2nd International Conference on Nanosciences & Nanotechnology

ICNN'23

19-21 June 2023
Hôtel MauriCenter
Nouakchott, Mauritania

Abstracts of Invited Lecturers and Abstracts of Oral Communications
Program and List of Participants

ICNN 2023 : Short Program

Lundi 19 Juin 2023	
08h30-09h00	**Inscription des participants**
09h00-09h30	**Ouverture officielle**
09h30-10h00	**Pause café**
10h00-10h40	**Conférence plénière 1: Mohammed Belaiche** Nanoscience et Nanotechnologie perspective pour le développementscientifique et technologique
10h40-11h20	**Conférence plénière 2: Mohamed Henini** Development of advanced semiconductor materials and devices for next generation photovoltaics: Opportunities and challenges
11h20-11h30	**OC 1: Khalidou Ba** Elaboration by conventional melt quench and sol gel method of new glasses with in the system $xTiO_{2-y}NiO\text{-}zP_2O_5$ with high chemical durability
11h30-11h40	**OC 2 : Aichata Kane** Synthèse des nanoparticules de ZnO et ZnO dopé au Co et Niet l'etude de leur prorpiétés d'adsorption
11h40-11h50	**Discussion sur les deux communications**
11h50-12h30	**Conférence plénière 3 : Lassaad EL MIR** Innovative technological applications based on nanoscaled materials
12h30-13h10	**Conférence plénière 4 : Ousmane Ly** Magnetic dynamics driven high harmonic generation in spin orbit-coupled systems
13h10-14h30	**Déjeuner**
14h30-15h10	**Conférence plénière 5 : Noureddine Raouafi** Nanomaterials-based biosensors for the monitoring of (Bio)Markers for Environment, Food Safety and Healthcare
15h10-15h50	**Conférence plénière 6 : Hamada Boudjema** Synthèse, fonctionnalisation de nanotubes de carbone et leur application
15h50-16h20	**Pause café**
16h20-16h30	**OC 3 : Khaled Ebeid** Synthesis and characterization of ME nanoparticles (M = Cd, Hg ou Zn ; E = S ou Se) capped with different phosphine oxides
16h30-16h40	**OC 4 : Mohamed Abdellahi AMI** DFT/TD-DFT investigation of the structural and spectral properties of nimetazepam: a psychoactive drug
16h40-16h50	**OC 5: Kebbada Salihi** Optimisation des méthodes et techniques de l'orpaillage en Mauritanie sur la base de l'énergie renouvelable
16h40-16h50	**Discussion sur les deux communication**
Mardi 20 Juin 2023	
09h00-09h40	**Conférence plénière 7 : Abaidia Siddik El HAK** Le développement des nanomatériaux dans le domaine de l'efficacité énergétique, l'écologie et le confort humain: Cas des habitations modernes
09h40-10h20	**Conférence plénière 8 : M. A. Sanhoury** Synthesis and characterization of metal chalcogenide nanoparticles for photovoltaics
10h20-10h30	**OC 6 : Cheikh Mohamed Samba Vall** Comparative study of the electrical properties of schottky diodes based on ZnT:Ni and CuO:Ni thin films
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11h00-11h40	**Conférence plénière 9 : Ahmadou Wagué** Les défis de l'énergie et de la transition énergétique et écologique pour un développement durable en Afrique
11h40-12h20	**Conférence plénière 10 : R. El Bouayadi** A new approach for the chemical and morphological analysis of nanoparticles based on HAADF-STEM image simulations at nanometric scale
12h20-12h30	**OC 8: Fatimetou Ebnou** Préparation des nanoparticules du type HgSe capées par R_3PO
12h30-13h40	**OC 9 : Elfahem Sakher** Studying the effect of high-energy milling on the morphological, structural, and magnetic properties of $Ni_{50}Ti_{50}$ powder and revealing the new phenomenon of particle folding during the milling process
13h40-13h50	**Discussion sur les deux communication**
13h50-15h20	**Pause déjeuner**
15h20-16h00	**Conférence plénière 11 : Mohamed Abdellah LemineKerim** Magnetic nanoparticles for biomedical and spintronics applications
16h00-16h10	**OC 10 : Ely Cheikh S'Id** Fabrication of ion-exchange ultrafiltration membranes for water treatment I. Semi-interpenetrating polymer networks of polysulfone and poly(acrylic acid)
16h10-16h20	**OC 11: Sidi Ahmed Bowba** Structural behaviors of Mg-Ti co-doped zinc oxide
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Mercredi 21 Juin 2023	
	Conférences Online
09h00-09h40	**Conférence plénière 12: Teyeb Ould Ely** Scaling-up nanomaterials for energy storage applications
09h40-10h20	**Conférence plénière 13: Mazin A. Khasawneh** Josephson junctions using a strong ferromagnetic interlayer and spin triplet superconductivity
10h20-10h50	**Pause café**
10h50-11h30	**Conférence plénière 14: M. Maaza** On novel smart nanomaterials for heat management & energy saving
11h30-12h10	**Conférence plénière 15: Irshad Hussain** Functional nanomaterials – Tuning the size and surface chemistry for applications in renewable energy technologies, biomedical and environmental sciences
12h10-12h50	**Table ronde**
12h50-13h20	**Clôture**
13h20	**Déjeuner et départ**

Avant-propos

Au nom du comité d'organisation et à mon nom, nous sommes heureux de vous accueillir à la seconde édition de la Conférence Internationale sur les nanosciences et nanotechnologies à Nouakchott en Mauritanie

ICNN 2023 se veut, à l'instar de la première version, riche en nouveautés dans le domaine du nano lié à la chimie. Quinze conférences plénières, dont 12 présentielles et 4 par visio-conférence ; ainsi que 11 communications orales seront présentées par d'éminents professeurs et de scientifiques en provenance de 09 pays (Sénégal, Maroc, Algérie, Tunisie, Arabie Saoudite, Pakistan, Grande Bretagne, U.S.A. et bien sûr la Mauritanie).

Nous espérons que ICNN 2023 soit aussi un espace passionnant pour discuter des dernières avancées de la recherche en nanosciences et nanotechnologies ; de même que nous souhaitons un séjour agréable pour nos hôtes.

J'adresse mes remerciements les plus sincères à tous les conférenciers et les participants qui ont accepté de prendre part à l'ICNN 2023.

Enfin, je ne saurais terminer ces paroles sans remercier également l'Agence Nationale de la Recherche Scientifique et de l'Innovation (ANRSI), l'Organisation Arabe pour l'Education, la Culture et les Sciences ainsi que la Société Chimique de Mauritanie qui ont contribué à la tenue de cette manifestation, pour leur soutien logistique et moral, à côté de leur aide à la diffusion de l'information.

Mohamed Said MINNIH

Doyen de la Faculté des Sciences et Techniques
Université de Nouakchott

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Mohamed Abderrahmane Sanhoury

Mohamed M'Hamed

Mohamed Mokhtar Dah

Mohamed Mohamed Lemine Yacoubi

Programme de l'ICNN-2023

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10h40-11h20	**Conférence plénière 2: Mohamed Henini** *School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD, UK* **Development of advanced semiconductor materials and devices for next generation photovoltaics: Opportunities and challenges**	Président : Med Abdallahi Kerim
11h20-11h30	**OC 1: Khalidou Ba** *FST, UN; Nouakchott, Mauritanie* **Elaboration by conventional melt quench and sol gel method of new glasses with in the system $xTiO_{2-y}NiO\text{-}zP_2O_5$ with high chemical durability**	
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11h50-12h30	**Conférence plénière 3 : Lassaad EL MIR** *Laboratory of Physics of Materials and Nanomaterials Applied at Environment (LaPhyMNE), Gabes University, Faculty of Sciences in Gabes, Tunisia.* **Innovative technological applications based on nanoscaled materials**	Président Chamekh Mbarek
12h30-13h10	**Conférence plénière 4 : Ousmane Ly** *University of Nouakchott* **Magnetic dynamics driven high harmonic generation in spin orbit-coupled systems**	
13h10-14h30	**Déjeuner**	

14h30-15h10	**Conférence plénière 5 : <u>Noureddine Raouafi</u>** *University of Tunis El Manar* **Nanomaterials-based biosensors for the monitoring of (Bio)Markers for Environment, Food Safety and Healthcare**	Président : M A Sanhoury
15h10-15h50	**Conférence plénière 6 : <u>Hamada Boudjema</u>** *Université M'Hamed Bougara Boumerdes, Algérie* **Synthèse, fonctionnalisation de nanotubes de carbone et leur application**	
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16h30-16h40	**OC 4 : Mohamed Abdellahi AMI** *Faculté des Sciences de Tunis, Universitaire Tunis- El Manar, Tunis, Tunisie* **DFT/TD-DFT investigation of the structural and spectral properties of nimetazepam: a psychoactive drug**	
16h40-16h50	**OC 5: Kebbada Salihi** *Laboratoire de Recherche Appliquée, FST, Université de Nouakchott, Mauritanie* **Optimisation des méthodes et techniques de l'orpaillage en Mauritanie sur la base de l'énergie renouvelable**	
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09h40-10h20	**Conférence plénière 8 : <u>M. A. Sanhoury</u>** *Materials Chemistry Research Uni, Chemistry Departmenet, Facukty of Sciences and Techniques, University of Nouakchott, Nouakchott, Mauritania* **Synthesis and characterization of metal chalcogenide nanoparticles for photovoltaics**	Président : N. Raouafi

10h20-10h30	**OC 6 : Cheikh Mohamed Samba Vall** *Faculty of Sciences Semlalia Marrakech, Morocco* **Comparative study of the electrical properties of schottky diodes based on ZnT:Ni and CuO:Ni thin films**	
10h30-10h40	**OC 7 : Hadjira RAFAI** *Faculty of Science and Technology, University of Adrar, Algeria* **Analyzing the morphology of nanocrystalline nickel-based materials using comparison between image segmentation and image**	
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11h40-12h20	**Conférence plénière 10 : R. El Bouayadi** *Université Mohammed V, B.P. 1014, Rabat, Morocco* **A new approach for the chemical and morphological analysis of nanoparticles based on HAADF-STEM image simulations at nanometric scale**	Président : Ahmed El Mouna
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16h00-16h10	**OC 10 : Ely Cheikh S'Id** *FST, University of Nouakchott, Mauritania.* **Fabrication of ion-exchange ultrafiltration membranes for water treatment I. Semi-interpenetrating polymer networks of polysulfone and poly(acrylic acid)**	
16h10-16h20	**OC 11: Sidi Ahmed Bowba** *Physics department, Faculty of sciences, Tunis El-Manar University, Tunis, Tunisia* **Structural behaviors of Mg-Ti co-doped zinc oxide**	
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09h40-10h20	**Conférence plénière 13: <u>Mazin A. Khasawneh</u>** *Physics Department, Shenandoah University, US9* **Josephson junctions using a strong ferromagnetic interlayer and spin triplet superconductivity**
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Abstracts of Lectures

Nanoscience et Nanotechnologie perspective pour le développement scientifique et technologique

Mohammed Belaiche

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Abstract

De nos jours, la compréhension fondamentale des processus physiques dans les ferrites et l'importance qu'ils revêtent dans de nombreux dispositifs technologiques ont suscité un intérêt considérable. Des progrès notables ont été réalisés dans l'exploration de l'effet optimisé des particules de taille nanométrique sur diverses propriétés électriques et magnétiques. Comparativement aux ferrites à l'état massif, une taille plus petite des particules peut apporter des variations novatrices aux propriétés des ferrites. Ainsi, une grande variété d'applications est envisageable, allant du stockage à haute densité jusqu'aux dispositifs énergétiques tels que les inducteurs, les transformateurs de puissance et les télécommunications. Soulignons que, les caractéristiques magnétiques des matériaux sont fortement affectées lorsque la taille des particules est fortement réduite et les effets de relaxation superparamagnétique sont dus à l'influence de l'énergie thermique sur l'orientation du moment magnétique à l'échelle nanométrique. En outre, l'anisotropie magnétocristalline est le paramètre vital qui influence l'orientation du moment magnétique dans les ferrites contrôlant le superparamagnétisme dans les nanodomaines. De nombreuses nouvelles applications ont vu le jour, impliquant des ferrites dans la gamme superparamagnétique, principalement dans le domaine biomédical, comme l'administration ciblée de médicaments, l'hyperthermie, le traitement des cellules tumorales, les agents de contraste IRM et la bio-imagerie. Notre conférence donnera un large aperçu sur tous ces applications et sur la valorisation des minerais marocains par le biais de la synthèse de ces nanoparticules de ferrites.

Development of Advanced Semiconductor Materials and Devices For Next Generation Photovoltaics: Opportunities And Challenges

Mohamed Henini

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Abstract

One of the most important devices in optoelectronics is the semiconductor laser because of its high quantum efficiency; its capabilities and the range of applications that have grown tremendously over recent years. The capability to fabricate novel materials on an atomic scale by using sophisticated epitaxial crystal growth techniques has contributed tremendously to the success of semiconductor quantum well (QW) lasers. The QW laser performances can be improved further by implementing new structures containing quantum dots (QDs).

QDs can be fabricated using several techniques including lithography-based technologies. However, the self-organisation process shows great potential for the fabrication of three-dimensional structures, which are formed by the Stranski-Krastanov heteroepitaxy growth mode using lattice-mismatched systems. The advantages of this fabrication technique where the QDs are grown in-situ include a homogeneous surface morphology and prevention of defects. In addition, there are no further processes required such as advanced lithography and chemical etching.

The low cost, high performance and high reliability of the QW laser contributed to its mass production within very few years of its invention. However, theoretical calculations expect that the QD lasers to have superior properties compared to those of conventional QW lasers. These include higher characteristic temperature T0, lower threshold (Ith) currents and narrower linewidth. In the last few years tremendous progress has been made in improving T0 and Tth of QD lasers. Recently, they have overcome the performance of the best QW lasers in terms for example of threshold current, which is one of the figures of merit of this key device. This implies that the QD lasers could potentially revolutionise the optical electronics industry and make them considerably energy efficient and therefore much more attractive from a commercial perspective.

In this talk, I will discuss the properties of self-assembled QDs and the progress in the development of QD lasers.

Innovativetechnological applicationsbased on nanoscaled materials

Lassaad EL MIR

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Abstract:
Advances in nanotechnology are strongly linked to other technologies, many of which have received greater attention. Nanotechnology will have applications for many technological domains such as additive manufacturing (3D printing), gene editing, artificial intelligence, energy, spacecraft, quantum computing, and water. However, the unique properties and processes of nanotechnology deserve greater attention. Narrow policies that treat nano-applications on a narrow basis will not address the unique characteristics and challenges of nanotechnology itself. In fact, systems based on nanoscaled materials have recently received much attention due to their interesting optical, magnetic, and electrical properties. Confining one or more dimensions to the nanometer scale, the physical properties of such materials exhibit dramatic changes. Those materials present intermediate behavior between bulk crystals and isolated molecules. In the nanoparticles, there is a strong spatial delocalization of valence electrons, and therefore a small crystallite must grow fairly large to achieve the limiting bulk electronic structure. The intermediate-size clusters can have unique properties, characteristic of neither the molecule nor solid-state limits. The main objective of this conference is to present our laboratory results in the field of synthesis and characterization of nanoparticles, nanocomposites, and thin films. These materials are used in a variety of technological applications like energy storage, gas sensing, hyperthermia, solar cells, optoelectronic devices, and electronic components.

Magnetic dynamics driven high harmonic generation in spin orbit-coupled systems

Ousmane Ly

University of Nouakchott

It has been predicted 20 years ago [1], that when a normal metal is subjected to magnetic dynamics, a pure spin current is pumped toward the adjacent paramagnet. The resulting pumped carrier dynamics is found to operate at the same frequency underlying the magnetic drive. In the actual work, we predict that in the presence of spin-orbit coupling, the interplay between the s-d exchange coupling and the relativistic interaction leads to the emergence of ultrahigh harmonics in the carrier pumping [2, 3]. We demonstrate that an enhancement of the initial dynamics by orders of magnitude can be achieved upon properly tuning the parameters of the drive and the spin-orbit strength. Using the non-equilibrium quantum transport platform TKwant [4], we examine the scaling laws of the proposed effect and present further theoretical insights on the proposed effect. Further, we predict that the effect seems to be universal and could be triggered in systems hosting noncollinear topological textures or magnetic impurities [5]. In the actual effect, magnetism is proposed as an alternative to light for the purpose of exciting highly nonlinear emission in solid state systems. Our proposal opens up an interesting perspective in utilizing adiabatic magnetic precession to trigger ultrafast carrier dynamics deep in the THz regime and beyond.

[1] Phys. Rev. Letters **88**, 117601 (2002)
[2] O. Ly and A. Manchon Phys. Rev. B **105**, L180415 (2022)
[3] O. Ly, Arxiv:2304.02619 (2023)
[4] T. Kloss et al., New. J. Phys. **23**, 023025 (2021)
[5] J. Phys.: Condens. Matter **35**, 125802 (2023)

Nanomaterials-based biosensors for the monitoring of (Bio)Markers for Environment, Food Safety and Healthcare

Prof. Noureddine Raouafi

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Abstract

In recent years, the advancement of science has led to a greater awareness among people about the importance of their health and the impact of their surroundings on their well-being. As a result, there has been a growing demand for tools and technologies that can monitor and measure key aspects of human health and environmental quality. One such technology that has emerged as a powerful tool for this purpose is biosensors. Biosensors offer a versatile and highly sensitive means of detecting a wide range of markers and biomarkers that can provide insight into disease, environmental pollution, and food safety. In this talk, I will provide an overview of our recent contributions to the field of biosensors, with a particular focus on the development of devices capable of detecting proteins, DNA, and RNA as biomarkers for disease, as well as pesticides, pharmaceuticals, and metallic cations, which represent a growing class of emergent pollutants in the environment and can contaminate food sources. Our work in this area has been driven by a commitment to advancing the state of the art in biosensor technology and addressing key challenges in the field, such as improving sensitivity, selectivity, and reproducibility. We believe that biosensors have tremendous potential to revolutionize the way we monitor and manage human health and environmental quality, and we look forward to sharing our latest findings and insights with you in this talk.

Synthèse, fonctionnalisation de nanotubes de carbone et leur application

Professeur Hamada Boudjema

Doyen de la Faculté des Hydrocarbures et de la Chimie
Université M'Hamed Bougara Boumerdes, Algérie

Abstract

Les nanomatériaux occupent une place importante dans plusieurs secteurs. Au vu de leur propriétés exceptionnelles les nanotubes de carbone trouvent des applications diverses et variées et ce en fonction de leur fonctionnalisation. Les dimensions nanométriques des CNTs, leur importantes surfaces spécifiques et leurs propriétés mécaniques, électriques, chimiques et thermiques exceptionnelles, telles la résistance mécanique, la flexibilité, la conductivité thermique et électrique… en font les candidats idéaux pour diverses applications, telle la synthèse de nouveaux matériaux composites à utilisation médicale ou autres, le stockage d'énergie, l'élaboration de capteurs chimiques et biologiques, la conception de nouvelles générations d'écrans plats pour téléviseurs, tablettes et téléphones portables. Dans la présente communication seront exposés les voies et moyens de synthèse (par voie pyrolytique) de nanotubes de carbone à partir de résidus pétroliers, leur fonctionnalisation et quelques domaines d'application à savoir: comme adsorbant pour la réduction du souffre dans les carburants, comme additif aux huiles lubrifiantes et en qualité de senseurs chimiques pour la détection de composés toxiques.

Mots clés: nanotubes de carbone, fonctionnalisation, caractérisation, application

Le développement des nanomatériaux dans le domaine de l'efficacité énergétique, l'écologie et le confort humain: Cas des habitations modernes

Abaidia Siddik El HAK

Université M'Hamed Bougara Boumerdes

Synthesis and characterization of metal chalcogenide nanoparticles for photovoltaics

Med Abderrahmane Sanhoury[a,b]

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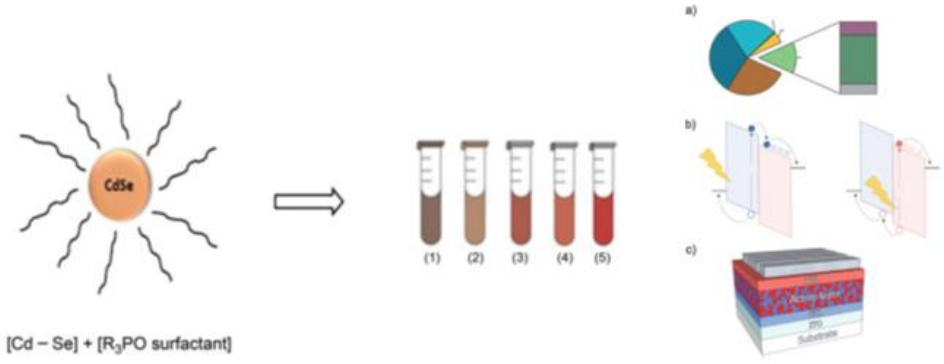
[b] *Lab of Structural Organic Chemistry, Synthesis and Physicochemical Studies, Department of Chemistry, Faculty of Sciences of Tunis, University of Tunis El Manar, Tunis, Tunisia*

In this work, the synthesis and characterization of nanoparticles (NPs), especially metal chalcogenide NPs, as well as their use in photovoltaic devices, including hybrid organic–inorganic solar cells are described. Such devices are known as potential candidates for low-cost and efficient solar energy conversion and belong to the so-called third-generation solar cells. The different methods of NP synthesis and their development for application in more efficient solar cell devices such as those involving perovskite NPs are also presented. Despite the fact that incorporation of oxides and metal nanoparticles has also been successfully achieved in this class of photovoltaic devices, we choose to focus here on metal chalcogenide NPs in light of their appealing optical and electronic properties. We describe herein a comprehensive detail of the synthesis and the combination of such nanoparticles with other inorganic materials (all inorganic) or with polymer matrices (hybrid systems) and their characterization techniques. Recent developments on more efficient photovoltaic devices and later strategies for surface chemistry modification and *in situ* NP synthesis are compared. This will include engineering of structure (e.g., energy-band alignment) and materials (e.g., selection and optimization of middle-layer materials).



Keywords : Nanoparticles · Metal chalcogenide · Ligand exchange · Photovoltaics Solar cells, TEM, PL

LES DEFIS DE L'ENERGIE ET DE LA TRANSITION ENERGETIQUE ET ECOLOGIQUE POUR UN DEVELOPPEMENT DURABLE EN AFRIQUE

Prof. Ahmadou Wagué

Université Cheikh Anta Diop
Dakar Sénégal

RESUME : L'énergie Énergies et les transitions énergétique et écologique constituent à l'heure actuelle de grands défis à travers le monde entier, particulièrement en Afrique où les effets du réchauffement climatique sont entrain de causer des dégâts énormes dans les écosystèmes environnementaux et agricoles. En plus la guerre en Ukraine est entrain de démonter l'importance pour l'Afrique de relever les défis de la souveraineté énergétique et alimentaire en Afrique par une approche appropriée de la gestion des sources énergétiques énormes du continent. Ici on aborde les questions de la gestion des sources d'énergie en Afrique et leurs implications géopolitiques et géostratégique pour un développement durable en Afrique. Nous insistons particulièrement sur l'importance du développement des énergies renouvelables et surtout l'énergie solaire où le développement des nanotechnologies dans la fabrications de nouvelles cellules photovoltaïques pourraient apporter des changements positifs considérables pour l'accès à l'énergie pour tous en Afrique.

SUMMARY: Energy and ecological transitions are currently major challenges throughout the world, particularly in Africa where the effects of global warming are causing enormous damage to environmental and agricultural ecosystems. In addition, the war in Ukraine is demonstrating the importance for Africa to address the challenges of energy and food sovereignty in Africa through an appropriate approach to the management of the continent's huge energy sources. Here we address the issues of energy source management in Africa and their geopolitical and geostrategic implications for sustainable development in Africa. We particularly insist on the importance of the development of renewable energies and especially solar energy where the development of nanotechnologies in the manufacture of new photovoltaic cells could bring considerable positive changes for the access to energy for all in Africa.

A new approach for the chemical and morphological analysis of nanoparticles based on HAADF-STEM image simulations at nanometric scale

R. El Bouayadi [1] and M. Benaissa [2], Ph. Vennégues [3]

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A new method based on the simulation of HAADF-STEM images at a nanometric scale is proposed to characterize the chemical composition and geometrical shape of low-dimensional systems. Since the intensity in HAADF images is roughly proportional to the average atomic number Z, this new technique, and by comparing simulation and experimental results, gives interesting insights of individual nano-particles' chemical composition and on its macroscale three-dimensional shape. The application of the HAADF technique in various fields of materials science has shown great potential as a fast and efficient tool for chemical and morphological analysis. HAADF was first applied on particles with simple geometric shape and homogeneous chemical composition: nitride precipitates in a ferrite matrix were chosen for the first analysis. To further simplify the study, we selected a sample that contains a single cubic-shaped particle of titanium nitride TiN and a single aluminum nitride particle AlN with a spherical shape. In this study, simulation results were found to be in good agreement with experimental results. To validate this method, we have analyzed particles that have a more complicated geometry. We have investigated the metal precipitation on defect induced by helium ions implantation in silicon. Results showed that helium implantation, followed by thermal annealing leads to extended defects formations, such as dislocations and nanometer-sized cavities in single-crystalline silicon. The created defects can be used as very efficient gettering sites of metallic impurities during device processing. It was suggested that empty cavities have a truncated octahedral shape, but the shape of a metal-filled cavity has never been subjected to a rigorous examination. The developed program provided detailed information about the filled-cavity morphology and the chemical composition of the precipitated phase within the voids. The technique was then used to check the inhomogeneous chemical distribution in complex quantum structures such as InAs/AlAs and GaN/AlGaN quantum dots.

Magnetic nanoparticles for biomedical and spintronics applications

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Abstract

Magnetic nanoparticles (MNPs)are promising nanomaterials for several applications ranging from photocatalysis, photonic, magnetic storage and electronic devices to nanomedecine. Among a variety of magnetic materials, iron oxides NP, is one the most promising and widely used due to their excellent magnetic and high chemical stability. For example, the presence of vacancies sites in maghemite (γ-Fe_2O_3 (≈12% Fe vacancy) compared to magnetite (Fe_3O_4)NPs, where no vacancy sites, imply that that saturation, Curie temperature and, subsequently the heating ability of the γ-Fe_2O_3 NPs can be tuned for specific applications such as magnetic hyperthermia by partial substitution of iron ions by alkaline earth, transition metals or nonmagnetic elements. Other types of magnetic nanostructure (dilute magnetic semiconductors (DMS)) have attracted a great attention due to their potential applications in spin-based electronics applications (spintronics).

In this talk, I will give few examples of our recent results related to the use of magnetic nanoparticles for cancer treatment, the development of dilute magnetic semiconductors nanostructures and preliminary results obtained on Mauritanoan'siron ore (Magnetite and hematite).

Scaling-up Nanomaterials for Energy Storage Applications

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Abstract

The current conflict between Russia and Ukraine and the looming global warming crisis impose rapid electrification of our transportation sectors. As a result, various renewable energies are under intense investigation (wind, solar, batteries, etc.). Lithium-ion batteries, in particular, are receiving a great deal of interest due to their high power and high capacity performances. However, their high cost, slow charging, low safety, and poor efficiency still hamper their large-scale adoption. Furthermore, the raw materials supply chain is strained due to the universal shift to electric transportation. We will discuss our recent attempts to scale-up energy-relevant nanomaterials using our homemade scale-up reactors. Furthermore, we will address the challenges facing the electrification of the worldwide transportation system.

Josephson junctions using a strong ferromagnetic interlayer and spin triplet superconductivity

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Abstract

We studied the interplay between superconductivity and ferromagnetism in hybrid S/F samples by fabricating Josephson junctions containing magnetic materials –S/F/S Josephson junctions for short. Hybrid systems consisting of superconducting (S) and ferromagnetic (F) materials brought into intimate contact with each other exhibit a wide range of properties not present in either S or F materials alone.

We have found strong evidence for a new type of superconducting pair correlations known as Long Range Triplet Component that exists in S/F hybrid structures in the presence of magnetic inhomogeneity at the S/F interface. Because of their spin-triplet character, these correlations are not suppressed by the exchange field of the ferromagnet; hence they penetrate deeply into F materials.

We have discovered strong evidence for spin-triplet correlations in Nb/"X"/Co/"X"/Nb Josephson junctions, where the "X" layers (PdNi or CuNi alloy) introduce the needed magnetic inhomogeneity

On novel smart nanomaterials for heat management & Energy saving

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Abstract:
As per today, ~55% of the world's population lives in urban areas. It is projected that it would reach ~2.5 billion by 2050, with ~90% of this increase in Asia & Africa. With such an of urban population and climate change increase of the average seasonal emperature, air-conditioning demand in urban areas is expected to skyrocket. The global stock of air conditioners in buildings & automotives sectors is expected to grow up to ~5.6 billion by 2050 from the current pool of ~1.6 billion today. The International Energy Agency (IEA)'s previsions [1] for the global energy demand in airconditioning is expected to triple by 2050, entailing the usage of a significant electricity supply, equivalent to the combined current electricity capacity of the USA, EU & Japan by today standards. Consequentially, sustainable technologies are urgently required to minimize the corresponding energy pressure as well as the related CO2 footprint.
Chromogenics and/or radiative cooling coatings in addition of advanced coolant fluidsare potential genuine solutions [1-4].Within this contribution, recent emboldening results of V2O5/V/V2O5 thermochromic coatings with a significant NIR-IR optical modulation will be presented. Likewise, biomimicry based paints for radiative coolings applications will be discussed. In addition, a mass production adapted novel engineering methodology for fabrication of nanofluids as a novel family of coolant & heat transfer fluids applications will be presented.

Functional Nanomaterials – Tuning the Size and Surface Chemistry for Applications in Renewable Energy Technologies, Biomedical and Environmental Sciences

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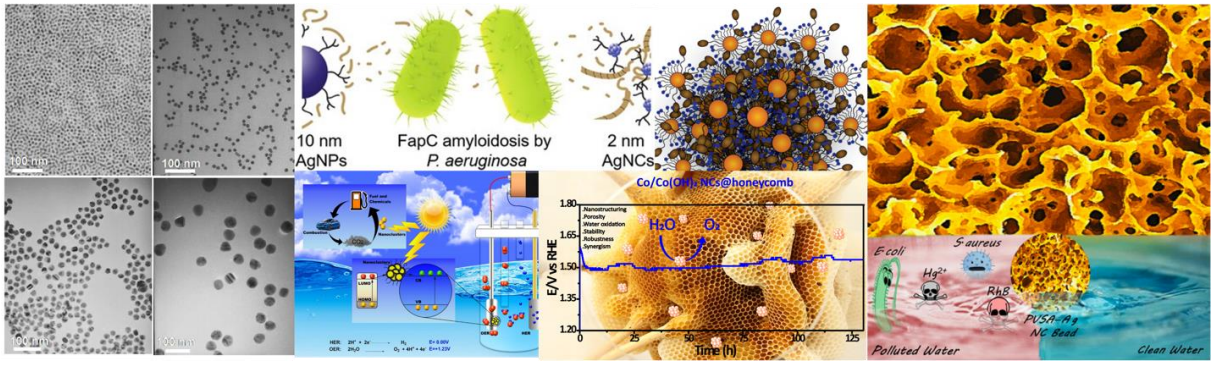
Abstract. The unique chemical and physical properties of nanoscale materials have triggered much scientific interest to explore their potential applications in biomedical sciences, energy technologies, agriculture, environment, catalysis and industry etc. The chemical and physical properties of metal/ metal oxide nanoparticles can generally be tuned by controlling their size, shape and surface chemistry. In this regard, we have developed several reproducible protocols based on chemical reduction and precipitation approach to prepare functionalized metal/metal oxide nanoparticles from subnanometer to over 100 nm in aqueous/organic media with a decent control over their size, shape, and surface chemistry. Many of these metal nanoparticles have been used as building blocks to design/synthesize new nanostructured materials with tunable nanoscale features using template-based and template-less strategies. The functionalized metal/metal oxide nanoparticles/nanoclusters possess interesting optical, recognition and catalytic/bio-catalytic properties and currently we are focusing on the applications of these nanoparticles and nanocomposites in biomedical sciences (i.e., bio-sensing especially bacterial detection, bio-imaging, drug delivery, killing drug resistant bacteria), environmental remediation (detection and removal of organic/inorganic pollutants from water, CO oxidation, and CO_2 capture and conversion) and renewable energy technologies (mainly H_2 production & storage and electrode materials for batteries). This talk would, therefore, be a brief overview of interdisciplinary research activities of Functional Nanomaterials Group at LUMS to synthesize customized inorganic/organic nanoparticles with tunable size and surface chemistry, and their composites having unique chemical and physical properties, and subsequent applications in biomedical sciences, environment, catalysis and renewable energy technologies.



Graphical image showing electron microscopic images/cartoons of different functional nanomaterials prepared in my group at LUMS.

Oral Communications

ELABORATION BY CONVENTIONAL MELT QUENCH AND SOL GEL METHOD OF NEW GLASSES WITH IN THE SYSTEM $xTiO_2$-$yNiO$-zP_2O_5 WITH HIGH CHEMICAL DURABILITY

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The aim of the present work concerns the development of a new and facile conventional melt quench and sol-gel synthesis route, structure, thermal properties and chemical durability for production of phosphate-based glasses in TiO_2-NiO-P_2O_5 systems. The structure of the prepared samples was investigated by XRD, 31P MAS-NMR, DSC, ICP-AES, density methods, FTIR and RAMAN spectroscopy that confirmed successful synthesis and production of phosphate-based glasses via the conventional melt quench and sol-gel method. In this study, ternary phosphate-based sol-gel derived glasses in the TiO_2- NiO- P2O5 system with a high TiO2 and NiO content of up to 12.5 mol% were synthesized. The elemental analysis showed that the loss of phosphorous upon drying and heat treatment is low. For samples containing no nickel oxide, crystalline patterns were observed, corresponded to titanium pyrophosphate (TiP_2O_7) (ICDD no. 38-1468). For samples containing NiO≥2.5 mol%, a broad peak at 2θ values of between 20 and 40° was observed and was free from any detectable crystalline peaks which confirmed the amorphous and glassy nature of these samples.Investigation of ternary glasses with the general formula $xTiO_2$-$yNiO$-zP_2O_5, were revealed, substituting Nickel in place of titanium significantly improves the stability and prolongs the degradation of these glasses, which opens up a number of potential applications.

Keywords : Glass, Sol-gel method, Thermal Analysis DSC, FTIR spectroscopy, chemical durability.

Synthèse des nanoparticules de ZnO et ZnO dopé au Co et Niet l'etude de leur prorpiétés d'adsorption

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Résumé:
L'augmentation rapide de la population mondiale et l'industrialisation continue ont rendu les chercheurs plus préoccupés par la gestion des eaux usées.Plusieurs techniques ont été utilisées pour le traitement de ces eaux. Parmi ces techniques l'adsorption a été identifiée comme l'approche la plus pratique pour leur traitement à faible coût et avec une grande efficacité. Dans ce travail, nous nous sommes intéressés à la synthèse et à l'étude des nanoparticules de ZnO, (Zn0.95Ni0.05O) et (Zn0.95Co0.05O) comme adsorbant potentiel pour l'élimination de colorants spécifiques, le méthylorange et la tartrazine, qui sont généralement présents dans les eaux usées de nombreuses industries.

Mots clé: Oyde de zinc, méthylorange, tartrazine, adsorption

Synthesis and characterization of ME nanoparticles (M = Cd, Hg ou Zn ; E = S ou Se) capped with different phosphine oxides

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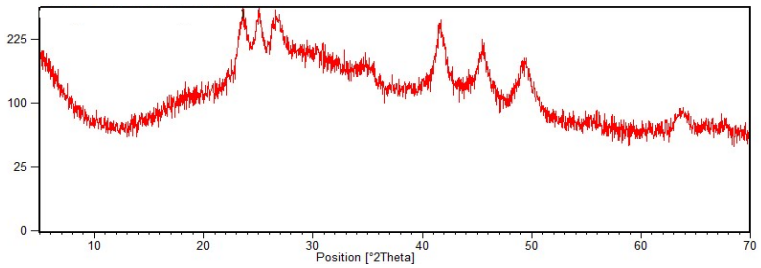
Phosphine chalcogenide complexes of the type $[MCl_2(R_3PPE)_2]$ (M = Zn, Cd ou Hg E = O, S, Se) have been widely reported and are attracting the attention of many research groups [1-5]. This is due to their diverse applications in bio inorganic chemistry and in particular as single source precursors for the preparation of binary metal chalcogenide thin films ME (M = Zn, Cd or Hg; E = S, Se or Te) as well as ME quantum dots [4, 5] Recently, we have prepared and characterized new complexes of zinc(II), cadmium(II), and mercury(II) with the ligands $Pyrr_3PE$ (Pyrr : pyrrolidinyl ; E = S or Se) [6]. Herein, we describe the synthesis of ME nanoparticles using different phosphine oxides as capping agents. These nanoparticles were characterized using UV-visible, PL, X-rays powder and NMR techniques. The effect of the nature of the caaping agent on the nanparticle size will be investigated and compared.



X-Ray spectrum of CdSe nanoparticles capped with $(Pyrr)_3PO$.

Keywords: Mercury, zinc and cadmium complexes, ME nanoparticules, IR, X-Rays analyses.

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DFT/TD-DFT investigation of the structural and spectral properties of nimetazepam: a psychoactive drug

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Abstract:
We investigate the potential energy landscape and the spectroscopic properties of nimetazepam using the density functional theory approach. Our calculations show that this molecule exhibits two conformational enantiomers, M and P. For the isomerization process, we find an activation energy of 16.7 kcal/mol and, consequently, the nimetazepam drug exists as a racemic mixture. The theoretical spectroscopic analysis of these enantiomers including IR, VCD, NMR, UV-Vis and ECD has been performed. The infrared spectrum of nimetazepam agrees well with the experimentally observed one, and vibrational bands have been assigned. Moreover, the ^{1}H and ^{13}C NMR experimental chemical shifts have been well reproduced using the gauge-independent atomic orbital method. The TD-DFT approach enables us to simulate the UV-Vis spectra, and the obtained results coincide satisfactorily with the observed spectrum. The M and P conformers show a complementary behavior in their predicted VCD and ECD spectra.

Keywords:
DFT, spectroscopy, nimetazepam, conformers, isomerization.

Optimisation des méthodes et techniques de l'orpaillage en Mauritanie sur la base de l'énergie renouvelable

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Résume

En Mauritanie les sites d'orpaillage se trouvent dans des régions isolées sans accès à l'électricité et sans infrastructure pour transporter et stoker des matières fossiles, ce qui fait besoin d'approfondir l'étude pour promouvoir cette activité sur la base de l'énergie renouvelable (solaire). Dans cet article, J'évalue la disponibilité des ressources solaires et la faisabilité économique pour installer un système autonome photovoltaïque/batterie avec générateur de secours dans les sites de l'orpaillage (lmjahir) en Mauritanie. La première phase de l'étude a consisté à utiliser la technologie de cartographie du système d'information géographique (SIG) pour évaluer le potentiel solaire dans les couloirs de MAADEN. Dans la deuxième phase, décrite dans cet article, Un dimensionnement d'un kit solaire a été réalisé pour subvenir les besoins énergétiques d'un groupe de quatre orpailleurs avec une consommation de 15,824 kWh/jour, situé dans le creusement d'Asouadan (25°38' 12.8" N 6°18' 42.5"W) à une distance de 714 km au nord-est de la ville Zouerate à la frontière algéro-malienne où le potentiel solaire atteint **3.52** kWh/m2/jour. De plus, une comparaison économique a révélé que le Cout total de cette conception pour une durée de 10 ans en utilisant l'énergie fossile CTgr = 10 218 184 A-UM est relativement élevé par rapport au cout total en utilisant énergie solaire photovoltaïque, CTpv =2112500 A-UM. La dernière phase c'était une conception optimale basée sur le logiciel Homer Pro a été réalisée, indiquant qu'une capacité PV plus faible peut réduire le coût unitaire de l'énergie à 0,356 USD/kWh tout en réduisant la fraction solaire à 54,9%.

Comparative study of the electrical properties of schottky diodes based on ZnT:Ni and CuO:Ni thin films

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Abstract:
Zinc telluride doped Ni (ZnTe:Ni) and Copper oxide doped Ni CuO:Ni thin films were deposited by radio-frequency reactive sputtering (RF- sputtering) on glass coated by (FTO) thin film representing the back-electrode, and they were subsequently electrically contacted with an silver (Ag) layer acting as the top-electrode. The RF-sputtering procedure was carried out at 200 W in argon (Ar) gas atmosphere kept at 2. × 10−6mbar working pressure for 75 min at a substrate temperature of 85○C kept constant during deposition. For the electrical investigations, current-voltage characteristics of the diodes have been studied at room temperature. Conventional (*I-V*) and resistance dynamic methods were used in order to determine the ideality factor, barrier height, and series resistance values. The capacitancevoltage (C-V) measurements were also performed.

Keywords: current–voltage (I–V); measurement Schottky diode; metal oxide, RF-sputtering.

Analyzing the Morphology of Nanocrystalline Nickel-Based Materials Using Comparison Between Image Segmentation and Image

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Abstract:
Nanocrystalline nickel-based materials are particularly beneficial in a variety of industries, including healthcare, energy storage, and electronics, because of their special features. Nanocrystalline nickel-based alloys were synthesized by high-energy ball alloying from elemental pure Ni powders as a function of milling time. The changes in structural, morphological, and ultrafine properties of the processed powders during mechanical alloying have been studied using scanning electron microscopy (SEM). The qualities and performance of these materials are significantly influenced by their morphology and particle size features. This work compares the image segmentation algorithm and ImageJ software to examine the morphology and particle size distribution of nanocrystalline nickel-based materials produced by mechanical alloying. The outcomes will offer useful knowledge for enhancing the synthesis and processing of these materials.

Keywords: Nanocrystalline materials, Mechanical alloying, Scanning electron microscopy, Image segmentation, Image.

Préparation des nanoparticules du type HgSe capées par R_3PO

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Les nanoparticules des chalcogénures des métaux du type ME (M = métal, E = chalcogène) ont attiré beaucoup d'attention au cours des deux dernières décennies [1] non seulement pour leur intérêt scientifique, mais aussi pour leurs nombreuses applications technologiques potentielles, leurs utilisations se situent à l'interface de trois grandes disciplines : la biologie, la physique, et la chimie. Ils sont utilisées en tant que marqueurs fluorescents pour la biologie [2,3] à la fabrication de matériau de gain optique pour lasers [4,5] en passant par les diodes électroluminescentes [6] ou encore les sources de photons uniques [7]. Dans notre étude nous nous intéressons à des nanoparticules semi-conductrices de type II-VI et appartenant à la famille de séléniure à savoir le séléniure de mercure (HgSe). Ces NPs sont préparées par voie à source unique à partir de complexes que nous avons déjà synthétisées [8] et en présence des oxydes des phosphine comme agents capants. Les NPs en HgSe ainsi obtenues sont caractérisée par UV-Vis, RMN et par DRX sur poudre. Les applications de ce type desNPs dans les cellules photovoltaïques hybrides seront discutées

$$Hg(R_3PSe) + R_3PO \xrightarrow[110\text{-}120°C,\ 12h]{R_3PSe} HgSe/R_3PO$$

R= piperidinyl ou morpholinyl

Keywords: les chalcogenure de phosphine, piperidinyl, morpholinyl, les nanoparticules du complexe de mercure, NMR, UV-Vis.

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Studying the effect of high-energy milling on the morphological, structural, and magnetic properties of $Ni_{50}Ti_{50}$ powder and revealing the new phenomenon of particle folding during the milling process.

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Abstract:

In this research, we investigate how the milling duration affects the physical characteristics of nanostructured Ni50Ti50 powders produced through mechanical alloying using a Fritsch Pulverisette 7 planetary ball mill. By utilizing scanning electron microscopy and electron dispersive X-ray spectroscopy, our innovative analysis uncovered a unique phenomenon of particle folding during high-energy milling, which differs significantly from conventional welding and fracture processes. As the milling time increased, we observed a reduction in particle size and the development of a more spherical and equiaxial shape. The powders consisted of a combination of the amorphous phase, NiTi-martensite (Ms), NiTi-austenite (As), and solid solution phases (SS). Rietveld refinements of X-ray patterns and magnetic measurements emphasized the crucial role played by the amorphous phase in determining the Ms and Mr (reversed martensitic) values of the synthesized Ni50Ti50 powders. After 72 hours of milling, the coercive field rose to 285.8 Oe, and the proportion of the martensitic phase reached 21.58496%. These findings provide valuable insights into the relationship between milling time and particle folding, facilitating the optimization of Ni50Ti50 powder synthesis for various technological applications.

***Keywords*:** Mechanical alloying; Nanoparticles; Folding phenomenon; Rietveld analysis; Magnetic properties.

Fabrication of ion-exchange ultrafiltration membranes for water treatment I. Semi-interpenetrating polymer networks of polysulfone and poly(acrylic acid)

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Abstract: This paper reports a simplified, efficient and economical method for fabricating ion-exchange ultrafiltration membranes for pollutant removal from water. To obtain these membranes by the phase inversion method, polysulfone (PSf) and poly(acrylic acid) (PAA) were separately dissolved in dimethylformamide (DMF), then the two solutions were mixed in desired proportions. The membranes have an asymmetric structure and rugous surface, as demonstrated by scanning electron microscopy (SEM) and atomic force microscopy (AFM) analyses. Their ion-exchange capacity was in the 0.70–1.0 meq/g range. The retention ratio of lead ions (Pb^{2+}) and Ponceau S dye were 99% and 90%, respectively, in the ultrafiltration process under 0.5 × 105 Pa (0.5 bar), with an average pure water flux of 18 L/(m^2 h).

***Keywords*:** Membrane preparation; Water treatment; Ultrafiltration; Lead ion; Ponceau S dye; Polysulfone

Structurale behaviors of Mg-Ti co-doped zinc oxide

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Abstract:
In this work, the electronic structure of the co-doped ZnO system $Zn_{1-x-y}Mg_xTi_yO$ has been studied using a Gaussian method and a plane wave bases set implemented in the CP2K code. Magnesium-doped ZnO has the quality of improving optical properties, but also reduces its electrical properties. The incorporation of a low concentration of Mg in Ti-doped ZnO should enable good electrical conductivity and high transmittance to be reached. To achieve this, it is essential to characterize the electronic structure of ZnO in order to study its physical properties. In this context, density functional theory (DFT) has been used for different configurations of ZnO co-doped with Mg-Ti. Electronic structure calculations have shown that MgZn-doped structures with a Ti co-doping of 2.778% exhibit a behavior that does not produce substantial lattice deformation compared to other dopants. It is hoped that the present and subsequent results will make this material a suitable candidate for transparent electronic devices.

Keywords**:** ZnO, co-doping, DFT, electronic structure.

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