recent progress in bioengineering, a field of research into bio-inspired new materials that has already seen the development of promising tools for medical applications in wound healing and regeneration of various tissues. For SCI treatment, biomaterials in the form of implantable hydrogels appears particularly interesting, and evidence is accumulating that future combinatorial approaches will need to integrate such "bio-scaffold" materials as substitute for lost neural extracellular matrix (ECM). Various biomaterials have been designed, both natural and synthetic, differing in their physical state, in situ biodegradability, and specific functionalization

Accordingly, we designed a scaffold material for SCI treatment containing only chitosan (derived from chitin) and water as fragmented physical hydrogel suspension (Chitosan-FPHS), with defined degree of acetylation, polymer concentration, and mean fragment size. Implantation of Chitosan-FPHS alone into rat spinal cord lesion promoted reconstitution of spinal tissue and vasculature, and diminished fibrous glial scarring, allowing the border between lesion site and intact tissue to become permissive for regrowth of numerous axons into, and for some even beyond the lesion site. Interestingly, Chitosan-FPHS also modulated the inflammatory response, and we show that this might contribute to tissue repair. Finally, this structural remodeling was associated with significant, long-lasting gain in locomotor function recovery. Because it effectively induces neural tissue repair, Chitosan- FPHS biomaterial may be a promising new approach to treat SCI, and a suitable substrate to combine with other strategies. Thus, implantation of Chitosan-FPHS into an acute SCI lesion site seems a very promising strategy, and our ongoing investigation and perspective is to test its relevance in a chronic lesion. Determination of the suitable time window for chitosan hydrogel implantation is also important when considering a combination with other strategies, such as cell therapy or drug delivery. Furthermore, for a proof of concept, we are testing our strategy in an experimental model more relevant to humans, i.e. a contusion lesion.

ID: 270041

And Then There Was Light: Advanced Biophotonic Tools to study Brain Networks in vivo

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Abstract: Survival critically depends on the ability of animals to select the appropriate behavior in response to sensory signals from the external world. However, the synaptic and circuit mechanisms by which the brain learns to encode accurate predictors from noise has long remained largely ignored, mostly because of technical limitation. Nevertheless, over the past decade, the emergence of optogenetic - the use of light-sensitive proteins to observe and manipulate neuronal activities - has profoundly transformed neurosciences. This has become possible through the development and application of new optical tools, particularly multiphoton imaging techniques that enable the monitoring and control of neuronal excitability and network activity in awake behaving animals.

Here, by using longitudinal two-photon (2P) calcium imaging in awake head-restrained mice, in vivo electrophysiological recordings and optogenetic conditional strategies, we show that frontal association cortex (FrA) dendrites discriminate sensory modalities through the recruitment of non-linear, NMDARs-dependent conductances. These active dendrites can further modify membrane potential dynamics by specifically integrating sensory cues and basolateral amygdala (BLA) inputs. This cooperative mechanism critically shapes the expression of discriminative memories generated from sensory cues that were not explicitly paired to an aversive event (e.g., a footshock) during associative learning. Taken together, our data reveal a dendritic mechanism for cue discrimination in FrA, thus providing a new framework for discriminative learning and related disorders.

Keywords : two-photon chronic imaging; optogenetic; in vivo; learning and decision-making; signal processing

ID: 270049

The revival of electron microscopy for biomedical research

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Abstract. The electron microscopy (EM) era began in the late 1920s and early 1930s with Ernst Ruska who conceived and built the first electron microscope. It was his brother, Helmut, who produced the first EM image of living organisms, bacteria and viruses, in 1939. Explorations of the cell's internal structure with transmission EM (TEM) were not realized until the development of thin sectioning methods with ultramicrotomy. These initial studies paved the way for the nanoscale analysis that elucidated cell and tissue ultrastructure.

Localising molecules is perhaps where EM has made its greatest achievements. Positioning molecules within a cell provides information about their function, and their arrangement is key to revealing how they can operate in a highly coordinated manner. These specific labelling methods require chemical fixation and ultrastructural immunohistochemistry to pinpoint molecule localisation. By using gold-conjugated antibodies, post-embedding approaches offer high specificity and a suitable resolution to accurately position molecules. One of the main limitations is the necessary compromise between preserving cell morphology and molecular structure, and getting access to the epitopes. To circumvent this issue, recent approaches have produced genetically encoded tags for EM contrast. These techniques can be used, in combination with fluorescent protein labelling for light microscopy, to correlate ultrastructural analysis of cells to their tissue environment. An important challenge is also to maintain the observed structures in their native state through the EM process. Cryo-methods aim to determine the molecular structure with unsurpassed resolution and without chemically induced artefacts produced by aldehyde fixation.

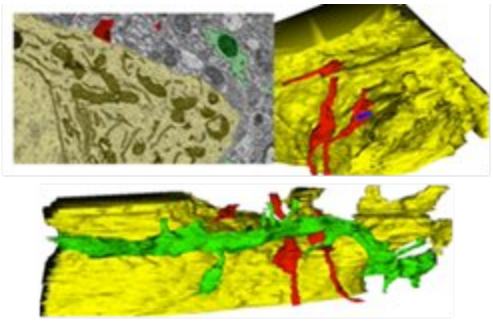

Fig. 1. SBF-SEM 3D reconstruction showing a double excitatory synapse (blue) made by an axon (red) on a dendrite (green) and a cell body (yellow) of the ACC.

By imaging volumes of brain using 3-dimensional EM, the details of neuronal shape and connectivity can be reconstructed. Depending on the anatomical extent of the circuit, or structure, to be characterized, it implies to choose between TEM- or SEM-based techniques. Small structures, ranging from a molecular complex to synaptic boutons, can be reconstructed from TEM acquisition of thin sections with electron tomography. Electron tomography is the highest resolution 3D technique for investigating pleomorphic structures that cannot be crystallized, such as certain molecules and cellular organelles. Beyond a single bouton, a complete map of an entire neural network would provide the basic connectivity blueprint through which an organism operates. The serial block-face electron microscopy (SBEM) method collects electrons backscattered from the surface of samples, allowing the surfaces of block-faces to be imaged (Fig. 1), and aiming to

determine the connectivity of a neuronal circuit, so that its wiring diagram or ‘connectome’, can be extracted.

Volume EM imaging is producing enormous amounts of data that can be hardly stored and analysed. In the medium-to-long term, we anticipate that the recent progress in automating and speeding the acquisition of volume EM data will carry over to automation of the analysis of these large datasets, eventually permitting complete reconstruction of mammalian circuits across millimeter scales.

Keywords: Cell ultrastructure, immunogold, correlative light-electron microscopy, cryo-methods, 3D volume reconstruction

ID: 270046

Biotechnological advances & applications: when reality is catching up with fictionion

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Abstract. Over the past decade, advances in biotechnology have led to the rapid development of precision medicine or personalized medicine, which is "an emerging approach for disease treatment and prevention that takes into account individual variability in genes, environment, and lifestyle for each person".

These advances have allowed physicians and researchers to more accurately predict which treatment and prevention strategies for a particular disease will be most effective and in which groups of people. This contrasts with the unique approach, used so far, in which treatment and disease prevention strategies are developed for the average person, not taking into account differences between individuals.

This presentation will review several examples found in several areas of medicine showing the role of these dramatic biotechnological breakthroughs and their impacts on daily health care and patient care. It will also review the situation in Morocco and prospects for the development of Moroccan precision medicine with the advent of NGS technologies, Nano-technologies, bioengineering and OMICS approaches.

Keywords: Biotechnology, Precision medicine, Omics Approach, personalized medicine

ID: 242651

Annealing temperature dependence of photovoltaic properties of solar cells containing Cu_3SnS_4 thin films produced by spin coating

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Abstract: Thin CTS film was elaborated using spin coating route on glass substrate. CTS thin films were prepared through the sulfurization of CuSnS alloy precursors at sulfurization temperatures of 200-500 °C for 1h in a Argon atmosphere with sulfur vapor. The structural, surface morphological and optical properties of thin films were studied by X-ray diffraction, a scanning electron microscopy (SEM) and an UV-Vis Spectrophotometer, respectively. These films exhibited p-type semiconductor behavior with the band gap energy decreased from 1.7 eV to 1.3 eV. This makes the material as a good candidate for low cost and friendly environment thin film solar cells.

ID: 244412

Structural, Electronic and Mechanical Properties of Two-dimensional Penta-GeCx monolayer via external electric field and strain engineering

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Abstract: Monolayer pentagonal germanium carbide pGeCx (with x=0,1 2,5 : nombre of C-atom in the unit cell) is a two-dimensional material composed entirely of pentagons, and it possesses novel electronic properties possibly leading to many potential applications. The objective of this work is the investigation a new two-dimensional nano-materials semiconductors pGeCx and predict that the (pentagonal Germanium carbideg) (pGeC2, pGeC5) can be operated as novel material for applications in novel generation electronic devices. Using theoretical calculations based on Density Functional Theory (DFT), the electronic structure, its optimization, the structural and electronics properties, the strain effect of band gap under Uniaxial and Biaxial strains (Compressive and tensile), the external electric field effect of band gap were methodically studied. The cohesive energy and phonon dispersion calculation confirms that the predicted structures are energetically and dynamically stable. By using Quantum Espresso codes our calculation show that pGeC2 and pGeC2 are a semiconductors with indirect band gap. We found that the band-gap of both structures can be adjusted by requesting stress in the X and Y directions or by applying an external electric field along +Z and -Z. Which offers a great latent for new electronic applications.

ID: 244314

DFT, Monte Carlo and QSAR approches for quantifiying the anticorrosive performance of some neutral and protonated macrocyclic polyether compounds, towards the iron surface, in vacuum and aqueous solution

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Abstract: The performance of some macrocyclic polyether compounds containing 1, 3, 4-thiadiazole moiety (n-MCTH) n=1-5, to inhibit the corrosion of iron surface was studied using theoretical and statistical calculations to investigate their electronic structures. Density Functional Theory (DFT) and molecular dynamic simulations (Monte Carlo) approaches were investigated, in vaccuo and aqueous solution. Firstly, quantum chemical and global parameters such as the highest occupied molecular orbital energy (EHOMO), lowest unoccupied molecular orbital energy (ELUMO), the energy gap between ELUMO and EHOMO (ΔE), chemical hardness, softness, proton affinity, and global nucleophilicity were calculated by B3LYP/6-31G**. Then,the local reactivity of the n-MCTH inhibitors has been studied through the Fukui indices and population analysis (NBO). Thereafter, binding energies on Fe (111) surface with the n-MCTH derivatives were performed by Monte carlo modeling to investigate the strength of their interactions with iron surface. The last part of our work was devoted to the QSAR study, for correlating the quantum descriptors with the effectiveness of inhibition. Our results showed that the inhibition efficiency of these derivatives increases with the oxygen's number on the molecules, the electronic and geometric proprieties favor the reactivity of 5-MCTH more than the other molecules. The complex 5-MCTHFe (N-N) which results in adsorption of nitrogens of 5-MCTH on iron surface, was found the most favorable by analyzing the quantum chemical descriptors, binding energy, and adsorption energy. QSAR results show good linearity between some quantum chemical reactivity descriptors and literature experimental inhibition efficiency ($R^2 \approx 1$) knowing that HOMO is the descriptor that influences mainly the inhibitory activity.

ID: 244933

Computational effective thermal conductivity of polyurethane foams

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Abstract: Polyurethane foam is a porous heterogeneous material; the microscopy parameters are function of the position of the point in the material. It is made of finely divided solid phase and cavities, the cavities are polyhedral cells with polygonal faces (in the case of closed cells) and edges. These edges constitute the link segments between the vertexes of the cell. The objective of this paper is to compute effective thermal conductivity of PU foam used in thermal insulation for building with new approach to generate representative elementary volume. The proposed approach seems more realistic because it simulates the real fraction of closed cells and open cells and it models the real phenomena which happen in closed and open cells. This study is investigated for polyurethane foam with 70 % of closed cells fraction and 30 % of open cells fraction, by using finite element method and numerical homogenization. The result shows that there is a systematic change in thermal conductivity when the position of the closed cell or open cell varies at fixed volume fraction. Simulation cases demonstrate the interest of this proposed approach; it brought new factors including the investigation of effective parameters which are position and fraction of closed cells and open cells.

ID: 244633

Theoretical study of electronic properties of nitrogen doped carbon nanotubes

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Abstract: We have studied the effects of nitrogen substitutional doping on the electronical properties of single wall carbon nanotube using the electronic density of states (eDOS) calculations based on the microscopic tight-binding. The results reveal that the nanotube changes from the semiconducting to the quasi-metallic state because of the dopants. Our calculations indicate that electronic properties of the doped nanotubes are sensitive not only to the concentration of nitrogen atoms but also to their distribution. The doping effects on the electronic properties of the carbon nanotube are discussed.

Keywords: nanotube, doping, nitrogen, DOS

ID: 245124

Performances Improvement of Doped-Pentacene-Based Organic Thin-Film Transistor with Top-Contact Geometry

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Abstract: In this work we report a simulation study on the performances of doped pentacene based organic thin film transistors (OTFTs), in bottom-gate top-contact geometry. The simulation was performed for a Gaussian distribution of density of states (DOS). The obtained results with numerical simulations show that the field-mobility in saturation regime, the threshold voltage and the sub-threshold slope are of about 0.063cm2/V.s, -6V, and 2.89V/dec, respectively. Thus, we noticed the performances improvement for doped pentacene compared to undoped pentacene based organic thin-film transistors. In addition, the reported values are interesting and remain in good agreement with those reported in the literature as well as to those reported experimentally.

ID: 245132

Synthesis and characteristics of polyaniline/tungsten trioxide conductive nanocomposite for hexavalent chromium ions adsorption application

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Abstract: The new nanocomposite polyaniline/ tungsten trioxide (PANI/WO3) was synthesized through the chemical method, using the sodium persulfate as an oxidant. PANI/WO3 was used as an eco-friendly adsorbent to remove hexavalent chromium from aqueous solution. The developed adsorbent was characterized using various analytical techniques such as X-ray diffraction, Fourier transforms infrared spectroscopy, X-Ray Energy Dispersive Spectroscopy (EDS) and Scanning electron microscopy (SEM). A batch adsorption system was applied to study the ability of the adsorbent to remove Cr (VI) ions from aqueous solution. The obtained experimental results showed that the Cr (VI) removal efficiency is significantly dependent on different physicochemical conditions including initial pH, contact time, PANI weight content in PAN/WO3 nanocomposite, adsorbent dose, Cr (VI) initial concentration and temperature. The adsorption follows Langmuir adsorption isotherm and second-order kinetic model. Thermodynamic parameters like free energy ($\Delta G°$), enthalpy ($\Delta H°$) and entropy ($\Delta S°$) were also calculated.

Keywords: Synthesis, Polyaniline, tungsten trioxide, Nanocomposite, Hexavalent chromium.

ID: 245616

Design of high-performance perovskite solar cells adapted to the tandem configuration

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Abstract: Thin film based solar cells offer great advantage of presenting a low temperature coefficient of power and are usually suggested for hot climates. Furthermore, Perovskite solar cells have reached today a record efficiency of 23.3%. In addition, perovskite solar cells demonstrated a great compatibility to be used as the top cell in tandem cells using CIGS, CZTS, perovskite and silicon heterojunction (HIT) as the bottom cell. In our case, our research will focus on developing perovskite/silicon heterojunction tandem solar cells, in order to enhance the performances of solar cells and to overcome the 29,4% silicon cell Shockley-Queisser limit .The purpose of this work is to design planar perovskite solar cells (PSCs) reaching high power conversion efficiency, using the SCAPS-1D software. First, the different layers constituting the PSCs, which fulfill the optimal conditions to be used in tandem configuration were selected, such as the transparency of the electrodes, the alignment of the band gaps and material showing higher stability. Subsequently, based on the results of the simulation we will be able to optimize each layer in the objective to obtain the best performances for the perovskite subcell. In this step, the materials, thicknesses, band gaps, sequence of the layers will be defined, to be integrated on top of heterojunction silicon solar cell and form a monolithic tandem cell suitable for Moroccan climate. Based on the preliminary simulation results, cell efficiency of 27.73% was achieved with an open circuit of 1.2 V, a short circuit current of 26.02 mA/cm^2 and a fill factor of 88.79%. These results were found with a perovskite absorber with double halide having a band gap of 1.55 eV and 3.9 eV electron affinity, with inorganic electrodes thus make the final devices more stable. In addition, the first results show that the materials used in these devices, their sequences and their thicknesses affect significantly the performances of the perovskite solar cell. Furthermore, a matrix of parameters will be investigated to boost the performances and to get improved perovskite subcell with high stability adapted to the tandem configuration.

These results will be a starting point for further experimental optimization of these kind of cells in our laboratory.

ID: 245655

Investigation of the dosimetric parameters of a new cobalt 60 source used in brachytherapy with Monte Carlo N-Particles Extended code (MCNPX)

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Abstract: High Dose Rate (HDR) Brachytherapy has been used over the past two decades, especially for the treatment of gynecological tumors and for tumors which are not easily accessible for Low Dose Rate (LDR) technics. HDR brachytherapy uses a single miniaturized source which moves step by step through implanted devices to achieve the desired dose distribution chosen by an appropriate number of dwell positions [1]. After the acquisition of the radiological image, the calculation should be done accurately for more compliance with the PTV (Planning Target Volume). Brachytherapy consists of a very local irradiation. The dose is delivered by one or several sealed sources.

The aim of this study is to obtain the dosimetric parameters of a new Co-60 source [2],

used in HDR brachytherapy, simulated by the Monte Carlo N-Particles Extended (MCNPX) code. So to validate the pattern, a comparison is required with the protocols of the updated TG-43U1 formalism of the American Association of Physicists in Medicine [3]. In the other hand we applied the developed code in the biological medium with its own characteristics. The newly obtained results can be used as input data for the Treatment Planning System (TPS).

Keywords: Brachytherapy HDR, MCNPX, cobalt 60, TPS.

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ID: 250249

Transport and magnetotransport studies in $CdAs_2$ semiconductor

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Abstract: We report a comprehensive study of the low temperature transport and magneto-transport properties that have been measured for Cadmium diarsenide material in the fields up to 1.5T. We focused, in this investigation, on n-CdAs2 semiconductor, located on the insulating side of the metal insulator transition. At zero magnetic fields, the effects of electron-electron interactions dominated the transport properties in agreement with the Efros-Shklovskii predictions of variable range hopping resistivity. In particular, applying magnetic fields, a new hopping conduction process governs the charge transport properties. Our new experimental crossover suggests that compensated CdAs2 is an important disordered system for probing hopping behavior and its crossover by applying the magnetic field. Moreover, an understanding of the low temperature magneto-transport properties is very important to improve the practical technology in these materials. This is obviously in contrast to the previous theoretical prediction because it is widely accepted that hopping transport is more pronounced at low temperature.

ID: 248011

Aspect of Mn-Doped forsterite ceramic pigments

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Abstract: The present work is a continuity of the investigation of the potential of M-doped forsterite as ceramic pigments, whose colours and technical behaviours were reported for M=Ni and Co. The current focus is on Mn-doped Forsterite. At an earlier stage of this work, Mn-doped Forsterite solid solutions $Mg_{2-x}Mn_xSiO_4$ were synthetized using a new sol-gel method. The latter allowed the obtaining of single-phased materials with a wide range of mole fraction xMn (from 0.2 to 1) and at a relatively low tem- perature. These advantages could not be reached through the conventional ceramic route, and consequently these materials remained unexplored as ceramic pigments. The obtained powders have a very nice lilac colour whose shade changes from bright to intense lilac with respect to the increasing Mn- doping rate. After application in different glazes, their developed colours depended on the glazes composition and firing temperature, and their used concentrations. These results, in addition to the high thermal and chemical stabilities of Forsterite, indicate that these $Mg_{2-x}Mn_xSiO_4$ solid solutions have a high potential as performing, less expensive and less toxic ceramic pigments. In this presentation, the aspect of these pigments both as powders and applied will be presented, and the correlation with results of Optical Spectroscopy and XRD and SEM analyses and will be made.

ID: 249788

First-principles calculations of electronic structure and optical properties of Be and Mg co-doped ZnO monolayer

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Abstract: The effect of Be and Mg co-doping on the electronic structure and optical properties of ZnO monolayer has been studied by first-principles density functional theory. It is found that (Zn, Be, Mg) O monolayer exhibits interesting tuning of electronic structure and optical properties with Be and Mg co-doping concentration. On one hand, the band gap increases with increasing Be and Mg concentration; and on the other hand, Be and Mg co-doping leads to a blue shift of the optical absorption peaks. Such modulation of the band gaps and optical properties provides (Be, Mg) co-doped ZnO monolayer with promising application in ultraviolet photoelectronic devices.

ID: 250344

Generation of generalized spiraling Bessel beams using Dark and Antidark Gaussian laser beams

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Abstract: The propagation and transformation of laser beams are fundamental topics of laser physics and its application domains. In recent years, the light beams with optical vortices have attracted much interest due to their relevant potential in optical micromanipulation and trapping of particles. Different technics have been introduced to produce such beams, among them one can mention methods using a phase spiral plate (SPP), helical axicon (HA) and curved fork-shaped hologram (CFH). This topic has inspired our research Laser Physics Group and some results have been reported. On the other hand, the Dark and Antidark beams (DADGBs), have been introduced and a method for their experimental realization has been investigated. These beams can serve as atomic traps; the atoms can be trapped in the vicinity of a dark notch of the beam where the optical field vanishes. More recently, the effect of the conical diffraction phenomenon on the intensity profiles of Dark and Antidark Gaussian beams by a biaxial crystal has been investigated. In this work, based on the Fresnel-Kirchhoff integral diffraction and by using the stationary phase method, the propagation properties of DADGBs spreading by a CFH is investigated in detail. Numerical calculations are performed to analyze the influence of some factors, including the base angle of an axicon lens g, the parameter m, topological charge p and the waist width of the Gaussian part, on the variation of the intensity distribution. Furthermore, it is shown that the obtained analytical expression of the outgoing spiraling Bessel beam can be regarded as a generalization to that one of the Gaussian beam.

Keywords: Fresnel diffraction; Curved fork-shaped hologram; Dark and Antidark beams; Generalized spiraling Bessel beams.

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ID: 250441

Ferroelectric, dielectric properties and electrocaloric effect of $Pb_xSr_{1-x}TiO_3$ thin films

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Abstract: Electrocaloric Effect (ECE) in $Pb_xSr_{1-x}TiO_3$ thin films is calculated from first principles based effective-Hamiltonian. The influence of the electric field and the concentration x on the dielectric and ferroelectric properties of $Pb_xSr_{1-x}TiO_3$ thin films are investigated. In particular, we have studied the polarization and the pyroelectric coefficient as a function of the temperature in order to examine the ECE. The increase of x shifts the critical temperature to higher temperature range. In addition, the temperature change due to the electrocaloric effect of $Pb_xSr_{1-x}TiO_3$ thin films is also predicted with particular focus on the applied electric field and the concentration x. The increase of the electric field enlarges the magnitude of T. However, by appropriately choosing the gradient field, the ECE can be enhanced. Investigations in a wide temperature range revealed large ECE observed and shift it toward higher temperature to achieve T~3.0 K for x=1.0.

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ID: 246131

The frustration behavior on the transverse antiferromagnetic ising model

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Abstract: In the presence of the uniform external magnetic field (h/J) and the transverse field (Ω/J) and using the effective field approximation, the thermodynamics properties of the transverse antiferromagnetic Ising model are studies. We have analyzed the behavior of the susceptibility and specific heat to study the frustration phenomena, and for the appropriate values of the system parameters, the divergence in the susceptibility and specific heat curves indicate the existence of this reentrant behavior. The same, the hysteresis behavior and coercetives field are also investigated.

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ID: 250510

MRT-LBM study of natural convection with surface radiation in a square inclined cavity

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Abstract: The present study reports numerical results of natural convection with surface radiation in an inclined square cavity filled with air, using the Multi-Relaxation Time (MRT) scheme of the Lattice-Boltzmann method (LBM). The cavity is heated from one side with a constant temperature and submitted from the opposite side to a temperature that varies linearly along the boundary, while the remaining parallel walls are considered adiabatic. The purpose of the study is twofold; testing the performance of the MRT scheme in the presence of convection-radiation coupling and analyzing the combined effects of thermal radiation, inclination angle of the cavity and Rayleigh number on the fluid flow. The obtained results show that the surface radiation has an important quantitative and qualitative effect on the fluid flow structure and can causes the appearance of an unsteady flow regime. For the inclination angle, results revealed that its effect on the heat transfer is important particularly in the absence of radiation. The results of this preliminary study confirm also that the MRT-LBM method is a robust tool of simulation that can be used instead of the classical methods to simulate problems of natural convection coupled with surface radiation.

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Ambiguity domain characteristics of newborn eeg seizure signals

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Abstract: Newborn EEG seizure signals may appear as piecewise segments in the time frequency domain. Improving the time frequency image can be done using a quadratic-time frequency distribution which has the disadvantage of introducing indesirable artifacts commonly called cross terms. Using a signal model which mimics some typical behaviours of newborn EEG seizure signals, cross-terms can be characterized in the ambiguity domain. A filter can then be defined and an improvement of the time frequency image quality of newborn EEG seizure signals can be made possible. The filter is tested on both simulated and real signals and compared with current ones.

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ID: 252170

FP-LAPW investigations of magnetic structure of ReB_2 compounds

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Abstract: We have studied the magnetic properties of hexagonal rare earth diboride ReB_2 using density functional theory calculations where the RE-F bands, which are difficult to include in DFT calculations, have been treated beyond the local density approximation (LSDA), within the LSDA+U formalism with the spin-orbit interaction. (i) We study magnetic stability of ReB_2 compounds, (ii) the band structure and density of state results prove that the coulomb potential and spin-orbit interaction are key factors to understand the electric and magnetic properties of this series of materials and (iii) we explained the behavior of chemical bond of ReB_2 compounds through the analysis of the density of state (DOS) and of charge density which are in well agreement with experiments and theoretical studies.

ID: 254921

Analaysis and characterization of phosphate sludge from Moroccan phosphate mines: Perspectives of valorization

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Abstract: During phosphate beneficiation, fluorapatite is separated from associated gangue minerals by a combination of successive mineral processing. These operations generate a large volume of phosphate sludge residue which is constructed ponds with a large surface area at the mine site. In the field of construction, waste resulting from phosphate beneficiation processing may be important raw material sources for the manufacture of ecological building materials. The aim of this work is to analysis and characterize these products in order to know the potential of valorization by identifying the important compounds. Physical, chemical and mineralogical characterizations (ICP, DRX, FTIR, MEB and EDX) show that sludge contains 40% of carbonates, 11% of silicates, iron and aluminum oxide and silica. Meanwhile, atomic absorption analysis shows that 80% of silica is reactive which is an important raw material for agricultural products.

Keywords: phosphate sludge, Silica, reactive silica, valorization, construction, agriculture

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ID: 255055

Microstructural study of SiO_2 aggregates and valorization

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Abstract: In this study two silica aggregates behaviors are investigated for the purpose of valorization in terms of structure and chemical composition, then their durability. The first one is almost pure silica and the second one contains silica and calcite. The relationship between the durability and microstructural changes is evidenced using XRD, TGA/TDA and TEM. Based on these results, the chemical, microstructural and mechanical properties of the starting aggregates are linked to the durability of the materials. In addition to the chemical content, the portlandite phase evolution seems to be a good parameter to follow the aggregate behavior. A relationship between the portlandite content and the water absorption is evidenced. The results are in good agreement with the reactivity of silica network and Alcali Silica Reaction process.

Keywords: SiO2 aggregates, Reactivity, Durability, Microstructure.

ID: 255449

Natural Convection Heat Transfer in an Open Cavity Provided with Multiple Discrete Heaters

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Abstract: The present study deals with numerical simulations of natural convection heat transfer and fluid flow in open square cavities heated with three discrete sources placed on the left vertical wall facing to the opening. The governing equations where solved based on a mesoscopic approach using the Multiple-Relaxation-Time Lattice-Boltzmann method (MRT-LBM). The Rayleigh number was varied from to and the Prandtl number corresponding to air used as a working fluid. The results are presented in terms of streamlines, isotherms, volume flow rate and average Nusselt number. It is found that the volume flow rate and Nusselt number are increasing functions of Rayleigh number.

Keywords: Natural convection, Heat transfer, MRT-LBM, Numerical study, Open Cavity, Discrete heating.

ID: 265631

Efficient removal of p-nitrophenol from water using natural materials: Insights into the adsorption mechanism, process optimization and regeneration

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Abstract: The present research highlights the use of Moroccan natural clay to remove p-nitrophenol (PNP) from aqueous solution. The clay mineral was characterized using powder XRD, FTIR, SEM-EDS, XRF, BET analyses and pH of zero-point charge in order to establish the adsorption behaviorproperties relationship. The physiochemical parameters like pH, initial PNP concentration and material dosage as well as their binary interaction effects on the PNP adsorption yield were statistically optimized using response surface methodology. As a result, 99.5% removal of PNP was obtained under the optimal conditions of pH 2, adsorbent dose of 2 g/L and initial PNP concentration of 20 mg/L. The interaction between initial concentration and adsorbent dose was the most influencing interaction on the PNP removal efficiency. The mass transfer of PNP at the solution/adsorbent interface was described using pseudo-first order and intraparticle diffusion models. Langmuir isotherm model well fitted the experimental equilibrium data with a satisfactory maximum adsorption capacity of 122.09 mg/g. The regeneration study showed that the mineral clay exhibited an excellent recycling capability. Overall, the clay mineral is very attractive as efficient, low-cost, eco-friendly and recyclable adsorbent material for the remediation of hazardous phenolic compounds in industrial effluents.

Keywords: p-Nitrophenol, Adsorption, Clay mineral, Response surface methodology, Regeneration, Water treatment.

ID: 263253

Role of a uniform electric field on the energy spectrum of an exciton in a core/shell spherical quantum dot

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Abstract: We have investigated the influence of an external electric field on the binding energy of an exciton in a GaN/AlN core/shell nanodot. The control of the confined exciton ground state energy by the nanodot size is also discussed. Our theoretical model, based on a variational calculation, predicts a remarkable shrink of the exciton energy when the electric field is switched on. Additionally, the present investigation shows that for a fixed GaN/AlN size, the energy redshift depends only on the external electric field strength. By contrast, it was established that as the nanodot size increases the lowest exciton energy decreases and vice versa.

Keywords: Exciton; Core/shell materials; Quantum dots; Electric field

ID: 241222

Influence of Manganese content on the structural and thermal properties of some manganese-phosphate glasses

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Abstract: Glasses of the compositions xNa_2O-yK_2O-zP_2O_5-$tMnO_2$, with $0 \leq t \leq 60$ %, have beenprepared using a solid state route followed by melt-quench process. The obtained glasses showed various colors which do indicate that the oxidizing state of manganese was composition dependence. In order to get insight to the physical and structure of these vitreous materials, we have determined some of their parameters such as density, molar volume and glass transition temperature. From Differential Scanning Calorimetry (DSC) scan on heating we evaluate the glass transition temperature (Tg) of each glass which correspond to the phase transition temperature from solid to viscous liquid. The density (ρ) as a structural index was found to increase while the corresponding molar volume decreases with MnO2 content. They were also characterized by FTIR spectroscopy and Raman. These vibrational techniques allowed us to identify the coexisting bond vibration modes in the glass network. It was evidenced from the present work that many phosphate structural units coexist, mainly pyrophosphate and metaphosphate structural groups are the most components of the network of these glasses.

ID: 243301

Toward understanding the anticorrosive mechanism of cytisine derivatives: molecular structure, nbo, nlo, mep and thermodynamic theoretical analyses

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Abstract: In the present work, the quantum Density Functional (DFT) calculation at the B3LYP levels using the aug-cc-pvdz basis set were performed on Cytisine and two of its derivatives namely N-methylCytisine and dehydro-Cytisine in order to understand their possible role as corrosion inhibitors of mild steel in hydrochloric acid (1M)**1,2**. Sensitivity to corrosion has been quantified using global electronic descriptors of the whole molecule and local ones at the atomic level. Moreover, stability of these molecules arising from charge delocalization and hyper conjugative interactions has been investigated using natural bond orbital (NBO) analysis. The polarizability and hyperpolarizability were computed to determine their nonlinear optics (NLO) behavior. Total electron density and molecular electrostatic potential were also evaluated. The thermodynamic parameters such as entropy, enthalpy, heat capacity and Gibbs free energy of the title compounds were also taken into consideration. Furthermore, in order to approach the interaction mechanics between molecule and the metal surface and quantify the nature and the adsorption force **3**, we have used quantum mechanics as well as Monte Carlo type dynamics. In total, the results of the calculations made it possible to show

a noticeable competition between the three inhibitors, with a priority of dehydro-Cytisine in both gas and aqueous phases.

Keywords: Density Functional Theory (DFT), corrosion inhibitors, global and local descriptors, NBO, NLO, MEP.

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ID: 243450

Conformational stability, Barriers to internal rotation, vibrational spectral assignments (FT-IR and FT-Raman), UV-Vis, NMR, NBO, HOMO-LUMO and NLO properties of 2, 2, 3-trimethyl pentane based on long-range (LR) corrected model's calculations

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Abstract: The structure of a hydrocarbon fuel has a profound impact on its ignition and other combustion properties. Empirical correlations between species molecular size and structure and ignition properties have largely been highlighted [1]. Based on experimental studies, the roles of fundamental kinetic properties of these hydrocarbon fuels on ignition rates have become clearer [2]. Trimethyl pentane compounds are of particular industrial interest as they are used in commercial gasoline to increase the octane number because of their ability to withstand compression and reducing the contribution to pollution. Then, it is necessary to identify the right computational method for modeling them, especially their conformational isomerism and their rich infrared and Raman vibrational spectra [3].

In the present communication, a theoretical study of 2.2.3-trimethylpentane (2.2.3-TMP) in the ground state were investigated using long-range (LR) corrected model's CAM-B3LYP and B97XD levels of density functional theory with aug-cc-pvtz basis set, in order to have insight into electronic properties of this molecule and to differentiate between its conformers. After the conformational optimization, the rotational barriers between the most stable conformers have been calculated. The Natural bond orbital (NBO) analysis have also been carried out to analyze the effects of intramolecular charge transfer. HOMO and LUMO frontier orbitals, molecular electrostatic potential (MEP), the polarizability (α) and first-order hyperpolarizability (β) and related properties were calculated. In addition to NMR and UV simulations, the normal mode calculations of the most and less-stable conformers using a scaled force field in terms of non-redundant local symmetry coordinates have been made to approach the vibrational spectra temperature dependency.

Keywords: long-range (LR) corrected, Density Functional Theory; Conformers; Natural bond orbital, hyperpolarizability; scaled vibrational analysis.

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ID: 244463

Thermodynamic investigation for synthesis of intermetallic compounds by thermal process

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Abstract: The nickel aluminide intermetallic compounds have attractive properties that make them good candidates for high temperature structural applications. In particular, Ni3Al-based intermetallic alloys have received considerable attention in recent years because of their unique physical and mechanical properties, including high melting temperature, high hardness, low density, also the good resistance to oxidation and corrosion. In addition, the elastic limit of Ni3Al increases with temperature up to 600-800° C. The goal of our work is to elaborate these materials and solid solutions (Al-Ni), that's why we proposed their synthesis at the laboratory scale from Al powders and Ni (NO3)2 salt taking into account their availability compared to the solid "Ni" pure. Thermodynamic parameters of the Ellingham diagram were defined. In addition, the tests of its elaboration were carried in furnace an inert gas to avoid the oxidation of the elaborated metals. The processed blends were prepared based on previously were developed phase diagrams that provide information on the phase nature, chemical composition, and stability temperature of the desired solid solutions. This approach allowed us to effectively elaborate solid nickel and to synthesize Ni3Al intermetallic compounds and solid solutions of oxide-free aluminium. In the perspectives, we will intend to control the parameters of the process and we will try to elaborate other materials whose aim is to evaluate their electrochemical and mechanical properties.

ID: 245111

Thermal Lattice Boltzmann Method for micro-Poiseuille gas flow

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Abstract: In this paper, the thermal Lattice Boltzmann Method (TLBM) is used for simulation of rarefied gas micro flows. The simulated gas is confined within an inlet/outlet micro channel and driven by a constant inlet velocity Uin. The bottom wall temperature is taken to be unity while the top wall temperature is decreasing from 1 to 0. For consistent results velocity slip and temperature jump boundary conditions at the walls are used. The rarefaction effects described by the so-called Knudsen number, on the velocity and temperature profile are investigated. The results obtained from the TLBM are compared with those obtained using the Finite Difference Method (FDM). In addition to the good agreement observed between the two methods, the results show an interesting sensitivity of velocity and temperature profiles with the gas rarefaction degree.

ID: 245367

Optimization of an organic solar cell based on P3HT-ICBA: Effect of p-type doping

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Abstract: This paper reports a study on the p-type doping effect on the performances of a photovoltaic organic solar cell structure based on P3HT: ICBA. Thus, numerical simulations have been investigated on ITO/PEDOT: PSS /P3HT: PCBM/Ca/Al structure with AMPS-1D (Analysis of Microelectronic and Photonic Structures the simulation one dimension) software. Indeed, we noticed that there is unintentional p-type doping associated to uncontrolled density in the active layer. In addition, an efficiency peak is obtained for a particular p-type doping density of 1017 cm^{-3} with an improvement of 6.12%. Moreover, the obtained results show a good fit to those experimentally reported in literature.

ID: 245433

Bioactivity and controlled drug delivery of mesoporous bioactive glass nanoparticles doped with magnesium

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Abstract: The effect of magnesium doping on binary glasses' (Si-Ca) particle texture, biomineralization process in Simulated Body Fluid (SBF) as well as drug release were examined. For this purpose, magnesium-doped binary bioactive glasses (85SiO 2 - (15-x) CaO x MgO, with x = 1, 3, 5 and 10 wt. %), were prepared by the sol-gel method. N2-adsorption isotherms analyses showed an enhancement in specific surface area as Mg-doping bioglasses increased. In addition, FTIR spectra of samples after soaking in SBF for various periods of time confirmed the presence of new chemical bonds related to apatite phase as was also confirmed by SEM observations while XRD revealed that the crystallization to form a more stable apatite-like phase was hindered with increasing magnesium content in the glass composition. Furthermore, it was proved that the kinetics of drug release was improved with increasing magnesium content. The porosity and the specific surface area were found to be responsible of this improvement.

ID: 245847

Analysis of polycrystalline silicon solar cells by Laser- Induced Breakdown Spectroscopy (libs)

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Abstract: The quality control of the solar cells in the industrial chain is necessary to detect the responsible defects on the efficiency of the solar panels. In this context, we analyzed a polycrystalline silicon solar cell by Laser Induced Breakdown Spectroscopy (LIBS). LIBS is an analytical technique based on atomic emission spectroscopy from laser-induced plasma, it allowed to determine the chemical composition of all types of materials including metals [1]. The target was irradiated by an Nd: YAG pulsed laser at the fundamental wavelength λ = 1064 nm with an energy of 20 mJ. Based on the color of the used solar cell, two zones were detected: a blue zone representing the silicon wafer and a white zone representing the contact metal ribbons. Seven elements were detected in the white zone and only four in the blue zone. The depth profiling of the detected elements versus the number of laser shots was investigated. These results demonstrate that LIBS is a promising tool for direct depth-resolved chemical analysis of solar cells.

Keywords: LIBS, Depth profiling, photovoltaic solar cells, polycrystalline Silicon, Calibration-free approach

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ID: 246251

Swelling Behaviour and Mechanical Properties in filled elastomeric nano-composites: A comparative study

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Abstract: The effect of physicochemical properties of solvents on the transport process and mechanical properties in elastomeric nanocomposite materials is reported. The investigated samples are formed by a semi-crystalline ethylene-co-butyl acrylate polymer filled with hard spherical carbon black (CB) nanoparticles. The swelling behaviour was studied at room temperature by immersion the dried samples in two selected solvents, i.e. Toluene and Xylene. Mass gain relative to the mass of dry material at specific times was recorded to probe the absorption kinetics. The transport of the molecules of a given solvent in these filled elastomeric composites is found to follow a Fickian diffusion mechanism. Mechanically speaking, the stress-strain curves of uniaxial tensile tests pre- and post- swelling highlight a remarkably decrease of the strength and elongation at break of the swollen samples. This behaviour can be attributed to the decrease of the load transfer density between the matrix and the CB in the presence of the solvent. The Mooney-Rivlin model is used to capture the physics of the stress-strain curves in both dry and swollen samples. We believe that the results reported in this experimental investigation can be useful for some demanding applications e.g. tires, sealing rubber...etc.

ID: 252572

Phononic-plasmonic interaction in the nano-opto-mechanical cavities

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Abstract: In this paper, we numerically simulate interaction between localized plasmon resonance mode of periodic system of 3 dimensional gold disc above a dielectric ribbon (Si3N4) with locally resonant elastic modes in phononic crystals slab. The goal of working on this specific structure is the possibility of exciting local resonance modes which are also called whispering gallery mode a.k.a WGMs. We find that our structure supports elastic plat modes which are non-dispersive modes to avoid losses and to localize the field on the gold nano-particle. We proceeded by studying the coupling of four WGMs with the plasmonic dipolar mode and we have demonstrated that the coupling between these two (the plasmonic mode and the WGMs) is relative to the symmetry of the phononic mode. The way we did the coupling is by shifting the wavelength of plasmonic mode under different kind of deformation of this four phononic modes. A detailed comparison between these four modes allows us to determine the one with the right coupling. Such structures are promising for the conception of detection generally and of nano-biosensors specifically. This simultaneous confinement of these two modes gives high coupling and innovation towards new acousto-plasmonic devices.

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The effect of tri and tetra-vacancies defects on the electronic and vibrational properties of (14, 5) chiral carbon nanotube

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Abstract: The spectral moment's method, can be applied to very large systems, whatever the type of atomic forces, the spatial dimension, and structure of the material were shown to be a powerful tool for determining vibrational properties (infrared absorption, Raman scattering and inelastic neutron-scattering spectra) of the harmonic systems. In this work, in order to obtain the Raman signature of Tri and Tetra-vacancies (TriV and TetraV) points defects, and the effect of such defects on the electronic and vibrational properties of carbon nanotubes. We calculated the non-resonant Raman spectra of pristine and defective (14,5) chiral carbon nanotube by using the spectral moment's method. In comparison with Raman spectra of pristine carbon nanotube, the D band is observed around 1350 cm-1. The Raman characteristics modes of TriV and TetraV defects are identified. The concentrations effect of TriV and TetraV was discussed. In the electronic part of our work, the electronic density of states of our systems is calculated.

ID: 248765

Raman analysis of sexithiophene encapsulated inside single-walled carbone nanotubes

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Abstract: In this work, the encapsulated effect of sexithiophene inside single walled carbon nanotubes (SWCNTs) is reported. We evidence by means of Raman spectroscopy calculations, the structural organization of the nanohybrid systems depend on the carbon nanotubes diameter. The optimum configurations of sexithiophene inside carbon nanotubes are derived from minimum energy calculations using a convenient Lennard-Jones expression of the van der Waals intermolecular potential. The calculated results indicate that the minima correspond to the Zigzag (12,0) and Armchair (7,7) configurations with diameter close to 0.94nm. The charges/energy transfer in the 6T@SWCNTs systems has been investigated by analyzing the Raman mode of 6T molecules and the RBM and G-band modes of SWCNTs before and after encapsulation.

Keywords: sexithiophene, SWCNTs, Raman

ID: 249554

Monte Carlo dose calculation for HDR brachytherapy source using GATE/GEANT4 code

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Abstract: Brachytherapy is a technique of irradiation for cancer treatment. It involves placing radioactive sources as close as possible to the tumor. The various types of available sources vary according to their geometry, and the isotope selected (192Ir, 125I, 60Co). Dosimetric parameters for brachytherapy source should be known before its effective clinical practice. For this reason, there are several source geometries and mediums where the authors calculate the parameters of brachytherapy sources recommended by TG-43U1 protocol, using Monte Carlo codes. In this work, the simulated geometry of the BEBIG 60Co HDR source model Co0.A86 was performed through the Monte Carlo method using the GATE/GEANT4 code, the purpose of this study is to obtain the dosimetric parameters of the new BEBIG 60Co brachytherapy source following by TG-43U1 recommendation, such as radial dose function g(r), anisotropy function F(r, theta). The results obtained show good consistency with the published data for the dosimetric parameters of the brachytherapy source and to measurements published and fixed as recommended values by the AAPM Task Group 43U1.

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Electronic and magnetic properties of the double perovskite Sr_2CrWO_6: ab-initio and Monte Carlo studies

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Abstract: The electronic and the magnetic properties of the double perovskite Sr_2CrWO_6 are studied by using ab-initio density functional theory (DFT) calculations with Generalized Gradient Approximation (GGA) and Monte Carlo simulation within the framework the Ising model. This compound is formed by two magnetic cubic sublattices, one occupied by Chromium Cr^{3+} with spin (S = 3/2) and the other occupied by Tungsten W^{5+} with spin (σ= 1/2). The density of states (DOS) and the band structure of the compound are investigated. The results show the half metallic behavior of Sr_2CrWO_6 with a total magnetic moment equal to 2μB. The degeneracy removed from the orbital d of the Chromium by the octahedral crystalline field was discussed. The exchange couplings Cr - Cr and W - W are ferromagnetic, while the super exchange coupling Cr - O - W is antiferromagnetic. Concerning the Monte Carlo study, it is seen that the system presents interesting phenomena. In particular, the compensation behavior, the first order transition and multiple hysteresis loops have been obtained.

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Effects of variation in autoclave pressure, temperature and vacuum-application on mechanical properties and void content of epoxy prepreg

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Abstract: Final mechanical properties of composites materials highly depend on their curing parameters in the autoclave. Voids are one of the most harmful defects in carbon/epoxy laminates since they weaken the matrix-dominated mechanical properties such shear and compressive strength. The curing parameters for autoclave processing of prepregs are curing pressure, curing temperature, curing time, and vacuum pressure. A series of [0/90/+45/- 45/-45/+45/90/0] laminates were fabricated, and various curing cycles with ramp rate curing of 3 K.min-1 were designed to study the effect of the combination of three pressures, three temperatures and two different vacuum-application on some mechanical properties of carbon fiber/epoxy prepreg, HexPly 8552S/AS4. The interlaminar shear strength (ILSS) and compressive strength at room temperature and at 120°C were used to evaluate the mechanical properties of the composites under different curing conditions. The correlation between the ILSS and void content was studied using experimental data and theoretical models.

ID: 250562

Effect of the nanostructuring on the thermoelectric properties of α-MgAgSb

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Abstract: Thermoelectric materials, capable to transform the heat energy into the electrical energy using Seebeck effect. Among the challenges of the nanotechnologies is to develop non-toxic thermoelectric materials with better performance at room temperature. Therefore, the bulk structure of MgAgSb has been explored recently due to its advantage properties. In this work, we have investigated the thermoelectric performance for both bulk and thin films α-MgAgSb by using the first principles pseudopotential method based on the density functional theory (DFT) and the plane-wave method combined with the Boltzmann transport theory. The results show that the thermoelectric performance for thin films is better compared to the bulk structure due to a difference of their density of states.

ID: 252243

Infrared phonon modes of double walled CBN nanotube: theoretical study

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Abstract: Since their discovery by Iijima 1991 [1], carbon nanotubes (CNTs) have been of great interest, both for the elucidation of fundamental one-dimensional science and for a wide variety of potential applications. Subsequent to the CNTs, boron nitride nanotubes (BNNT) have attracted much attention due to their stable insulators, high thermal conductivity, superb oxidation resistance, distinguishable chemical stability and extraordinary mechanical strength [2]. They may be nano-electromechanical potentially found applications in electronics, optoelectronics and energy storage systems [3]. The structure of boron-nitride nanotubes (BNNTs) is very similar to that of CNTs, and they exhibit many similar physical and chemical properties [4]. Both experiments and theoretical calculations have shown that nanopeapods formed by encapsulating C60 and C70 with BNNTs can exist stably [5]. In this work, we focus on coaxial structure composed of an inner CNT and an outer BNNT (CNT@BNNT), these materials have a stable structure and a practical application. We report the structures and the infrared spectra of hybrid systems CNT@BNNT. The optimal structure of these systems are derived from total energy minimization using a convenient Lennard- Jones expression of the van der Waals intermolecular potential between the inner carbon nanotube and outer boron-nitride nanotube. The infrared spectra have been calculated as a function of nanotube diameter and chirality using the spectral moment's method. These results should be useful for the interpretation of the experimental data of boron nitride nanotubes encasing carbon nanotube.

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Energy and exergy analysis in a salt gradient solar pond for the assessment of three heat exchanger designs

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Abstract: Structural, electronic and magnetic properties of GdNi5, GdNi3Cr2, GdNi3Co2 and GdNi3Fe2 intermetallic compounds have been studied in the spin-polarized case by employing the fullpotential linear augmented plane waves (FP-LAPW) within the density functional theory (DFT) implemented in the WIEN2k package. In this approach, we have chosen the generalized gradient approximation with Hubbard U-correction (GGA+U) as exchange-correlation potential. The structural properties such as the structural equilibrium parameters of these alloys have been calculated and show that equilibrium volume (v0) are increasing with the increase of the metal transition sphere atomic radii. The band structure and density of states have been investigated; the results show that the densities of states and bands structures of the pure GdNi5 compound are changed by substitution with d metals. These changes are clearly observed in the appearance of others peaks on the spectral data. The total and local magnetic moments of $GdNi_5$, and $GdNi_3T_2$ (T=Cr, Fe and Co) are also affected in this work by the substitution of Cr, Co and Fe by Ni in 2c position.

Keywords: Salt gradient solar pond, solar energy, Heat extraction, Energy and exergy analysis

ID: 255577

Soret and Dufour effects on the onset of thermosolutal convection in a shallow horizontal Brinkman porous layer

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Abstract: The study of thermosolutal convection in porous media has been motivated by its presence in many engineering applications, such as in hydrology, petrology, geophysics, solar ponds, material processing technology, contaminant transport in saturated soil and drying processes. This type of convection caused by the combined inuence of thermal and solute buoyancy forces lead to the onset of the other phenomena, namely Soret and Dufour effects, which describe the mass transport in a temperature gradient, and heat flow due to a concentration gradient, respectively. The present investigation, conducted analytically and numerically, deals with the determination of the onset of thermosolutal convection in a horizontal Brinkman porous layer heated and salted from below in the presence of both Soret and Dufour effects. In the N-Du (buoyancy ratio-Dufour Number) plane, up to six regions, describing different flow behaviours, are delineated and the location of each region depends on the value of Soret number. The supercritical and subcritical Rayleigh numbers corresponding to the onset of the parallel flow convection are also determined. The analytical solution is derived based on the parallel flow approximation and validated numerically using a finite difference method.

ID: 255613

Study of thermal aging of a polymer matrix nanocomposite on mechanical behavior

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Abstract: In recent years, there has been a great deal of enthusiasm for the development of nanoreinforced polymeric materials called nanocomposites. Different types of particles, of various types, factors and shapes can thus be incorporated into the polymer matrices. These are usually inorganic particles, such as mineral fillers. The addition of the nanoparticles, bring great interest, because they have unique properties, namely, the improvement of mechanical properties, thermal, electrical and optical ... etc. In this work we developed nanocomposites with polymer matrix by in situ polymerization at different charge percentages, then we focused on the study of the capacity of a biodegradable filler played the role of a thermal barrier. In this sense, we performed accelerated thermal aging, then performed a morphological analysis using the optical microscope and studied the mechanical behavior using the tensile test and the hardness test. From the results obtained, we have been able to deduce that a mineral filler delays the thermal degradation of the polymer and improves the thermal stability of the nanocomposites. The presence of carbonates as a well dispersed reinforcement in the matrix has been an obstacle to the diffusion of the degradation products, which reduces the mass loss of the nanocomposite.

Keywords: Synthesis of polymers, waste, nanocomposites, nanoparticles, thermal aging.

ID: 255623

Physico-chemical characterization of a regional clay: application to the adsorption of phenol

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Abstract: Morocco is among the African countries most threatened by the pollution of aquatic environments. The main sources of this contamination are of urban, agricultural and industrial origin. These rejections are generally organic and microbial. Agricultural development in recent decades has contributed to the pollution of water resources through the use of fertilizers and phytosanitary products. In addition, the discharge of domestic wastewater from urban and rural centers without prior treatment or after insufficient treatment in the natural environment adds a negative impact on the quality of water resources. This during the earth and its rocky and clay present a real filter to purify wastewater. In this context, this paper studies the ability of local clay to remove organic pollutants such as phenol. The elimination of this pollutant has been achieved by adsorption which is a suitable technique for the removal of organic pollutants. The support used was characterized by X-ray fluorescence spectroscopy, X-ray diffraction and infrared spectroscopy. The results obtained showed that the adsorption equilibrium is fast. The adsorption kinetics of phenol on this clay follow the pseudo-second order model. The adsorption isotherm is described by the Langmuir and Freundlich model. The important retention capacity has been explained by the structure of this clay.

Keywords: adsorption, clay, phenol, isothermal, characterization.

ID: 261987

NANOMD software for Molecular Dynamics study of nanomaterials

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Abstract: We have developed and implemented Molecular Dynamics software (called NANOMD) to study the vibrational properties of carbon nanomaterials. Using the spectral moment's method, NANOMD offers the possibility to calculate the linear responses for large systems (up to 100.000 atoms) and for different dynamical models. Thanks to graphical interface, NANOMD allows to visualize the structures of many carbon nanomaterials: Graphene, SWNCTs, DWCNTs, and MWCNTs. To perform molecular dynamic simulations, different interaction potentials (FCM, Lennard-Jones…) are incorporated in order to calculate the dynamical matrices of the nanostructures. The software requires a reasonable CPU time and memory to determine the neutron; Raman and IR spectra.

ID: 245050

Global indicators of the quality of the diffraction data

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Abstract: To get a good quality crystal structure, we should first do the initial analysis of the diffraction data. There are many global indicators of the quality of the diffraction data. Accentuated in this paper are the nominal resolution d*min* , the completeness C, the merging factor R merg , the effective resolution deff and the redundancy independent merging R factor Rr.i.m . Based on the results obtained and these global indicators of the quality of the diffraction data, this paper will overview the above-mentioned indicators and accordingly discuss, using practical examples, the usefulness of the data.

Keywords: Diffraction data, initial analysis, global indicators

ID: 246425

Reticular plasmon resonance detection properties of metal nanoparticles

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Abstract: The theoretical study of the detection properties of network plasmon resonances, supported here by gold, nanoparticles (form T) and graphene expressed in terms of sensitivity and figure of Merit (FoM). The expressions of sensitivity and FoM for changes in geometric parameters of surface nanostructures are derived to establish the relationship between sensor detection performance parameters and enabling biosensor design of nanoparticles with optimum detection performance. The sensitivity of the proposed biosensor is improved using two methods. First, the layers of graphene are covered with nanoparticles, which have been discussed and, it has proved that the sensitivity can be improved. Second, the influence's angle of incidence of the wave excited the network on the sensitivity. Finally, the improvement of the sensitivity and the FoM using the structure is revealed these two methods. The maximum sensitivity ~ 505.47 nm/RIU is obtained with coating of graphene layers and angle of incidence oblique to the surface.

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ID: 247856

Sorption of contaminants into thermoplastic pipes: critical review

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Abstract: For several decades, polymeric materials are increasingly used in various fields, particularly in the distribution of drinking water in the form of pipes or fittings, thanks to the various advantages represented by polymers such as light weight, low cost, easier to install and without any problem of corrosion compared to metal pipes. One of the main concerns of researchers is the sorption of the constituents of drinking water through the pipe. Many studies have found that the mass transfer of a liquid into the polymer has consequences such as the change of crystallinity, the yellowing of the polymer, decrease of mechanical resistance and the swelling of the polymer. The aim of this study is to carry out a critical review about the sorption of the constituents of liquid transported into the material in order to summarize what is already done in this field and to serve as a source of background information. We started with the description of the transfer process, we discussed the theoretical study of sorption then the experimental one by showing the different methods used to measure the diffusivity of a contaminant towards the polymer then we enumerated the empirical and analytical models developed for predicting diffusivity and solubility coefficients and finally we showed the influence of this transfer on the mechanical characteristics and the morphology of thermoplastic pipes.

ID: 249144

Petroleum potential assessement of energetic oil shale material originated from central Kongo basin of the Democratic Republic of the Congo

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Abstract: Oil shale sedimentary rocks (OS) constitute substantial natural resources that can be converted by pyrolysis or burning to produce energetic materials useful for power generation and heating purposes. Morocco and Democratic Republic of the Congo (DRC) are the most known African countries for their vast reserves of OS. In the present research, mineralogical characterization and assessment of the hydrocarbon potential of OS, originated from the western part of Central Kongo basin were carried out and compared to Moroccan oil shales. The mineralogical characterization showed that Central Kongo oil shale (CK) is mainly composed of mineral quartz and low portion of montmorillonite clay. In addition, scanning electron microscopy (SEM) revealed the presence of pyrite in framboid form and pores filled by carbonaceous organic matter (OM). The thermal analysis (TG/DTA) showed that the CK sample contains 11.5% of volatile OM corresponding to kerogen. The assessment of petroleum potential of CK sample and its comparison with Moroccan oil shales, such as Timahdit (TI), Tarfaya (TA) and Arbaa Ayacha (AA), were performed using the Rock-Eval analysis. The results show high total organic carbon (TOC) contents in all samples, which is assigned to favorable conservation environments of the OM. Furthermore, the S2 parameter value of 80.4 mgHC/g is higher than Moroccan oil shales and indicates an excellent potential for producing hydrocarbons from the source rock at the maximum pyrolysis temperature (Tmax) of 438°C. The HI and OI index values imply that the OM is exclusively composed of type I kerogen, which was deposited in anoxic marine. While, TI and TA oil shales are dominated by type I, and AA oil shale is exclusively formed by type II. Hence, the studied CK sample has a great potential for generating oil with appearance similar to crude oil.

References:

R. Bouamoud, A. El Hamidi, M. Halim, R.M. Masamba, R.A.K. Nlandu, S. Arsalane, Mineralogical characterization and preliminary assessment of the hydrocarbon potential of sedimentary rock from the western part of the Central Kongo, Mediterr. J. Chem. 7 (2018) 936104.

ID: 249623

Modelling and thermophysical characterization of a new clay-based construction material from the Atlas region

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Abstract: As part of the revaluation of local materials used in construction and the search for energy efficiency in the building sector, a thermal performance study is being carried out on a new clay-based material extracted from the Atlas region and peanut shells which constitute an abundant untapped ecological product. The study consists in studying the thermal performances of this composite material. For this purpose, samples prepared from clay and different percentages of a certain granular class of peanut shells. The thermal characterization of these samples is done by the method of the hot plane in steady state, and in transient state then by the ash method, also a numerical simulation for validation The results are encouraging and show the influence of these natural additives on improving the thermal insulation of the clay, which promotes a reduction in energy consumption.

ID: 249679

A study on the influence of process parameters on the thermal, mechanical and morphological properties of 3D printed Poly (phenylene sulfide) material

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Abstract: Poly (phenylene sulfide)(PPS) is a semi-crystalline engineering polymer and an attractive material for high-performance applications, frequently used in high-performance application due to its solvent resistance, thermal performance, and ease of processing. Many parameters of fused deposition modeling (FDM) influence the resulting properties. Processing parameters during the manufacturing process of PPS can implement a significant impact on its crystallinity and mechanical properties. In this study, we have focused firstly on the effect of nozzle temperature and speed of printing to determine the effects of each parameter on the mechanical, thermal and morphological properties. Maximum tensile properties are attained for a nozzle temperature of 330°C and a speed of 30 mm/s. These two parameters were selected for probing the effects of infill orientations and raster width. Among the two orientations tested, the combination [0°, 15°, -15°] relative to the long axis of the test bar yields exhibited the higher levels of tensile properties than [45°, 135°] orientation. 0.15 mm of raster width exhibited the best surface finite and high mechanical properties. Annealing treatment can also affect the level of crystallinity, as a consequence, improvement of elastic modulus of manufactured parts. Through differential scanning calorimetry analyses (DSC), the degree of crystallinity was assessed for samples annealed under various conditions. Results show that annealing increase crystallinity in PPS samples. The Young's Modulus exhibits higher values for annealed parts than the others. With a lower cooling rate yielding higher modulus values; this is attributed to a relaxation of the material structure as well as an improvement of alignment of polymer chains in the crystalline region causing great strength and rigidity.

ID: 252177

The effect of M1 and M3 polymorph on the rate of hydration of Cement, using Rietveld analysis

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Abstract: Rietveld analysis has been increased in in the recent years. It is an effective tool for identifying and quantifying cement Portland phases. The Rietveld method is used in this study to follow the rate of hydration of M1 and M3 polymorphs on the alite phase synthetized in laboratory. The result of this method is compared by other technics as ATG and Si-NMR. Here we present the study of the correlation between the crystallographic structure of cement and its reactivity. This work describes the use of rietveld analysis to study the effect of alite polymorphism on the rate of hydration. Two polymorphs were studying M1 and M3 which are the most often found in commercial clinkers.

ID: 254969

Simulation of soret convection flows in a square cavity with internal heat generation and opposite buoyancy forces

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Abstract: Thermosolutal natural convection heat and mass transfer in a 2D square cavity is studied numerically in the presence of Soret effect and uniform volumetric heat generation. A hybrid scheme with simple relaxation time lattice Boltzmann method (SRT-LBM) is used to obtain the velocity field while the temperature and concentration fields are deduced from energy and species balances using a finite difference method (FDM). The study focuses on the effect of two parameters, which are the Soret parameter (Sr=-0.5, 0 and 0.5) and the internal to external Rayleigh numbers ratio (**$0 \leq R \leq 80$**). Combined effects of these parameters on fluid flow and heat and mass transfer characteristics are examined for the buoyancy ratio **N = -1**, Lewis number **Le = 2**, Prandtl number ***Pr = 0.71*** and external Rayleigh number $Ra_E = 10^5$. The interaction between the heat generation and the thermodiffusion may play an important role in purifying/charging the confined fluid from/with species by considered positive/negative values of ***Sr***.

Keywords: Thermosolutal convection, Binary mixtures, Lattice Boltzmann method, Soret effect, internal heat generation.

ID: 255042

Effect of the integration of hemp wool as an insulation material for the construction of the roof and external walls of a typical Moroccan building

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Abstract: This paper deals with the integration of thermal insulation in Moroccan buildings roofs and external walls in order to reduce the energy consumption due to the use of air conditioning systems. The insulation material under investigation is the hemp wool, an eco-friendly material whose use allows the storage of the Carbone and help reducing greenhouse gas emissions. In order to assess the dynamic thermal performance of the typical Moroccan insulated building, a life cycle cost analysis is conducted based on annual cooling transmission loads specific to the climate of Meknes, Morocco. Optimum insulation thicknesses, energy savings and payback periods are determined for a building life-span of 20 years. Investigations are carried out based on an implicit finite difference method using a home-made code developed in Matlab®.

Keywords: energy consumption; energy savings; hemp wool; optimum insulation thickness; payback period.

ID: 255627

Elaboration of solid biocombustibles from biomass waste

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Abstract: Face of the growing energy demand and the resulting environmental problems, the use of alternative energy sources is essential to continue meeting our global energy needs while preserving the environment. Among the different forms of renewable energy, we find biomass with its different types. Biomass is defined as a renewable energy source, mainly composed of hydrogen, carbon and oxygen and having a low calorific value compared to fossil-based resources seems to be the best alternative. In this study, biomasses and their derived solid biofuel were evaluated for their energy characteristics. The solid biofuel samples were produced by slow pyrolysis at a temperature of 400 °C for a reaction time of 2 h. Properties such as the combustion process, the combustion index, the ignition index, the heating value of biomass waste and their solid biofuel have been determined. The results showed that solid biofuel has better fuel qualities than its parent biomasses, the combustion properties of solid biofuels are influenced by their structure.

Keywords: Biomass, Food waste, Pyrolysis, Energy recovery.

ID: 255591

Corrosion inhibition of E24 steel in acidic medium by composite coating with biodegradable charge

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Abstract: The majority of metals and alloys placed in various environments are affected by different forms of corrosion, uniform or localized corrosion is found. These attacks are particularly dangerous when they are localized. Preventive measures against corrosion are therefore necessary and the use of inhibiting coatings is an appropriate and practical method to protect metals. Recently, bio-filled polymer matrix composites have gained considerable interest due to their physical properties, chemical unique compared to polymers alone. Applications of these environmentally friendly composites include anticorrosive coatings, which is due to their inherent stability, improved impermeability, high resistance to solvents and heat, and their ability to act as a physical barrier against corrosive elements (for example H_2O and O_2). In this context, the use of natural lignocellulosic fillers from agricultural biomass (Bio-charges) offers a good alternative to conventional fillers such as synthetic, mineral or organic fillers while maintaining an attractive and environmentally friendly technology. The olive oil industry, which is well established in Morocco, generates huge quantities of chemical olive waste (COW) which represents approximately 25% of the primary material annually. This waste is a major source of pollution that can have several environmental impacts. The recovery and treatment of COWs would help to limit the negative impact of this industry on the environment. The objective of our work is to apply a polymeric matrix composite coating charged with COW nanoparticles on the surface of E24 carbon steel specimens, in order to test its inhibition efficiency in a 1M hydrochloric acid solution. The effect of the addition of the COW charge on the anticorrosive performance of the composite coating was investigated by gravimetric tests, polarization tests and electrochemical impedance spectroscopy (EIS). The kinetic activation parameters and adsorption isotherm were evaluated. The results showed that the addition of COW nanoparticles improved the inhibitory properties of the coating by providing excellent corrosion protection.

Keywords: Chemical olive waste (COW), corrosion, composite coating, electrochemical impedance spectroscopy (EIS), adsorption isotherm

ID: 249236

Electronic, magnetic and electric proprieties of Cobalt-Iridium based double perovskite

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Abstract: Electronic, magnetic and electrical proprieties of Cobalt-Iridium based double perovskite have been studied in this work by means full-potential method based on density functional theory. For exchange-correlation, we use PBE and exact exchange for correlated electron (EECE) to compute the strange correlation in d orbital, For instance using PBE approximation we found the half-metallicity behavior with high spin polarized in minority spins, on the other hand EECE shown a semiconductor behavior with different gap energy for both polarization of spins, This change in behavior owed to the localization of d electrons by a strong Coulomb repulsion. Since, the magnetic moment up to 8.0 μ_B per formula unite due to the high spin in cobalt ion Co^{2+} (S=3/2) and low spin in Ir^{4+} (S=1/2) for a ferromagnetic phase, band structure and density of state revealed that our simple is semiconductor or spin gapless semiconductor with a gap energy of 2.6 eV and 0.5 eV for majority and minority spins respectively.

Keywords: Double perovskite, DFT+ EECE, strong correlation, semiconductor with gapless

ID: 249865

Comparison between a simple smart facade and a smart double skin facade in terms of energy saving performances

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Abstract: The concept of smart walls and roofs has known a high interest in the last few years due to the potential gains that presents in terms of thermal insulation and the resulting energy savings. This concept is based on the application of smart materials on the external surface of building wall. Several materials such as phase change materials (PCMs), thermochromic (TC) and electrochromic (EC) materials are intensively studied. In this work, we present a benchmark study in the aim of comparing the energy performances of two smart wall configurations integrating a TC material which is the tungsten (W) doped vanadium dioxide (VO_2). The first smart configuration is composed respectively from outdoor to indoor of a thin film of W doped VO_2 deposited on a glass substrate fixed on a massive wall composed of cement plaster and brick. The second smart configuration is a double skin facade (DSF) composed of a thin film of W doped VO_2 deposited on a thick glass substrate forming the first skin (outdoor), an enclosed air cavity and a second skin composed on thin coating of Aluminium Nitride (AlN) stuck on a massive wall. Results have shown that the smart DSF configuration presents a high potential energy savings during both, hot and cold seasons with a nearly 0% energy consumption for heating and cooling loads. It was noticed that this configuration have the capacity to generate and control a greenhouse effect in the air cavity. The generation of this phenomenon is due to the natural convection-radiation interaction which is controlled by the smart W doped VO_2 by modulating the incident solar radiation depending on the outdoor temperature. On the other side, the smart simple facade had shown interesting results during the hot season with 70% decrease in energy consumption. However, this configuration presents heating energy penalties around 1% during the cold season due to the massive wall absorptivity limitation.

Keywords: Smart materials, Thermochromism, Double skin facade, Thermal insulation, Energy savings

ID: 250425

Hysteresis behavior of a nanographene sandwich-like structure

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Abstract: Within the classical Heisenberg model and Monte Carlo simulation, we have studied the hysteresis behavior of a nanographene with sandwich structure. The system consists of a ferromagnetic layer of spin-5/2 and an antifferomangetic layer of spin-3/2. The influence of the anisotropies, the exchange coupling and also the temperature on the hysteresis properties of the system is examined. It is found that the hysteresis loop area decreases when we increase the value of the interface exchange interaction and the temperature.

Keywords: Nanogrphene, Monte Carlo simulation, Heisenberg model, Hysteresis behavior.

ID: 250498

Oscillating magnetocaloric effect of a multiwalled nanotubes

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Abstract: The oscillating magnetocaloric effect of multiwalled nanotubes in hexagonal structure is investigated to extend the previous knowledge of the effect on a single walled nanotube. We started from results of an Ising model and obtained analytical expressions for the order parameters and for the entropy change and adiabatic change. The last exhibits the same dependence on field and temperature observed for other diamagnetic systems; it oscillates with the inverse magnetic field and presents a maximum value at a given temperature. The amplitude of the oscillating entropy change decreases with the number of layers and the stacking sequence rules the magnetocaloric properties of the system.

ID: 250524

Magnetic, Magnetocaloric and Hysteresis behavior of Cd doped $Nd_{1-x}Cd_xMnO_3$ perovskite: Monte Carlo study

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Abstract: In this work we study the effect of Cd doping on the magnetic and magnetocaloric properties of $Nd_{1-x}Cd_xMnO_3$ using Monte Carlo simulation based on heath bath algorithm. The variation of magnetization with the external magnetic field h is given for different values of x (x= 0.0, 0.1, 0.2, 0.3). The magnetic entropy change S, the adiabatic temperature change T are obtained for different external magnetic fields. The isothermal magnetizations versus magnetic field are obtained at different temperatures. Finally, the magnetic hysteresis cycles have been obtained for different values of x and temperature.

ID: 254613

The photo catalytic hydrogen formation on the hetero-junction Ag/$NiFe_2O_4$ prepared by chemical route

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Abstract: The photoelectrochemical ability of Ag/$NiFe_2O_4$ for H_2 evolution under visible light irradiation was studied. The hetero-junction prepared by sol-gel method, shows a much higher activity than the physical mixture (hetero-system: Ag + $NiFe_2O_4$). The electrons of $NiFe_2O_4$ activated by visible light are focalized toward Ag clusters, intimately contacted to the spinel. The spinel was characterized by X-ray diffraction (XRD), spectroscopy Attenuated total reflection (ATR) and scanning electron microscopy (SEM). The optical gap of $NiFe_2O_4$ (1.59 eV) is due the crystal field splitting of d-d transition of Fe^{3+}: 3d orbital in octahedral site. p type conductivity of $NiFe_2O_4$ was demonstrated from the capacitance measurements in neutral solution (Na_2SO_4, 0.1 M). The conduction band is more cathodic than H_2 evolution and hetero-junction was successfully used for the photochemical hydrogen production under visible light irradiation. The photo-activity is dependent on the nature of the hole scavenger (NO_2^-, $Fe(CN)_6^{4-}$ and I^-).

Keywords: hetero-junction Ag/ NiFe2O4, spinel, hydrogen, photocatalysis.

ID: 242119

Profilometric method used to characterize the mechanical properties of optical materials

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Abstract: Fracture toughness is one of the important mechanical properties of optical materials. It can be determined by Vickers indentation which allows generating cracks along the diagonals of the indent whose length depends of the loading rate. Subsequently, a relationship between the crack length and the corresponding indentation load is applied to calculate the indentation fracture toughness. Therefore, the precision of this propertie will depend on the accuracy of the crack length measurement. In order to minimize the uncertainties of this parameter, we propose its measurement more precisely by a profilometric method. In this paper, we use an optical profilometer in conjunction with indentation experiments to estimate the length of a crack to determine the fracture indentation toughness of four optical glasses. Unfortunately, this method is done after the Vickers indentation test, which took a lot of time. However, this method proves to be a more accurate method for determining the crack length. On the other hand, the surface quality of the optical materials, ie the roughness and the presence of surface defects, can greatly affect the measurement. This is why special attention is paid to the lapping and polishing processes to prepare the sample.

Keywords: Optical glass; toughness; interferometric measurement; polishing method; indentation.

ID: 244405

Exploration of electrical conductivity of Fe-doped foresterite synthesized by a new sol-gel method

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Abstract: Recently Forsterite Mg_2SiO_4 has solicited thanks to its high potential use in different applications, such as lasers, bioceramics, pigments, etc. Concerning electrical properties and electrochemical performance, the literature shows that this silicate is a good candidate as a cathode of the rechargeable batteries. Furthermore, the reported results indicate that the electrical conductivity of the doped forsterite is very sensitive to the synthesis parameters (e.g. doping type and rate, sintering temperature, etc.). In this work, a new sol-gel method was followed in the synthesis of Fe-doped forsterite ($Fe_xMg_{2-x}SiO_4$) and its effect on the electrical conductivity of the latter was studied. The different analysis including electrical impedance spectroscopy was carried out. The results reveal the obtention of high pure materials whose electrical conductivity increases with increasing of doping rate. This result has not yet been reported. In this communication, the mentioned method, as well as the most important obtained results, will be presented.

ID: 244447

Enhancement of localized surface plasmon resonances of a silver nanoparticle array upon the presence of graphene coatings: LSPR biosensor

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Abstract: The resonance of localized surface plasmon (LSPR) on silver nanoparticles (AgNPs) deposited on a glass substrate and coated with a graphene by the finite element method (FEM) is studied. The resonance peaks in the absorption spectra of the nanostructure SiOx/AgNPs/Graphene, show significantly different profiles such as the thickness of the graphene, and the refractive index of the surrounding environment is, gradually, varied. Numerical simulation reveals that movements in plasmon resonance peaks result from coupling between the AgNPs networks and the covering graphene layer. In addition, the LSPR modes shift to red from 412 nm to 588 nm when the thickness of the graphene layer deposited on silver nanoparticles changes from 0.34 nm to 10 nm. Light coupled with LSPR modes propagating along a AgNPs-graphene interface is calculated and compared to a conventional AgNPs-based LSPR biosensor. The result of the comparison shows an improvement in the sensitivity of the biosensor from 26 to 106 nm RIU-1.

Keywords: Localized Surface Plasmon Resonance; silver nanoparticles; Graphene; Biosensor; Sensitivity.

ID: 244671

CFD simulations and experimental investigation of nucleate pool boiling of liquid nitrogen

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Abstract: Pool boiling heat transfer is a very efficient mode of heat transfer. It is used in various energy conversion and heat exchange systems and in the cooling of high energy density electronic components. In this work, heat transfer during nucleate boiling for a brass ribbon horizontally immersed in liquid nitrogen is experimentally and numerically studied. An experimental apparatus was built to conduct a pool boiling heat transfer study .the capabilities of CFD boiling mode in pool boiling heat transfer is investigate. The computational model used combines the Euler/Euler two-phase flow. The general measurements of the super-heat, the influences of super-heat on the triggering of the boiling, as well as the critical flux which represents an important issue for the security of the systems were specially analyzed. The results of numerical simulations were compared by experimental data.

Keywords: Pool boiling; experimental study; CFD boiling model; Refrigerant LN2

ID: 245435

Temperature's impact on bitumen ageing during storage

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Abstract: The mechanical properties and the chemical composition of bitumen are affected by the temperature fluctuations applied, and we cannot avoid these temperature fluctuations, while using renewable energies in bitumen's heating. Therefore, it is important to identify the less harmful fluctuation range on bitumen properties. The study is divided into two important parts. Starting with the evaluation of different thermal cycles impact on the quality of a 40/50 bitumen sample. The second part is to investigate the effect of bitumen storage at ambient temperature. Aging of bitumen was characterized using laboratory tests: needle penetration at 25°C, softening point, ductility, and NIR (Near-Infrared). The thermal cycles were chosen to cover three critical temperature ranges for bitumen: its storage range, a lower temperature that can occur if the renewable energies are not supplying enough heat, and a higher temperature that we may need to use during the heating process.

ID: 245498

Effect of hexa-vacancy defects on a double wall carbon nanotube

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Abstract: Double-walled carbon nanotubes (DWNTs) are an emerging class of carbon nanostructures. A DWNT consists of exactly two concentric carbon nanotubes. DWNTs, provide the ideal model for studying the influence of interlayer interaction on the physical and chemical properties of nanotube systems [1,2]. Compared to single-walled carbon nanotubes (SWNTs), DWNTs have higher mechanical strength and thermal stability and they also possess interesting electronic and optical properties. In contrast to theoretical considerations, the experimental results it is found that CNT and DWCNTs are not as perfect as it seems. Defects such as kinks, junctions, and impurities may be presented in as-prepared SWNTs. These defects can significantly change the electrical, chemical, and mechanical properties of CNTs [3,4]. Carbon nanotube and nanopeapod characterization and identification relies extensively on their vibrational properties such as Raman spectroscopy [5,6]. This technic is widely used by theoretician and experimentalists as a fast and non destructive method to identify the type of nanoparticle and to study their vibrational properties and their electronic structures. This work focuses on defective DWNT where the inner and outer wall are bonded through van der Waals interactions. In this study, we calculated the nonresonant Raman spectra of DWCNT to determine the effect of vacancy defects, in this aim we use a spectral moment's method together with a bond polarizability model. Essentially, the Raman vibrational properties are closely coupled with the atomic structure of the system. The evolution of the Raman spectrum as a function of the distribution of the vacancy defects in the outer carbon nanotubes is discussed. This work provides benchmark theoretical results to understand the experimental data of defective DWCNT.

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ID: 245841

Vibrational properties of black phosphorene: Raman study

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Abstract: In this paper, the non-resonant Raman spectra of phosphorene are calculated in the framework of spectral moment's method, together with a bond-polarizability model. New force constant model using DFT calculations to calculate the dynamical matrix of phosphorene was developed. We have found a good agreement with group theory concerning the number of the Raman-active modes of black phosphorene.

Keywords: Raman spectra, phosphorene, spectral moment's method

ID: 247568

Scale effect on wave propagation of double – walled carbon nanotubes with initial axial loading

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Abstract: This work studies the vibrational characteristics of double – walled carbon nanotubes (DWNTs) with initial stress using a nonlocal Euler – Bernoulli beam model. Both the effect of initial stress and the effect of small length scale are discussed in detail. The effect of van der Waals forces is incorporated in the formulation. The corresponding resonant vibrational characteristics are presented in detail, which are shown to be very different from those predicted by classical elasticity theory when nonlocal effects are significant. The influence of initial stress in carbon nanotubes on their flexural vibration modes is dependent on the tension or compression forms of the initial stress. The investigation of the effects of initial stress on transverse wave propagation in carbon nanotubes may be used as a useful reference for the application and the design of nanoelectronic and nanodrive devices, nano-oscillators, and nanosensors, in which carbon nanotubes act as basic elements.

Keywords: Carbon nanotubes, Wave propagation, Euler Bernoulli beam model

ID: 252117

Infrared-Active Modes in Finite and Infinite Hexagonal Boron Nitride

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Abstract: Hexagonal boron nitride (h-BN) is an interesting quasi two dimensional insulator [1]. It has attracted intense scientific and engineering interest due to its excellent lubricity, high thermal, chemical stability and especially remarkable electronic properties. The band structure engineering of h-BN extends the exploitation of its potential applications. The spectral moment's method (SMM) [2] was shown to be a powerful tool for determining vibrational spectra (infrared absorption, Raman scattering and inelastic neutron-scattering spectra) of harmonic systems. This method can be applied to very large systems, whatever the type of atomic forces, the spatial dimension, and structure of the material. In this theoretical work, we study the Infrared spectra of h-BN as a function of their diameters, chiralities, and lengths. Calculations are performed in the framework of the force constants model, using the spectral moments method. This original approach allows us to consider not only infinite h-BN sheet as usual in most theoretical models but also tubes with finite lengths. These predictions are useful to interpret the experimental data.

Keyswords: Infrared, boron nitride, spectral moment's method

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ID: 248771

Noncovalent functionalization of carbon nanotubes by Polyaniline molecules: Raman analysis

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Abstract: PANI/SWCNT composite has been studied using Raman spectroscopy calculations. We evidence that the structural organization of the nanohybrid systems depend on the carbon nanotubes diameter. To study the stability of PANI molecules encapsulated in the cavity of the SWCNTs, the optimum configurations of PANI inside carbon nanotubes are derived from minimum energy calculations using a convenient Lennard-Jones expression of the van der Waals intermolecular potential. The calculated results indicate that the minima correspond to the Zigzag (16,0) and Armchair (9,9) configurations with diameter close to 1.2nm. We investigated also the charges/energy transfer in the PANI@SWCNTs systems by analyzing the Raman mode of PANI molecules and the RBM and G-band modes of SWCNTs before and after encapsulation.

Keywords: PANI, SWCNTs, Raman

ID: 248910

Comparisons of Raman and IR spectra of quercetin Anhydrate and dihydrate in order to use ther antioxidant effects

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Abstract: Quercetin is a flavonoid that has been the subject of dozens of scientific reports over the past thirty years. She seems to have multiple beneficial effects on human health, including cardiovascular protection, anti-cancer activity, anti-ulcer effects, antiallergic activity, antiviral and anti-inflammatory, but its use as a drug is affected by its low solubility in the formulation milieu, and its instability to light and heat. To solve these problems we used the excipient Gelucire 50/13. For this reason, the objective of our study is to characterize the mixture quercetin-Gelucire 50/13 at room and body temperature, using Raman and IR spectroscopy to determine their physicochemical properties and especially their solubility and the influence of Gelucire 50/13 on the quercetin, and befor to start we are invited to choose the appropriate conformation of quercetin (anhydrate or dihydrate) to mix them with the gelucire

ID: 249251

Electronic and magnetic properties of two dimensional ferromagnetic semiconductor: Ab-initio calculations and Monte-Carlo simulation

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Abstract: Electronic and magnetic properties of two dimensional chromium oxide chloride CrOCl are performed using first principles calculations and Monte-Carlo simulations. According to the phonon dispersion spectra, it is found that the CrOCl monolayer is dynamically stable. The density of state and the band structure are analyzed. Our study reveals that the CrOCl sheet is a ferromagnetic semiconductor with band gap of 0.6ev and a total magnetic moment of 3μβ/f.u. additionally, the corresponding Curie temperature is 160K and, it increases up to 190K under appropriate strain. Our calculations indicate that the two dimensional ferromagnetic semiconductor CrOCl can be a promising candidate for nanoscale spinotronic devices.

Keywords: 2D Materials, semiconductor, ferromagnetic, Ab-initio, Monte Carlo.

ID: 250435

Quantum Monte Carlo simulation study for hysteresis properties of a ferromagnetic thin film

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Abstract: In this work, we have investigated the hysteresis loops and hysteresis related properties (like exchange bias, coercive field and remanent magnetization) of an Ising ferromagnetic thin film by means of quantum Monte Carlo simulation. The effects of the temperature T and the transverse field Ω on the hysteresis behavior of the system are studied. It is shown that exchange bias can exhibit non-monotonic behavior depending on the value of the system parameters. Also, the results indicate that as the temperature and the transverse field Ω increase the coercive field decreases and the remanent magnetization presents a maximum with changing the value of T and Ω, respectively.

Keywords: Thin film, Quantum Monte Carlo simulation, Hysteresis behavior

ID: 250581

Magnetocaloric effects of a binary alloy multilayer grapheme

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Abstract: The magnetic properties and magnetocaloric effects of ferromagnetic binary alloy multilayer graphene characterize by a random arrangement of spin-2 A and spin-5/2 B atoms of ApB1-p type and a positive A − B coupling are studied within the framework Monte Carlo simulation. The influences of the concentration parameter p, the surface exchange coupling and the system thickness on magnetic entropy change are examined. Our study indicates that the binary alloy multilayer graphene may be as very promising magnetocaloric material for varying applications

Keywords: Binary Alloy, Graphene, Magnetocaloric effects, Monte Carlo simulation

ID: 255604

Adsorption of Crystal Violet from aqueous solution onto two agricultural waste residues: corncob and almond shell

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Abstract: Recently, many approaches have been explored for the development of low-cost and effective non-conventional adsorbents, including waste and by-products from agriculture and other industries, have been suggested by several researchers. This work aimed at examining the potential of corncob and almond shell, as low cost adsorbent, for the removal of a cationic dye; Crystal Violet from aqueous solutions. Adsorbents were first analyzed by Fourier transforms infrared spectroscopy (FTIR), and then the adsorption was studied in batch system, with an artificial effluent. Experiments were carried out, as function of the adsorption parameters (contact time, initial dye concentration, dose of adsorbent, initial solution pH and temperature. Adsorption data were well described by the Langmuir's model. The adsorption process followed the pseudo-second order kinetic model. The thermodynamic parameters indicated that the adsorption is spontaneous ($\Delta G^\circ < 0$), and endothermic ($\Delta H^\circ > 0$).

Keywords: Adsorption; almond shell; Corncob; Textile dyes

ID: 250586

Magnetocaloric effects of mixed ternary nanoparticle

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Abstract: In this paper, we have investigated the magnetic and the magnetocaloric properties of mixed ternary spherical nanoparticle of the type AB_pC_{1-p} with spins (S_A=1/2, S_B=1, S_C=3/2) by means of Monte Carlo simulation based on Metropolis algorithm, the both ferromagnetic and antiferromagnetic interactions are considered. The effect of the concentration of the p atom between two atoms A and B on the magnetization and the magnetic entropy change of the system are discussed. The results revealed that the ternary nanoparticle as a promising condidate for the potential applications in the magnetic nanomaterial field.

Keywords: Ternary Alloy, Magnetocaloric effects, Monte Carlo simulation

ID: 253372

Effect of mould temperature, grain refinement in Al-9Si alloy

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Abstract: The present work aims to study the influence of grain refiner addition and the effect of mould temperature for some Al-Si foundry alloys Grain refining and modification are two common liquid metal treatments applied to Al-Si alloys. This treatment only concerns the primary phase of aluminum-silicon alloys. It consists in adding a grain refiner in small quantity in the liquid bath before the casting. The grain size depends on the state of refining of the bath. That is to say, more germs will be numerous, the more the number of crystals will be high and the latter will be fine.

In practice, the seeds consist of titanium and boron compounds. We will focus on hypoeutectic alloys the results and analyzes that have been observed and which are: Casting at a relatively high temperature has an effect on the structure of the alloy – it leads to an increase in the size of the dendrites. The addition of the grain refiner increases the germination and growth temperatures of the α-Al dendritic phase and eliminates the phenomenon of supercooling. The total time of solidification and the time of aluminum-silicon eutectic solidification in $AlSi_9$ alloy was decreased when titanium was added. Moreover, it has been shown that the thermal analysis does not take into account the variation of the initial temperature of the mould.

ID: 255624

Vibrational properties of linear carbon chains inside single-wall carbon nanotubes

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Abstract: The discovery of carbon nanotubes (CNTs) initiated extensive studies on the nanotube structure for a variety of applications in nanotechnology. Linear carbon chains (LCCs) are consisting of sp-hybridized carbon atoms and considered a fascinating 1D system. LCCs could be used in the fabrication of the next-generation molecular devices because of its ideal linear atomic nature. The LCCs encapsulation in the 1D nanospace of single walled carbon nanotubes (LCCs@SWCNT) have been used to stabilize LCCs, still theoretical studies show a strong coupling interaction between LCCs and SWCNT would alter significantly the electronic properties of CNTs [1]. In this work, the effect of the entrapped LCCs on the vibrational properties of SWCNTs is discussed. The optimal structure of the encapsulated LCCs inside nanotubes is derived from minimum energy calculation using a convenient Lennard-Jones expression of the van der Waals intermolecular potential. Using the spectral moment's methods (SMM) [2], we calculate the Raman spectrum of LCCs@SWCNT. The relative Raman intensity from the LCCs to that from the tube as a function of the chain concentrations is analyzed. These predictions are useful to interpret the experimental data.

Keywords: linear carbon chains, carbon nanotubes, Raman spectroscopy, simulation.

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ID: 241225

Optical and spectroscopic properties of Er^{3+} doped oxy-fluoro tellurite glasses: effect of BaF_2 and BaO

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Abstract: Er3+ doped tellurite glasses are promising materials for photonic devices, due to their important optical properties such as a their broad transmission band and high refractive index which make them suitable in optical amplifier devices, paricularly at 1.5 µm through the transition [1,2]. In the present work, we are interested by the optical and spectroscopic properties of two series of tellurite glasses having chemical composition of (100-x) TZLBF-xEr_2O_3 and (100-x) TZLBO-xEr_2O_3 where. These materials are prepared by conventional melting quenching method. A series of experimental measurements were performed. Absorption and transmission spectra in the UV-Visible and IR were measured to evaluate the effect of BaF_2 and BaO in the optical and spectroscopic properties such as the absorption cross section for different substitution ratio of Er_2O_3 to La_2O_3. These measurements permit us to calculate the spectroscopic intensity parameters described by the Judd-Ofelt theory. Then, the intensity of transitions between different energy levels of Er^{3+}, their probabilities and the branching ratios of excited states, were calculated. Finally, the emission spectra of Er3+ under excitation at 532 and 662 nm were measured and the intensities of emitted transitions are compared to those calculated previously and predicted theoretically.

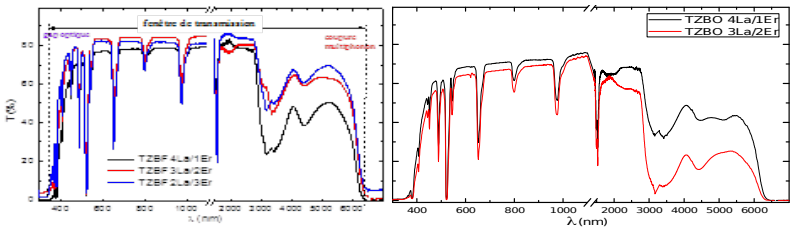

Fig.1.Transmission spectra of Er^{3+} doped TZLBF and TZLBO glasses

Keywords: Er3+, tellurite glasses, spectroscopic properties, Judd-Ofelt parameters

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ID 243468

Effect of frequencies on the change of electrical Impedance in sand dunes of Ouargla region

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Abstract: The previous research in the field of sand dunes knowledge of Ouargla region primarily focused on the diagnostic side, this research did not address the study to the measurement of physical properties of sand dunes. This paper focused of the measurement of the real and imaginary parts of electrical impedance and effective loss tangent respectively, and in sand dunes of Ouargla region at a range of frequency intervals between $4{,}6849 \times 10^{-2}$ Hz and $1{,}8593 \times 10^{+6}$ Hz with AC voltage 1.000 V using the impedance spectroscopy. The impedance spectroscopy is a powerful proven method of analysis in research and development of materials. This method is relatively simple and non-destructive. This technique is based on the modeling results by equivalent electrical circuits which have the same frequency response as the sample.

The experimental results revealed that the real and imaginary parts of electrical impedance and effective loss tangent have strong frequency dependence. In the lower frequencies range ($4{,}6849 \times 10^{-2}$ — $4{,}9385 \times 10^{-1}$) Hz and change between ($4{,}8118 \times 10^{+2}$ — $5{,}0422 \times 10^{+1}$), in the frequencies range ($5{,}4877 \times 10^{+1}$ — $2{,}3426 \times 10^{+4}$) Hz change between 146,04Ω and 4,8193Ω and 0 Ω. In the high frequencies range ($1{,}2599 \times 10^{+5}$ — $1{,}8593 \times 10^{+6}$) Hz change between 4,5359 Ω and 5,0567 Ω. The effective loss tangent values are decreased from $1{,}5956 \times 10^{+3}$ to $3{,}5081 \times 10^{+1}$ in frequencies range between $4{,}6849 \times 10^{-2}$ Hz and $1{,}8593 \times 10^{+6}$ Hz. The nature of impedance electric variation indicated a possibility to knowledge the polarization of sand dunes of Ouargla region and acquaintance the frequencies when the material is passive devices (consumes power) or active devices (produces power). It is also possible to know the quality of equivalent electrical circuit, whether to knowing if it is induction or capacitance.

Keywords: electrical impedance, effective loss tangent, frequency, impedance spectroscopy, sand dunes of Ouargla region

ID: 243334

Facile wet chemical synthesis of different shape-controlled copper oxide nanoparticles at low-temperature solution

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Abstract: In this work, CuO nano-crystals and their nano-architectures, with various morphologies, via a simple solution method process, were successfully synthesized, at a low reaction temperature (60°C). The effect of NaOH molars concentrations on structural and morphology properties was studied. XRD results confirmed the formation of pure single-phase CuO, with a monoclinic structure, in all preparation conditions. Additionally, in all the samples, FTIR spectra show three identical Cu-O vibration modes that indicate the presence of crystalline CuO monoclinic structure, which confirm the XRD results. SEM observations show homogeneous and uniform sand-flowers-like CuO nanostructures, which have been successfully synthesized by a simple wet chemical method at a low temperature of 60°C, without the addition of NaOH. Self-assembled three dimensional (3D) and unique nanostructures have average diameters in the range of 4-5 μm. Moreover, the addition of NaOH (1M) leads to a successful production of nano-flake-like CuO nanostructures, with an average size length of about 500 nm. As a result, this reliable low cost method was simple and can be completed in the absence of any surfactant.

ID: 244416

Hydrogen adsorption and storage of alkali metal ion-decorated Boron Phosphide with topological defects: A first-principles study

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Abstract: As a candidate for hydrogen storage medium, geometric stability and hydrogen capacity of Alkai metal atom-decorated boron phosphide with topological defects are investigated using the first-principle based on density functional theory (DFT). It is found that Alkali metal atom can be stabilized on above defective boron phosphide since Alkali metal ions binding energy on vacancy defect is much larger than its cohesive energy. Up to six H molecules can stably bind to an Alkali metal atom on defective boron phosphide with the average adsorption energies of 0.2-0.4 eV/H2. The hybridization of the Alkali metal 3d orbitals with H2 2-sorbitals and the electrostatic interaction between the Alkali metal cation and the induced H dipole both contribute to the H molecules binding. Double-side Alkali metal-decorated boron phosphide with defects can theoretically reach a gravimetric capacity of 6.1 wt% hydrogen, indicating that Alkali metal atom-decorated defective boron phosphide can be used as a promising material for high density hydrogen storage.

ID: 244419

Anti-perovskite Mn3(Sn,Zn)C : Potential candidates for an application in magnetic refrigeration

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Abstract: We have investigated the thermoelectric, magnetic-electronic and magneto-caloric properties of the anti-perovskite Mn_3(Sn, Zn)C using Ab initio and Monte Carlo calculations within the GG approximation, the LD approximation and heat bath (HB) algorithm for the exchange correlation potential. The energy (BS) band structures and (DOS) density of states are calculated and analyzed in comparison with the available theoretical and experimental data. We also investigate the equilibrium thermodynamics properties under the magnetic field by heat (C) capacity studies and determine the entropy-change S, the adiabatic temperature T change and as well as the relative cooling power about the transition of the Antiperovskite Mn_3(Sn, Zn)C Compounds. Our predicted results may be a reference for future experiment and theoretical studies of the nanostructures. These theoretical studies predict that this antiperovskite could be efficient material for thermoelectric generators and need further experimental and theoretical studies.

ID: 245460

Chirality dependence of electronic properties in single walled carbon nanotube

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Abstract: Application of carbon nanotubes (CNTs) to nanometer-scale electronic devices of the next generation is being highly expected owing to their prominent electronic properties and mechanical and chemical stability. In this work, we investigate the effect of chirality on the electronic band structure and the density of states in single-walled carbon nanotubes. Using nearest-neighbor tight binding approximation theory in association with the zone folding technique, the electronic band structures and the density of states for various chirality values has been analytically studied. We demonstrate that when the chirality increases, the total number of bands in the electronic band structure gets increased and Van Hove singularities appear in its density of states. Our results also show the semiconducting or metallic property of CNTs is linked to chirality.

Keywords: Single-Walled Carbon Nanotube, Electronic band structure, Chirality indices, Zone folding technique

ID: 245738

Structural, electronic and optical propreties of deltamethrin ($C_{22}H_{19}Br_2NO_3$) using Density Functional Method and IR spectrum

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Abstract: Pesticides are one of the most common pollutant groups in the world, and they have a major drawback such as toxicity. A long-term exhibition can be harmful for the human life and can disrupt the functioning of various organs of the body. Epidemiological and toxicological studies show that most neurodegenerative diseases, such as Parkinson's disease, associated with chronic exposure to pesticides. Deltamethrin (DM) is one of the most used pyrethroids and is currently the most widely used class of pesticides. The vibrational frequencies of Deltamethrin ($C_{22}H_{19}Br_2NO_3$) have been reproduced in the 500-4000cm-1 range. The modified Urey-Bradley-Shimanouchi force field was used, combined with an intermolecular potential energy function that includes van der Waals interactions, electrostatic terms, and an explicit hydrogen bond function. The vibrational frequencies of Deltamethrin were calculated and assigned to the experimentally observed vibrational frequencies. Overall, there was good agreement between the observed and calculated frequencies. In addition, the molecular orbital calculations such as Natural Bond Orbitals (NBOs), HOMO-LUMO energy gap and Mapped molecular Electrostatic Potential (MEP) surfaces were also performed with the same level of DFT. Electronic stability of the compound arising from hyper conjugative interactions and charge delocalization were also investigated based on the natural bond orbital (NBO) analysis.

ID: 246558

DFT investigations of the effect of intercalated atoms in layer graphene

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Abstract: The modulation of electrical, optical and magnetic properties in two-carbon materials is important for their applications as electronic devices and energy storage. We report here a comparative study of the effect of intercalated atoms of lithium, figure.1, and hydrogen systematically in graphene layers, within density functional theory. The structural, electronic band structures, the total and partial electronic density of states are investigated. We have shown that both the electronic and magnetic properties can be influenced by the type of atom which intercalated. Our results show that tunable values of band gap can be useful in applications. In optoelectronics, for instance, this property might be employed to control absorbed light wavelengths.

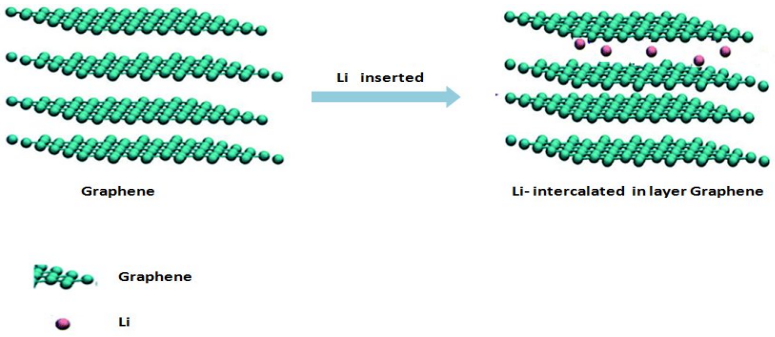

Fig.1: Li intercalated in layer graphene

Keywords : Graphen, Lithium, Hydrogen, band gap, Density functional theory

ID: 250657

Variable range hopping transport in insulating resistivity of doped InP

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Abstract: On the insulating side of the metal-insulator transition, we report the experimental results on low and high field magnetoresistance in InP sample at low temperatures. The relative magnetoresistance is negative for and is found to be positive in high fields (). Study of the temperature dependence up to of the positive magnetoresistance is made on n-type InP where conduction by the variable range hopping (VRH) mechanism is observed. The resistivity is well described by the Mott VRH model for and it's varies like in good agreement with Efros and Shklovskii model for in the presence of a coulomb gap in the density of stats created by the magnetic field. From the review of the literature, it appears that efforts have been made mainly to understand the mechanism in insulating disordered materials responsible for the temperature and field dependence of the magnetoresistance in the variable range hopping regime.

ID: 253286

Geochemical modeling of water contamination in the pit lakes of the abandoned Zeida mine (Morocco)

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Abstract: In the upper Moulouya watershed, the exploitation of the Zeida mine between 1972 and 1985 generated huge volumes (millions of tons) of metal-rich mining residues (Pb, Zn) and divided into three large dams. This activity had generated large excavations currently filled with water in permanent contact with the remaining ore deposit. In this area, the climate is arid to semi-arid with 300mm / year of rainfall and a scarcity of water resources, leading peoples to take water directly from the contaminated pit lakes. These resources need to be preserved and protected. An inverse geochemical modeling using Phreeqc carried out on water samples from ZA and ZL1 pit lakes made possible to highlight the chemical reactions occurring between the rainwater and the ore deposit/mining residues and which would control the geochemistry of the studied water lakes.

Keywords: Contamination, Heavy metals, Phreeqc, Modeling, Zeida mine

ID: 260963

Preparation of Ni^{2+} exchanged Zeolite NaY (FAU, Si/Al=2.56) for Efficient adsorption of phenol from Aqueous solutions

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Abstract: In this work, the removal of phenol from aqueous solutions onto synthesized zeolite NaY, and Ni modified zeolite NaY (FAU, Si/Al=2.56) were investigated. The excessively Ni^{2+} exchanged zeolite NaY (Si/Al=2.56) was prepared by ion-exchange method at 873 K and 5.8 pH. To know the amount of Ni in the modified zeolite, EDX elemental analysis was performed. The crystal structure of modified sample was determined by x-ray powder diffraction analysis using the Monte-Carlo approach by the hand of FOX program. The results reveal that, their unit-cell formula is $\left|Ni_{16}Na_8\right|[Si_{134}Al_{58}O_{384}]$ -FAU in the cubic space group $Fd\bar{3}m$. The physicochemical characterization of adsorbents was carried out by FI-TR, ATD/ATG, BET, and SEM. Afterwards, the results indicate that the phenol adsorption reached equilibrium within 2h at pH=4. Comparative study reveals that the Ni-NaY zeolite exhibited a high adsorption capacity than NaY zeolite. The experimental isotherm data were fitted by Frendlich, Langmuir models. The pseudo-first order, pseudo-second order, intra-particle diffusion models were used for the kinetic data and define the adsorption mechanism. It was determined from the correlation coefficient (R^2) that Freundlich model was more appropriate to depict the isotherm equilibrium adsorption approach and the phenol uptake process by the pseudo-second order expression on raw and modified zeolites. The adsorption study indicates that the adsorption of phenol is controlled by two steps and the thermodynamic studies reveal that the adsorption approach was exothermal and spontaneous.

Keywords: NaY zeolite, Ion-exchange, Characterization, Phenol, Adsorption.

ID: 245052

Numerical assessment of a Phase Change Material: Sizing the PCM's envelope with fluxmetrics measures

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Abstract The use of phase change materials (PCMs) in buildings has widely increased in recent years due to their high energy storage capacity compared to conventional construction materials, and their isothermal nature of the storage process. The main aim of this work is to define and size an envelope of Plexiglas containing PCM in order to perform a deep analysis of thermal energy storage of a brick incorporating microencapsulated PCM. The validity of the numerical code used is ensured by comparing our results with theoretical results. The effect of different parameters such as the height of the PCM sample and also the envelope thickness on the thermal behavior of the brick is investigated.

Keywords: Phase change material; Building construction; Energy storage; Fluxmetric experiments.

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ID: 252245

Optimisation of prostate balistic used in conformation radiotherapy with ELEKTA SYNERGY accelerator

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Abstract: Recently new technics of irradiation like IMRT (Intensity Modulation RadioTherapy) and VMAT (Volume Modulation Arc Therapy) are used for optimization of ballistics [1], but the conformational radiotherapy is the most used treatment for the prostate cancer. The 3D view of the ballistic is carried out by the TPS (Treatment Planning System). The delivered dose for the PTV (Planning Target Volume) and the critical dose deposed around the tumor are calculated by using the fast superposition algorithm [2]. The aim of this study is to compare two ballistics of the prostate treatment by using five and six beams. The difference appears in the dose delivered to the rectum. The TPS used is XIOcms with the linear accelerator ELEKTA SYNERGY PLATFORME

Keywords: Conformational radiotherapy, prostate ballistic, XIOcms, TPS.

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ID: 240512

Sodium zinc tris (dihydrogenphosphite) hydrate NaZn $(H_2PO_3)3.H_2O$

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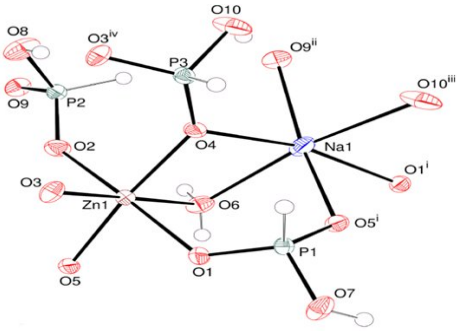
Abstract: The structure of $NaZn(H_2PO_3)3.H_2O$ belongs to the isotypic dihydrogenphosphite monohydrate series $NaM(H_2PO_3)3.H_2O$ (M = Mn, Co and Mg), with alternating NaO_6 and MgO_6 octahedra, crosslinked by H_2PO_3 pseudo-pyramids. In the mixed phosphate system NaO–MO–H_3PO_3, where M is a bivalent 3d metal, only three compounds are known, viz. $NaM(H_2PO_3)3.H_2O$, with M = Mn, Co, and Mg. In the present work, we describe the synthesis and crystal structure of the fourth member of the family, $NaZn(H_2PO_3)3.H_2O$, as part of our systematic investigation of this system. The crystal structure of the title compound can be described as a three-dimensional network made of [NaO_6] and [ZnO_6] octahedra sharing edges by way of O3…..O8 and O6…..O7 pairs, as shown in the figure below. Zn2+ is octahedrally coordinated by five O atoms of the phosphite anions and one oxygen (O7) of the water molecule. Average Zn—O is 2.086 Å, similar to that of 2.098 Å in $Zn(H_2PO_3)2.6H_2O$. The Na+ ion has a distorted octahedral coordination, with one Na—O distance longer than the others. The average Na–O, 2.466 Å, is similar to values found in isostructural phosphites: $NaCo(H_2PO_3)3.H_2O$ (2.451 Å), $NaMn(H_2PO_3)3.H_2O$ (2.442 Å). The bond-valence sum for sodium, 1.15 (ideal value = 1.00), indicates that its valence is fully saturated. An IR study has confirmed the presence of HPO_3 dihydrogenephosphite groups.



Details of bonding in the structure of $NaZn(H_2PO_3)3.H_2O$

Keywords: Inorganic-organic compounds; Chemical synthesis; IR; Raman; X-ray diffraction

ID: 246270

Processing and dielectric properties of multiwall carbon nanotubes filled polymers

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Abstract: The dielectric properties of particulate polymer composites are of great practical importance. It is known that the dielectric response can be varied over a wide range by an appropriate choice of the shape, size and the connectivity of the constituents in the polymeric matrix. In this study, we will explore the effect of the strong anisometry (length to diameter ratio) of the multi-wall carbon nanotube MWNT when they are dispersed in an epoxy matrix on the effective complex permittivity at low frequencies. The spectral data are examined as function of the nanotube content and the presence or not of a non-ionic surfactant (Tergitol NP7). The main results imply attractive interactions between the carbon nanotubes inducing the formation of the agglomerates that are observed by atomic force microscopy AFM, even in the presence of surfactant.

ID: 260974

Impact of Different Preheating Ambient on the Microstructural, Compositional and Optical Properties of Cu_2ZnSnS_4 (CZTS) Thin Films Deposited by Sol-Gel Technique

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Abstract: In this investigation, we report the effects of different preheating ambient on the microstructural, compositional and optical of sol-gel deposited CZTS thin films. CZTS precursors were deposited by spin-coating method, and subsequently preheated at 150ºC under different ambient (air, Ar and N2) prior to sulphurization process at 580ºC. Xray diffraction (XRD) pattern confirms the formation of crystalline CZTS compound with different crystallite sizes, meanwhile the Raman spectroscopy shows that the synthesized films are composed of stannite CZTS phase. CZTS films preheated in Ar and N_2 show better crystallinity, larger grains, suitable band gap and improved surface morphology compared to as-deposited and film preheated in air, which indicates that preheating ambient of Ar and N_2 are more suitable for fabrication of CZTS materials for solar cells application.

ID: 255347

The thermal fluctuations on the charge density wave dynamics in a one-dimensional conductor in the presence of the free-carriers: Numerical result

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Abstract: The effect of thermal fluctuations on the charge density wave dynamics properties of a one dimensional conductor in the presence of the free-carriers is studied numerically in the weak pinning limit. In good agreement with a recent experimental work on the CDW conductor K_3MoO_3, the addition of thermal fluctuations affects the CDW dynamics of the system. The results are discussed in the context of damping mechanisms of the collective mode arising from dissipative normal currents induced by dynamic deformations of the CDW and in the context of CDW dislocations.

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ID: 264042

Numerical simulation of the microclimate of an olive cuttings greenhouse

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Abstract: Olive cultivation is of great socio-economic importance in the Mediterranean basin. At the national level, it is the main cultivated fruit sector, covering an area of more than 1.07 million hectares. In order to meet national needs for olive seedlings and to ensure the development of this sector, several methods of multiplying these seedlings are used on a commercial scale. Semi-wood cuttings propagation in greenhouses is one of the most common techniques used to vegetative propagate woody plants. Environmental conditions outside and inside the greenhouse play a key role in this process. This research project is therefore aimed at developing a digital model to simulate the microclimate of an olive cuttings greenhouse. This study is based on experimental and numerical approaches: which aim to be applied to several situations, corresponding to the problems producers have to face: temperature and relative humidity management with a concern to reduce water and energy consumption. The numerical simulations will be carried out in 3D, the evolution of the climatic parameters will be validated on the basis of experimental data.

ID: 245401

Mechanical properties of titanium oxynitride thin films prepared for biomedical coatings

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Abstract: Titanium oxynitride (TiN_xO_y) films or thin films have recently attracted much attention because of their remarkable optical, electronic and mechanical properties. Sputtering is known to be a very effective method used to deposit uniform thin films and high-quality coatings. The work we have done is based on the elaboration of thin titanium oxynitride (TiON) layers by the PVD technique on stainless steel substrates by varying negative polarizations from 0 to -100Volts. SEM observations show that the surfaces of the TiON layers deposited at -50, -75 and -100 volts are uniform without relief. The crystallographic study is conducted using an X-ray diffractometer with which we find that the application of negative polarization at -100 and -75 V promotes the growth of the TiON phase to the detriment of anatase and rutile depending on the direction (111). The hardness measured by nanoindentation of TiON films increases with increasing substrate bias voltage. From the micro-scratch tests, we note two critical load values for all samples, crack initiation load and total delamination, while the coefficient of friction is stable at 0.58.

ID: 280000

Quantitative analysis and microstructural study of commercial clinkers using Rietveld analysis

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Abstract: A Full analysis of cement Portland requires the identification of all phases' mineralogy presents and microstructure estimation; since the hydraulic properties of cement are related to the mineralogy of phases, their microstructure presented in cement. The quantification of different cement components is a key step in determining the structure, properties and applications of a given material. Therefore, the study of the amount of crystalline phases present in a material represents an important parameter to control the microstructure and the correlation of the properties associated with the developed stage in the process. Rietveld analysis has been increased in construction domain and it considers as an effective tool for quantifying and identifying of cement Portland phases. This method makes it possible to qualify and quantify the material phases. The characterization of crystalline microstructure, regarding the density, atomic distribution and unit cell dimensions, contributes to the control of the manufacturing process.

Keywords: Cement Portland, microstructure, crystalline phases and Rietveld analysis.

ID: 280001

Nonresonant Raman spectroscopy analysis of bithiophene and quaterthiophene chains confined in graphene bilayer: A theoretical study

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Abstract: In this work, we focus on the confinement of polythiophene (nT) inserted between two sheets of graphene where the confined oligomer molecules and the bilayer graphene are bonded through van der Waals interactions. The nonresonant Raman lines of these hybrid nanomaterials were simulated using the spectral moment's method and the bond polarizability model. The optimum structures of thiophene molecules with graphene layers are derived from minimum energy calculations using a convenient Lennard-Jones expression of the van der Waals intermolecular potential. The changes of the Raman spectra as a function of the concentration of the confined oligomers are identified and the relative intensity ratio between a Raman mode of nT molecules and the G-band of graphene has been analyzed. This work gives benchmark theoretical data to interpret the experimental Raman spectra of graphene/conjugated oligomers hybrids.

Keywords: polythiophene, graphene, Raman spectra.

ID: 280002

Wall thikness effects on the infrared spectra of multi-walled carbon nanotubes

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Abstract: In this theoretical work, we investigate the infrared vibrational features of multi-walled carbon nanotubes (MCNTs). We calculate the polarized infrared spectra of multi-walled carbon nanotubes using the spectral moment's method. This original approach allows us to consider MCNTs with a large number of walls. We discuss the evolution of the low, intermediate and high wavenumber regions of these spectra as a function of the inner diameter and the size of MCNTs. Both the XX and ZZ polarisations are devoted. Our results provide benchmark theoretical data for understanding the experimental infrared spectra of MCNTs.

Keywords: MCNTs, infrared spectra.

ID: 255544

Lead-free materials for the storage of electrical energy

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Abstract: The goal of our research is to develop and characterize new lead-free materials for capacitors with high energy storage capacity. Capacitors that currently exist, allow to board high energy densities, but unfortunately, they are based on the lead derived from PZT (toxic materials.For this reason, we have proposed to direct our research to materials the same type of structure, but lead-free, inoentives for health, for the environment and in addition to an applied nature.To achieve our objective, our choice fell on lead-free ferroelectric materials of perovskite type structure, which They could normally have high dielectric permittivity, low dielectric losses, stable in frequency and temperature, and in addition, able to withstand a high electric field.These materials with high dielectric permittivity and low dielectric losses can be considered paraelectric state and at room temperature as potential candidates.

ID 243695

Elaboration, structural and vibrational studies of lacunar apatites of $APb_{3-x}Ca_xCd(PO_4)_3$ with A= Na, K and ($0 \leq x \leq 1$)

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Abstract: The major interest of researchers is the design and discovery of new materials that can be used in various fields of science and technology. Many people around the world have been interested in the study of lacunar apatite materials. The compounds of this family generally crystallize in a symmetrical hexagonal Centro structure and are reported in the literature in various applications, such as catalysts [1], ionic ion exchangers [2] and luminescent materials [3] , as well as optoelectronics [4] and biomaterials [5]. In the present work, we have designed the new phosphate material series $APb_{3-x}Ca_xCd(PO_4)_3$ with A= Na, K and ($0 \leq x \leq 1$) with a gap apatite structure of $P6_3/m$ space group with a number of motifs by crystalline mesh Z = 2. The crystal structures were studied using X-ray powder diffraction, Raman and IR spectroscopic techniques at room temperature. The refinement of crystalline structures was carried out using the Rietveld method using the FULLPROF software integrated in the WINPLOTR program [6]. The structure can be described as being constructed from $[PO_4]^{3-}$ tetrahedra and $Pb^{2+}/Ca^{2+}/Cd^{2+}$ ions found in six coordinate sites (6h positions) which delimit empty hexagonal tunnels, along the direction [001]. These tunnels are linked by the cations of the mixed sites (4f) which are half occupied by $Pb^{2+}/Ca^{2+}/Cd^{2+}$ and half by the Na^+ cations. The vibratory spectra of all the compositions are similar and show, as a function of the composition, the linear displacements towards the low frequencies following the substitutions of Pb^{2+} by Ca^{2+} of smaller radius. We have also studied the thermal stability of these materials using Gravimetric Thermal Analysis (GTA) and Differential Scanning Calorimetry (DSC) techniques.

ID: 238935

Rheological and physicochemical studies of new nanocrystalline apatite bioceramics developed by low temperature consolidation

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Abstract: The main objective of this work is to develop a new low-temperature ceramization technique for nanocrystalline apatite particles, whose structure is close to that of biological apatites. This technique makes it possible to obtain porous bioceramics having the advantage of being machined in rather complex forms, without altering the advantageous characteristics of the apatite phase similar to the mineral phase of the bone. The first part of this study deals with the synthesis and physico-chemical characterization of nanocrystalline and non-stoichiometric apatites. The second part is dedicated to the study of a new nanoparticle consolidation protocol using silicate solutions. The evaluation of the physicochemical properties of the obtained materials confirms that the low temperature ceramization takes place without structural modification of the initial apatitic phase, and retains the nanometric size of the particles. The third part evaluates the effect of the morphology of apatitic nanoparticles, synthesized by four different methods, on the mechanical properties of the consolidated materials.

Keywords: hydroxyapatite, nanoparticles, low temperature consolidation, ceramics.

ID: 245710

Performance of zeolite membranes type A and Y deposited on a clay support for the removal of heavy metals

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Abstract: Zeolitic membranes are used in several fields namely catalysis, petrochemistry, selective separation of gases ... The use of membranes in micro and ultrafiltration has been the subject of several research projects because of their good thermal stability, high surface area and high mechanical and chemical resistance. The objective of this work is the development and characterization of zeolite-based membranes deposited on local clay supports in the Meknes region for the purpose of the retention of heavy metals from industrial liquid effluents. for membrane were developed from clay of the region of Meknes, then characterized by different techniques (ATD, ATG, DSC, DRX, IR, BET) indeed the sintering of the raw supports was at 1000 ° C, ideal temperature for obtaining good performance media. Membrane deposits of zeolite A and Y were carried out by the hydrothermal method on the prepared supports, the application of the membranes developed in the filtration of liquid effluents containing heavy metals in particular: Pb^{2+}, Zn^{2+}, Cd^{2+} and Co^{2+} showed interesting results.

Keywords: Clay, Characterization, Support, Membrane, Zeolite, Filtration, Heavy Metals.

ID: 252861

Effects of metabolic syndrome on the oral cavity

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Abstract: Metabolic syndrome (MS) is a set of cardiovascular risk factors, including abdominal obesity, dyslipidemia, hypertension, insulin resistance, and proinflammatory and prothrombotic conditions. MS is considered pre-diabetes because it may not include hyperglycemia, but is usually associated with insulin resistance and a strong prediction of newly diagnosed Type 2 diabetes. The oral manifestations of MS are related to the severity of the associated metabolic disorders, and the dentist is often faced with a fairly complex clinical picture and therefore the obligation of multidisciplinary care of these patients. It is well established that diabetes is an independent risk factor for periodontitis. In addition, recent clinical studies have shown that MS is associated with an increased risk of periodontitis. In addition, studies have linked obesity to periodontitis suggesting that lipid metabolism disorders, present in both MS and obesity, may increase the risk of developing periodontitis. However, the underlying mechanisms linking MS and alveolar lysis remain largely unknown. Through this work we will define the metabolic syndrome, the mechanisms of alveolar bone resorption and establish the causal relationships described through a review of literature.

Keywords: metabolic syndrome, oral cavity, alveolar lysis.

ID: 244476

Development and characterization of ceramic tubular supports for the filtration of wastewater

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Abstract: This work describes the development and characterization of macroporous supports based on Moroccan clay. In this study, X-ray diffraction (XRD), X-ray fluorescence (XRF), infrared spectroscopy (IR), thermal ATG, and ATD analysis were used to characterize the clay minerals found in our samples. The FRX analysis results revealed high percentages of silica, aluminum, and moderate to low percentages of hematite, calcium oxide, and magnesia. The XRD analysis indicated that the above elements appeared in the form of quartz minerals, dolomite, calcite, kaolinite and illite. The tubular membrane supports of internal diameter 18 mm, thickness 24 mm and 3 mm were obtained using an extruder and then sintered at 1000 ° C. The characterization of these supports was measured by the flow rate using a tangential filtration pilot. And for that we realized a set of measures such as: the variation of flow as a function of the final sintering temperature (D = f (TF)), of the percentage of the added organic matter (D = f (% MO)), and finally according to transmembrane pressure (D = f (P)). The results obtained show that the flow rate increases with the percentage of organic matter, with the final sintering temperature and with the pressure. The flow rate is also very high (680 l / h.m^2 at a pressure of 2.5 bar) for the supports at 10% of the sintered organic material at 1000 ° C for 2 hours.

Keywords: Clay, Elaboration, Sintering, Membrane support, Flow.

ID: 263999

Phase diagrams for Yukawa fluids

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Abstract: Yukawa fluids are colloidal solutions consisting of solid nanoparticles suspended in a carrier liquid. The aim of this work is to determine, by a theoretical and numerical calculation, the conditions necessary and sufficient for the stabilization of the liquid phase in these colloidal solutions. We considered as theoretical model a monodisperse colloidal system containing spherical and mesoscopic molecules. The energy of the system consists of a kinetic energy and a potential energy of pairwise interaction. The latter consists of a repulsive part (repulsion of hard spheres), an attractive isotropic part of the Yukawa type. Using the generalized van der waals theory, we first calculated the Helmoltz free energy of this system. We have shown that this energy depends on two parameters: the range of interaction, and the amplitude of attraction. In a second time we calculated, according to these two parameters. The different phase diagrams and we have therefore studied and analyzed the different possible phase transitions. We have shown that the phase diagram depends on the scope of the interaction and that the liquid phase is always stable if the solid phase is not introduced.

Keywords: Free Energy, Phase Transition, Critical Point.

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ID: 244828

Development and characterization of three clay varieties from different regions of Algeria

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Abstract: This work aims to characterize and valorize three varieties of Algerian clay materials coming from three different regions (West, East and West Center), which can be used in the field of the elimination of pollutants such as dyes. The values of the cation exchange capacity CEC and the specific surface show that the three clays present a mixture between Illite and Kaolinite varieties, and the results obtained by FTIR and X-ray analysis confirm this heterogeneity. The raw materials contain a mixture of clay compound (aluminosilicates) and non-clay compound (quartz and calcium carbonate). Scanning electron microscopy analysis showed that most clay particles are globally flake or slat. The predominant constituents are silicon, Aluminum and Calcium. From an economic point of view, these materials may well be used as adsorbents of certain pollutants.

ID: 245018

Overview of the advantages of laminated perovskite molecular composites and their photovoltaic properties in the field of conversion of photon energy into electrical energy

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Abstract: The development of new non-polluting energy sources is retained as an essential strategy to meet these energy and environmental challenges, whatever efforts the national and international community may make in controlling energy demand. An alternative is the conversion of solar energy to produce electrical energy via photovoltaic cells.

Perovskites cells have marked the world of photovoltaics, however in most studies that have been conducted in this direction, problems of toxicity of the materials used (Ti, Si, ... etc.), and cost of realization have been met. In order to reduce these difficulties, laminated perovskite molecular composites of general formula $[R\text{-}NH_3]_2MX_4$ or $[NH_3\text{-}R\text{-}NH_3]MX_4$ have the ability to combine the properties of a subnetwork at the molecular scale organic to that of an inorganic subnetwork.

The diversity of structure and dimensionality of these composites motivated us to initiate several research paths in order to improve the electro-optical behavior of these molecular composites.

Previous studies that we conducted on materials of type $[R\text{-}NH_3]_2MC_{14}$ (M = Cd, Cu and Hg; R is an amino acid) have a diversity of very interesting structural properties, in particular the influence of the nature of the metal on the interlayer distance. This distance decreases from Cd to Hg through Cu.

In this work we will focus on the study of the band structure as well as the calculation of electronic state densities of its systems. Our goal is the determination of the corresponding energy gap.

Keywords: Perovskite, crystalline structure, density of states, energy gap, photovoltaic, solar-electric energy

ID: 242600

Effect of cooling rate and the addition of refining on the microstructure of Al-Si alloys

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Abstract: The present work aims to study the influence of grain refiner addition and the effect of mold temperature for some Al-Si foundry alloys. Grain refining and modification are two common treatments liquid metal applied to Al-Si alloys. This treatment only concerns the primary phase of aluminum silicon alloys. It consists in adding a grain refiner in small quantity in the liquid bath before the casting. The grain size depends on the state of refining of the bath. That is to say the more germs will be numerous, the more the number of crystals will be high and the latter will be fine. Practically, germs consist of titanium and boron compounds. We will be interested in hypoeutectic alloys the results and analyzes that we have seen and which are: The casting at a relatively high temperature has an effect on the structure of the alloy. It leads to an increase in the size of the dendrites. The addition of the grain refiner increases the germination and growth temperatures of the -Al dendritic phase and eliminates the phenomenon of supercooling. The total time of solidification and the time of aluminum-silicon eutectic solidification in AlSi9 alloy was decreased when titanium was added. Furthermore, it has been shown that the thermal analysis does not take into account the variation of the initial temperature of the mold. According to the results obtained, the decrease of the mold temperature from 700°C to 500°C is observed, leads to the decrease of the solidification time which implies the decrease of the size of the dendrites. And also the increase in mold temperature leads to a uniform distribution of dendrites