Université de Monastir
Faculté des Sciences de Monastir
École Doctorale Matériaux, Dispositifs et Microsystèmes

JDD
Journée des Doctorants

03 Juillet 2019

Recueil des Résumés

j2d2019.scienceconf.org

BIENVENUE à la JDD 2019

Journée des Doctorants 2019

Première édition

03 Juillet 2019

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Au nom du comité scientifique et pédagogique de l'École doctorale Matériaux, Dispositifs et Microsystèmes et du comité d'organisation, nous vous souhaitons la bienvenue à la Journée des Doctorants «JDD 2019» qui se tient à la Faculté des Sciences de Monastir. Nous remercions l'ensemble des participants et le comité scientifique, sans eux l'organisation de la JDD 2019 n'aurait pas été possible. Nous remercions particulièrement le Professeur *Adel Kalboussi,* Doyen de la Faculté des Sciences de Monastir et Monsieur *Mabrouk Ben Zaied,* Secrétaire Général de la Faculté des Sciences de Monastir pour leur aide à l'organisation de cette journée.

Pour le comité d'organisation,

Le président du comité d'organisation

M. Koussai Lazaar

Le Directeur de l'École Doctorale

Pr. Abdelaziz Bouazizi

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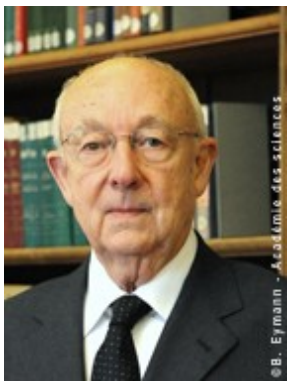
Conférenciers invités

Professeur Robert Guillaumont (IPNO, Orsay)



Professeur honoraire de chimie à l'université Paris-Sud à Orsay où il a enseigné de 1969 à 1998. Il a dirigé le groupe de radiochimie à l'Institut de physique nucléaire d'Orsay (IPNO) de 1979 à 1990.
Depuis 1994, il est membre de la Commission nationale d'évaluation des recherches sur la gestion des déchets radioactifs.
Robert Guillaumont est un radiochimiste spécialiste de la chimie des actinides, ce qui l'a conduit notamment à étudier les problèmes liés à la gestion des déchets radioactifs.

➢ **Titre de la conférence : Transition du Tableau périodique conduisant aux Actinides.**

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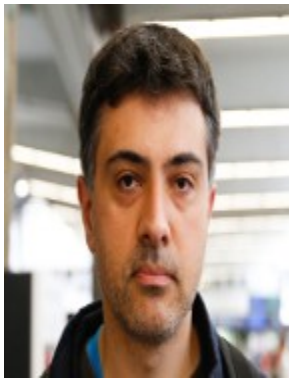
Docteur Sébastien Lebègue (LPCT, Nancy)



Directeur de Recherche CNRS, développe et utilise les méthodes de calculs ab initio pour la compréhension de la structure électronique des composés solides, avec une attention particulière pour les interactions de van der Waals et les états excités.
Après une thèse (2000-2003) à l'IPCMS (Strasbourg) sur le développement de l'approximation GW sous la direction de M. Alouani et un postdoc a Uppsala (Suède) dans le groupe de O. Eriksson, S. Lebègue a rejoint le CNRS en 2005 au laboratoire LCM3B puis depuis janvier 2018 au Laboratoire de Physique et Chimie Théoriques (LPCT) de l'université de Lorraine.

➢ **Titre de la conférence : Quelques avancées récentes en nanosciences vues par le biais du calcul ab initio.**

Programme

Heure	Mercredi 3 juillet 2019
8:00	(8:00 – 8:45) Accueil & Inscriptions des doctorants
9:00	(9:00 – 9:30) Ouverture de la JDD 2019 > Amphi 1
9:30	(9:30 – 10:45) Conférence plénière 1 **Transition du Tableau périodique conduisant aux Actinides** *Pr. Robert Guillaumont* > Amphi 1
10:45	(10:45 – 11:15) Pause café
11:15	(11:15 – 12:30) Conférence plénière 2 **Quelques avancées récentes en nanosciences vues par le biais du calcul ab initio** *Dr. Sébastien Lebègue* > Amphi 1
14:00	(14:00 – 16:00) **Session posters** *- Activités des structures de recherche* *- Posters des doctorants*
16:00	(16:00 – 16:30) **Clôture** > Amphi 1

Modélisation et calculs ab-initio

Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – MCA01

Electronic band parameters for zinc-blende III-V-Bi

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Abstract :

Band-structure calculations are performed for cubic III-V-Bi alloys using the empirical pseudo potential method. The band gaps variation are calculated as a function of the bismuth fraction x. It is found that there is no significant change in these electronic band parameters on taking into account the alloy disorder. On the basis of a model solid theory, we have calculated the band discontinuities for hetero-interfaces between strained III-V-Bi/III-V materials. As a result we obtain the approximate analytical expressions for the conduction and valence bands discontinuity that agree with experimental results. These results derived from this investigation will be useful in the design of lattice-mismatched heterostructures in optoelectronics applications.

Keywords: Band structure, III-V-Bi alloys, optoelectronic characteristics, band offset, discontinuity.

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École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – MCA02

DFT and TD-DFT Investigations on Optoelectronic and Nonlinear Optical Properties of New Cyclopentadithiophene (CPDT) Derivatives

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a. Université de Monastir, Faculté des Sciences de Monastir, Nom de Structure de Recherche, Code de Structure de recherche, Av. de l'Environnement 5000 Monastir, Tunisie.

b. Laboratory of Physical Organic Chemistry, Graduate School of Science, Osaka City University, 3-3-138 Sugimoto, Sumiyoshi-ku, Osaka 558-8585, Japan.

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Abstract :

Two types of di-fluorinated conjugated systems incorporating bridged cyclopentadithiophene (CPDT) **(1)** alternating fumaronitrile **(2)** and oxadiazole **(3)** have been designed and purely theoretical studied by Density Functional Theory (DFT) and its Time-Dependent extension (TD-DFT) at hybrid density functional, B3LYP, with 6-311g(d,p) basis set in THF solution. The first type is denoted FCFO-1 (X=>C=O) and the second one is the FCFO-2(X=>C=C-(C N)2. DFT and TD-DFT methods are powerful tools enabling the theoretical prediction of the ground and excited state properties of organic electronic materials with reasonable accuracy. The optical band gap of the studied materials ranges from 2.46 eV (FCFO-1) to 2.31 eV (FCFO-2) and they have been examined as green emitters (519-564 nm). The difference in optical behaviors may be due to the bridging group effect on CPDT. Thus, conformational geometry changes from ground (S0) to excited (S1) states varies from 11° (19°)(S0) to 39°(48°)(S1) and $_2$ from ~2°(S0) to ~3.5°(S1) for FCFO-1 and FCFO-2, respectively] leading a more twisted excited states of materials. In addition, a considerable decrease in the excited state dipole moment compared to that of ground state is certainly related to substantial redistribution of -electron densities in a polar excited state for the conjugated systems. Therefore, the molecules with large dipole moments (~ 11 Debye) based on the electric dipole moment calculation, show excellent nonlinear optical (NLO) properties. Static polarizability, first and second order hyperpolarizabilities were examined and compared for both structures.

These materials have shown improved optoelectronic properties making them interesting candidates for OLEDs and NLO optical devices.

Keywords: CPDT derivatives, DFT, Electronic properties, green emitter, OLED.

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JDD 2019 – MCA03

A theoretically study on the optical properties of ZnSe/ZnS core-shell quantum dot

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Abstract :

The core shell quantum dots (QDs) have been receiving enormous interest in the last few years. In this work we focus on ZnSe/ZnS core shell quantum dots (CSQDs) and we theoretically study their optical properties by two ways. First we have resolved the three dimensional Schrödinger equation in the spherical coordinate system. The second approach is based on a combination of the finite difference method and coordinate transformation.

The electron and hole energy levels, the transition energy as well as wavelength are investigated.

Keywords: Core shell, ZnSe/ZnS, Cordinate transformation, Optical propertie, Wavelenght.

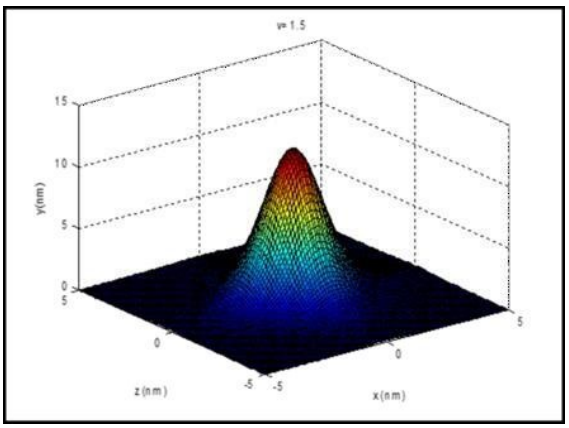

Figure 1 : Influence of the parameters on the shape of the quantum dot A = 0.5, D = B = 1, C = 1.5nm, K = 0.3

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JDD 2019 – MCA04

Molecular insight into water and benzoic acid adsorption on (001) WO_3 surface

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b. *Université de Lorraine, Laboratoire Physique et Chimie Theoriques, 54506 Vandoeuvre-lès-NancyCedex, France.*

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Abstract :

As an inexpensive n-type semiconductor, Tungsten trioxide (WO_3) is of great interest in different fields, such as photocatalysis and photovoltaics. However, studying the adsorption of water on WO_3 surface is a primordial step toward understanding the molecular mechanisms behind the wetting [1]. Interestingly, functionalization, with dye molecules, improves the absorption of the solar spectrum, refining the performances of the metal oxide in photovoltaic devices [2]. The first step in studying dye–surface interactions is to consider adsorption of the dyes' anchoring groups [3]. Indeed, we consider carboxylic acid functional group, such as benzoic acid, interacting with WO_3 (001) surface.

Here, density functional theory simulations, including a correction for dispersion interactions, were performed to investigate in details the surface hydration and the mode adsorption of benzoic acid on WO_3 surface. Ab initio molecular dynamics (AIMD) approach conducted at 300 K was also used to complete our results. These studies of anchoring group adsorption paved the way to studies of adsorption of complete dyes.

Keywords: WO3 ; Ab initio ; Adsorption ; Water ; Anchoring groups.

[1] Albanese E., et al. ACS Appl. Mater. Interfaces, 9, 23212 (2017).

[2] Galoppini, Chem. Rev., 248, 1283 (2004).

[3]Martsinovich N., et al. Energy Environ. Sci., 4, 4473 (2011).

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JDD 2019 – MCA05

Mathematical modeling of heat and mass transfers of a packed bed of shrinking particles during drying

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b. University of Monastir, National School of Engineers of Monastir, Research Laboratory of Thermal and Thermodynamics of Industrial Processes (LR18ES20), Rue Ibn El Jazzar 5000 Monastir, Tunisia.

Abstract :

The aim of this work is to describe the heat and mass transfer during the drying of a packed bed of shrinking particles with humid air. The granular bed is formed by moist spherical deformable particles through which humid air is flowing. The description of the thermal transfer necessitates a model of two temperatures. The mass transfer is described by a drying kinetics deduced from a single particle model. The numerical result was validated from the experimental data reported in the literature[1].

Keywords: Packed bed; humid air; drying kinetics; shrinkage.

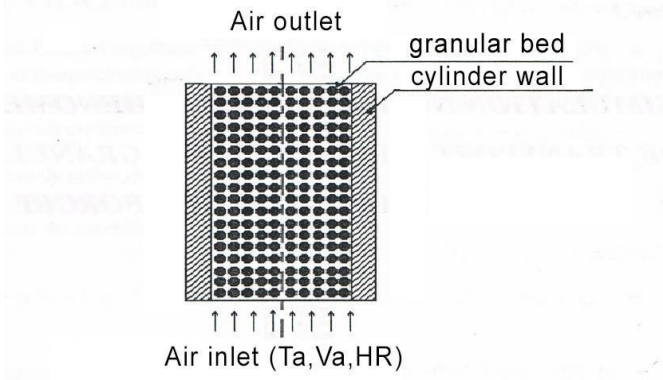

Figure 1 : Packed bed

[1] P. Dzaomuho, E. Verdin, N. Jacquet, P. Malumba, and M. Crine, "Mathematical modelization of fixed-bed corn drying and experimental validation," no. April 2012.

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JDD 2019 – MCA06

Ab Initio Study Of New Organic Solar Cell Acceptors

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b. Univ. Bordeaux, CNRS, LOMA, UMR5798, 351 cours de la Libération, 33400 Talence, France; c. *LPCT, UMRCNRS 7019, Université de Lorraine, Boulevard des Aiguillettes 54506 Vandoeuvre-lès-Nancy, France.*

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Abstract :

There are indications that the replacement of modified C60 by alternative electron-acceptor materials could improve the organic hetero junction solar cells that were pioneered by A. Heeger. Indeed, the electron -acceptor molecules, DBFI-T and PDI of non planar 3D architecture have shown better photovoltaic performance than cells based on C60 as acceptors.

Based an ab-initio calculations, we studied organic crystals that are candidates for new acceptors in such cells. We begin by studying the electronic structure of fullerene in different forms (isolated and fcc). Then we study electronic properties (band structure and DOS) both of fullerene and the new acceptors DBFI-T and PDI.

Keywords: DFT, SIESTA, Electronic structure, Organic Solar.

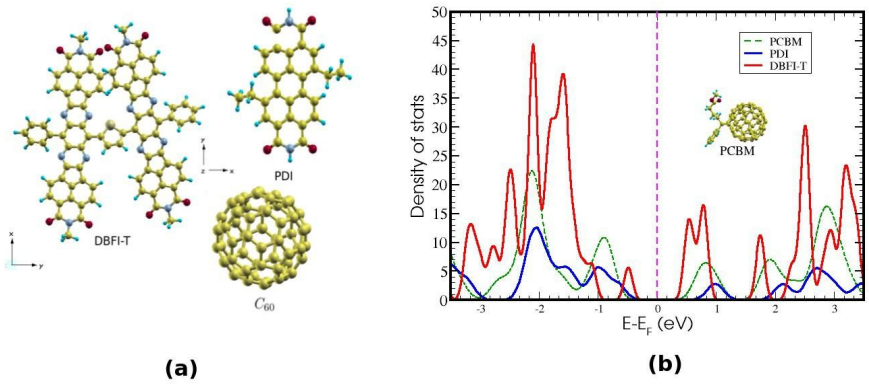

Figure 1 : (a) Molecular structures overlaid with the space filling structure of DBFI-T, PDI and C60. (b) Total density of states of PCBM, PDI and DBFI-T.

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JDD 2019 – MCA07

Solvation of alkali cations in helium via Density Functional Theory calculations

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Abstract:

Pure and sodium doped helium nanodroplets have been carried out using DFT calculations. As a starting point, potential energy curve of Na^+-He is calculated by using several DFT functionals and basis sets to find out the most reliable and accurate method for studying these clusters. The calculated potential energy curves showed that the Minnesota functional M05-2X associated to the extended 6-311+ +G(d,p) basis set fit correctly the experimental curve. At this level of theory, the lowest energy structures of Na^+He_n clusters (up to n=25) have been calculated. The obtained results are in good agreement with those found in the literature. The icosahedral geometry is obtained for Na^+He12 cluster ensuring the closure of the first solvation shell with a 'Snowball' shape. The relative stability of Na^+He_n clusters are discussed in terms of structural and energetic trends. These finding can be generalized for the solvation of the alkali cations in helium cluster.

Keywords: Doped helium clusters, Snowballs, DFT calculations, Structural and energetic stabilities.

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JDD 2019 – MCA08

First-Principles Study of CdS Nanoparticle Capped by Thiol Ligands

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a. *Université de Monastir, Faculté des Sciences de Monastir, Laboratory of Interfaces and Advanced Materials (LIMA), LR11ES55, Av. de l'Environnement 5000 Monastir, Tunisie.*

b. *Institute of Light and Matter (ILM) – UMR5306 CNRS, University of Claude Bernard Lyon 1 (UCBL1), 69622 Villeurbanne CEDEX, France.*

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Abstract :

Structures and properties of CdS quantum dots (QDs) clusters were investigated by combining experimental absorption, FTIR, TEM and X-ray diffraction (XRD) spectroscopies as well as ab initio DFT calculations. From the ground state geometry optimization results we conclude that thiol ligands preserve the wurtzite structure of the QDs. The DFT calculations were performed at the B3LYP/Lanl2dz level and followed by time-dependent TDDFT calculations to estimate n energy singlet transitions. On the basis of the results of these experimental and theoretical studies, we determine the relation between the CdS QDs and the organic ligands. The coupling between the CdS QDs and ligands (R-SH) was based on thiol chemistry. Thiols (S-H) are probably the most utilized functional groups for stabilizing and modifying CdS QDs. Thiol groups form stable bonds with metals on the surface of QDs such as cadmium. 3-mercaptopropionic acid (MPA), thioglycerol (TG) and 2-mercaptoethanol (ME) have a similar effect because the essential influence comes from thiol.

Keywords: Ligand binding, DFT, TDDFT, Quantum size effect, Semiconductor nanocrystals

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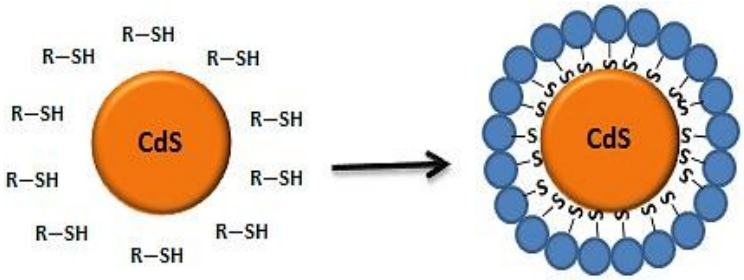

Figure 1. Thiol Ligands (R-SH) modified the structure of CdS QDs.

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JDD 2019 – MCA09

Density Functional Theories study of the non covalent interactions in 1-Phenylpiperazine-1,4-dium bis(hydrogen sulfate): Molecular Structure, NBO, AIM and RDG analyses

Olfa NOUREDDINE[a*], Sofian GATFAOUI[b], Houda MAROUANI[b] and Noureddine ISSAOUI[a]

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Abstract :

In the present work, we are interested in the theoretical study of 1-Phenylpiperazine-1,4-dium-bis (hydrogen sulfate). The attention was fixed to study the intra and intermolecular interactions in the 1-Phenylpiperazine-1,4-dium-bis (hydrogen sulfate) package. The ground-state molecular geometry has been reported by using the density functional theory (DFT)/B3LYP methods and 6-311++G(d, p) as a basis set. Here, the predicted geometrical parameters by using theoretical B3LYP/6-311++G (d, p) calculations show very good correlations with the corresponding experimental ones [1-2]. Intra and Intermolecular interactions were analyzed by Natural bond orbital NBO and topological AIM approaches.

The NBO analysis revealed a greater number of intermolecular hydrogen bonds in the title compound. He gives information on link stabilization and "quantifies" the electronic transfer, while the AIM allows to complete these studies by analyzing the topology of the density to extract its distribution in the link. RDG, atoms in molecules (AIM) and NBO calculations predicted high stabilities for the studied compound in gas and aqueous solution phases.

Keywords: Density functional theory; hydrogen bonds; Non covalent interaction; NBO; AIM and RDG analyses.

[1] G. Varsanyi, Assignments for Vibrational spectra of Seven Hundred Benzene derivatives, vol 1 and 2 Academic Kiaclo, Budapest (1973).

[2] G. Socrates, Infrared Characteristic Group of Frequencies, John Wiley & Sons, New York

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JDD 2019 – MCA10

The Dunkl-Coulomb problem in three-dimensions: Energy spectrum, wave functions and h-spherical harmonics.

Sami Ghazouani [a*], Insaf Sboui [b], M A Amdouni[b]
and Mounir Ben El Hadj Rhouma[b]

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b. Université de Monastir, Faculté des Sciences de Monastir, Laboratoire d ' Etudes des Milieux ionisés et réactifs (EMIR), UR 17ES31, Av. de l'Environnement 5000 Monastir, Tunisie.

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Abstract:

We present a study for the relativistic effect of hydrogen atom in presence of perturbation intensity on the dynamical stability. The energy spectrum and the wave functions of the system are solved by means of spectrum generating algebra techniques based on the so(1,2) Lie algebra. We observe that as soon as the perturbation rises any symmetry will be destroyed and the energy levels will be crossed. The effects of the relativistic corrections on the energy spectra are analyzed. Discrete and continuous energy spectra of a hydrogen atom with perturbation are studied. This study can be extended for hydrogenoïd atom.

[1] Sami Ghazouani, Insaf Sboui, M A Amdouni and Mounir Ben El Hadj Rhouma ,The Dunkl-Coulomb problem in three-dimensions: Energy spectrum, wave functions and h-spherical harmonics, Journal of physics A: Mathematical and Theoretical, 52, 225202, (2019).

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JDD 2019 – MCA11

Adsorption of ethanol onto biomass derived activated carbon: Modeling and consequent interpretation based on statistical physics treatment

Wouroud SGHAIER *, Yosra BEN TORKIA and Abdelmottaleb BEN LAMINE

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Abstract :

In the past few decades, thermally driven adsorption cooling and heat pump systems have gained considerable attention because it can be powered by renewable heat sources (heat waste, the sun…). This system can uses environmentally friendly adsorbent-refrigerants pairs. In the present work, a theoretical study was done to elucidate the adsorption mechanism of ethanol on Waste Palm Trunk (WPT) and on Mangrove Wood (M). For this investigation, the monolayer model with one energy treated by the grand canonical ensemble in statistical physics was successfully applied. Three parameters of the model are fitted, namely the number of adsorbed molecule per site n, the density of the receptor sites N_M and the energetic parameter $P_{1/2}$ .the results show that the ethanol molecules were fixed by angled position on the two type of adsorbent. Moreover, we determined the adsorption energies which are varies from 1, 40 to 3, 64 (KJ/mol) for WPT-AC and 3, 2 for 3, 81 (KJ/mol) for the M-AC reflecting a physisorption process. Also, the isosteric heat of adsorption is calculated from equilibrium uptake at different temperatures using monolayer model with one energy.

Using this isosteric heat of adsorption predicted from the isotherm data [1], we can study the performance of adsorption cooling cycle employing the coefficient of performance (COP).

Keywords: Adsorption isotherms, statistical physics, modeling, ethanol, biomass

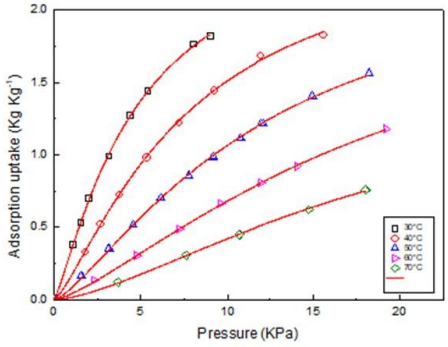

Figure 1: Fitted adsorption isotherms of ethanol on WPT-AC by HILL model in statistical physics.

[1] Pal, Animesh, et al. "Study on biomass derived activated carbons for adsorptive heat pump application." *International Journal of Heat and Mass Transfer* 110, 7-19, (2017).

Monolayer and multilayer adsorption of pharmaceuticals on activated carbon: Application of advanced statistical physics models

Amira Yazidi *, Lotfi Sellaoui and Abdelmottaleb Ben Lamine

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Abstract :

In this paper, the advanced statistical physics models (ASPM) were used to provide reasonable interpretations of the adsorption of pharmaceuticals Ketoprofen (KTP) and Ibuprofen (IBP) on raw and ultrasound activated carbons. Monolayer and multilayer models were selected to explain the adsorption mechanisms of these pharmaceuticals. Based on the values of the captured pharmaceutical molecules (n), it was concluded that multi-molecular ($n > 1$) and multi-docking ($n < 1$) processes were possible for IBP and KTP adsorption on AC and UAC. A detailed thermodynamic analysis was performed demonstrating that the adsorption mechanism was endothermic and associated to physical forces. The thermodynamic analysis confirmed the feasibility and spontaneous nature of the adsorption of these pollutants on tested adsorbents.

Keywords: Pharmaceuticals, Activated carbon, Advanced statistical physics models

[1] Andressa Cristiana Fröhlich, Glaydson Simoes dos Reis, Flavio André Pavan, Eder Claudio Lima, Edson Luiz Foletto, Guilherme Luiz Dotto. «Improvement of activated carbon characteristies by sonication and its application for pharmaceutical contaminant adsorption». Environnemental Science and Pollution Research (2018) 25 : 24713-24725.

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JDD 2019 – MCA13

Biaxial tensile effect on band structure and absorption coefficient of GaN x As 1 -x-y Bi y /GaAs strained DQWs calculated using k.p method

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Abstract

In this work, we derive the 16 band strain-dependent $\boldsymbol{k \cdot p}$ Hamiltonian using finite difference method for dilute bismide-nitride compound GaNAsBi. The influence of strain in conventional [001] crystal orientation on electronic band structure and optoelectronics properties of GaNAsBi/GaAs double quantum wells (DQWs) are examined. We apply the band anti-crossing model, envelop function formalism and Bir-Pikus theory in conjugation with $\boldsymbol{k \cdot p}$ perturbation method to describe the optoelectronics properties behavior of these structures. From the stimulated results, we have found that the biaxial strain induces opposite behavior at the level of the valence band offsets. In addition, we have presented the results of the GaNAsBi-based tensile strained DQWs. We have deduced that the combined effects of strained and coupling between two wells enhance considerably the absorption coefficient compared to uncoupled DQWs.

Keywords:

GaNAsBi-based tensile strained DQWs; Bir-Pikus theory; BAC model; Valence band offsets; Absorption coefficient.

Adsorption of acid red 1 and acid green 25 on grafted clay: Modeling and interpretation

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Abstract :

A grafted clay with 3-aminopropyl-trietoxisilane was employed to investigate the adsorption of acid red 1 (AR-1) and acid green 25 (AG-25) dyes [1]. Adsorption isotherms elucidating the variation of the adsorption capacity as function of equilibrium AR-1 and AG-25 dyes concentrations were performed at six temperatures (298- 323 K) clearly demonstrated that the adsorption process of both dyes was stopped after the formation of a certain number of layers. The estimated number of dyes formed layers, the density of receptor sites, and the adsorption capacity. The adopted model provided two adsorption energies characterizing the possible interactions between AR-1, AG-25-grafted clay adsorbent, and dye-dye. They were estimated and interpreted for a better explanation the present adsorption mechanism reflecting that only physical interactions are possible for all defined systems.

Keywords: Grafted clay, Acid red 1, Acid green 25, Multilayer model with saturation, Modelisation.

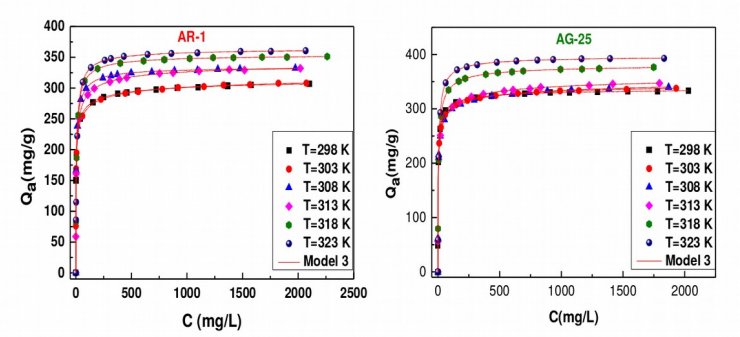

Figure 1: Adsorption isotherms of both dyes on grafted clay adsorbent at all operating temperatures

[1] Pascal S. Thue, A. Carmalin Sophia, Eder C. Lima, Alfred G.N. Wamba, Wagner S. de Alencar, Glaydson S. dos Reis, Fabiano S. Rodembusch, Silvio L.P. Dias, 2018. Journal of Cleaner Production,271, 30-44.

Cooperativity of hydrogen bonds O-H and Conformational preferences in calix[n= 4,6,8]arene : A DFT and QTAIM study

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Abstract :

Understanding the interactions of cage molecules with a variety of invited molecules is getting very important. The shape, the size and the diameter of the cavities are one of the main factors to know the environment of the interactions of these molecules with cation or neutral guests in sensor applications. But, the hydrogen bonds can also play a crucial role in the interaction phenomenon. In this work, vibrational spectroscopy study, molecular electrostatic potential (MEP) surface, Natural Population Analysis (NPA), chemical shifts and Atom in Molecules (AIM) analysis have been used to identify the role of hydrogen bonds in the stability of CX[n] molecules. Our calculations show clearly that, the chemical shifts of H atoms and IR spectra are very sensitive to the strength of hydrogen bonds. The red-shift of OH band increases when the hydrogen bond becomes stronger, explaining why the observed OH band in CX[6] is more red shifted than those of CX[4] and CX[8]. According to our calculation, the 13C NMR spectra are also sensitive to the nature of hydrogen bonds. We note that the DFT calculations have reproduced with a very good agreement, the experimentally observed chemical shifts of CX [4], the OH band frequencies of IR spectra for CX[4], CX[6] and CX[8] molecules.

Keywords: Calix[n]arene, hydrogen bonding, cooperativity, molecular electrostatic potential, intermolecular interactions.

Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – MCA16

Self-consistent vertical transport calculations in $Al_xGa_{1-x}N$/ GaN based resonant tunneling diode

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Abstract :

Heterostructures based on wurtzite III-nitride compounds are characterized by a large conduction band discontinuity and a presence of an internal electric field, both of which have important effects on the electronic transport.

In This work, we present a room temperature simulation of the vertical electron transport in GaN/AlGaN resonant tunneling diode (RTD). By using the transfer matrix formalism, we investigate the effect of the aluminum composition on the resonant current: We show an increase in the peak to valley ratio (PVR) with increasing Al content of the barriers which arises from the large decrease in the valley current.

Mots-clés : Wurtzite Nitrides, Resonant tunneling diodes, Self-consistent calculations, Ballistic transport.

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JDD 2019 – MCA17

Study of the electronic properties of two-dimensional ZrOS and ZrOTe materials by ab-initio calculation

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Abstract :

Based on density functional theory (DFT), we investigated the structural and electronic properties of novel two-dimensional ZrOS and ZrOTe-based materials. First, we optimized the total energy of the ZrOS and ZrOTe monolayers and bilayers, which allowed us to determine the structural properties of these materials. Subsequently, we calculated the partial and total electronic state densities as well as the band structures of these systems. This allowed us to determine the value and the nature of the band gap of the mono and bilayer ZrOS and ZrOTe. The gap values of these new 2D materials are 0.70 eV and 1.30 eV for the ZrOTe and ZrOS monolayers, respectively with the GGA approximation. For the ZrOTe bilayer the value of the band gap has increased by a value of 0.80 eV whereas for ZrOS the value of the gap is 0.50 eV which is lower than that of a monolayer.

We can conclude that these new two-dimensional materials can be useful for optoelectronic applications.

Keywords: two-dimensional materials, ab-initio, electronic structure, ZrOS, ZrOTe.

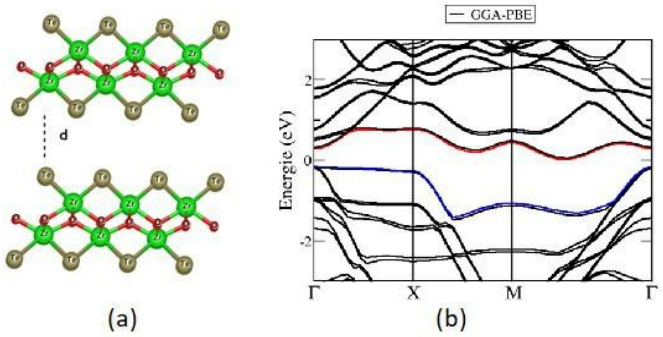

Figure 1: (a) Schematic representation of a ZrOTe / ZrOTe bilayer system,
(b) E (k) band structure of a ZrOTe bilayer structure obtained in the GGA approximation.

Synthèse, réactivité et substances naturelles

Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – SRSN01

SYNTHESIS OF NOVEL PYRROLES AND PHTHALIMIDES FROM EUGENOL MOLECULAR DOCKING INVESTIGATIONS

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Abstract

This work consists in the synthesis of novel pyrrole and phthalimide derivatives (Fig. 1) *via* the reaction of a previously synthesized hydrazide with aliphatic diketones and cyclic anhydrides. To do this, we used eugenol as a starting natural synthon, which is the major constituent of the essential oil of cloves and many other aromatic plants. This well known compound has been widely used as a starting material to access to a variety of products with potential biological properties.

Structures of all obtained compounds were determined using spectroscopic methods including ^{1}H NMR and ^{13}C NMR.

A molecular docking analysis was carried out to predict the inhibition potency of the new prepared phthalimide derivatives against target protein tyrosinase receptor (**1**). In the other hand, to evaluate their anticancer activity, docking studies were performed to fit pyrrole derivatives into the active site of target protein (**2**) (Fig. 2).

Keywords: Eugenol, pyrrole, phthalimide, docking

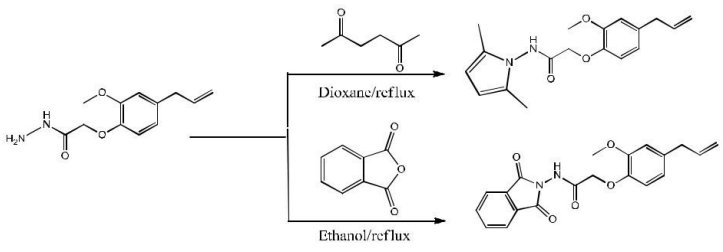

Fig. 1. General pathway for the preparation of pyrroles and phtalimides

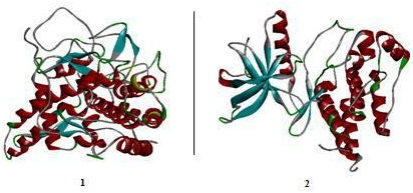

Fig. 2. Target proteins of studie activities

Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – SRSN02

Étude phytochimique de la plante *Crithmum maritimum* et évaluation de ses activités antioxydante et allélopathique

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Abstract :

Dans le cadre de notre contribution à la valorisation du patrimoine végétal Tunisien et découvrir de nouvelles substances naturelles à intérêt biologique, nous nous sommes intéressés au cours de la présente recherche aux études biologique et chimique de l'espèce *Crithmum maritimum*. Cette étude a été commencée par l'extraction de l'huile essentielle (HE-F) des feuilles. Les séparations chromatographiques que nous avons envisagées ont permis de simplifier cette HE-F en cinq fractions. L'identification de leurs constituants a été faite par la CPG-FID et la CPG/SM. Cette étude nous a permis d'identifier pratiquement la totalité des constituants, le dillapiole s'est trouvé le composé majoritaire.

L'évaluation de l'activité antioxydante de l'huile essentielle et de ses fractions a été envisagée en utilisant le test de DPPH. Les résultats obtenus ont montré que cette huile présente une activité modérée avec une CI_{50} = 731 µg/mL. Quant aux fractions, nous avons constaté que la 5^{éme} fraction a manifesté l'activité relativement la plus élevée avec une CI_{50} = 272 µg/mL. D'autre part, l'activité allélopathique de l'huile essentielle a été envisagée en se basant sur l'évaluation de la germination et la croissance des graines de laitue (*Lactuca sativa* L.). Les résultats obtenus ont montré que cette huile paraît un bon inhibiteur de la croissance des graines de Laitue utilisée comme plante cible vue sa sensibilité.

Keywords: *Crithmum maritimum*, huile essentielle, dillapiole, activité antioxydante, activité allélopathique

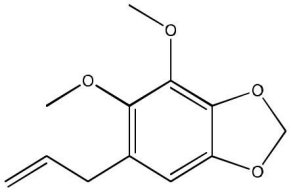

Figure 1 : Structure du dillapiole

Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – SRSN03

Synthesis of a novel bio-based monomer derived from Isosorbide and biphenyl

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Abstract:

Over the last decades, the usage of bio-based polymeric materials has been significantly developed, as a more sustainable alternative to those based on fossil-resources [1,2]. In this context, Isosorbide, which is one of the most promising renewable diols, has emerged a spiraling growth of interest required to its bioavailability, rigidity, thermal stability and non-toxicity. Due to those exceptional and attractive properties, we have synthesized a bio-based monomer derived from Isosorbide and 4,4'-biphenol. AA-type monomer, having two hydroxyl functions in exo-exo position, therefore with the same reactivity and thus more suitable to be used in polymer synthesis. The chemical structure of this monomer was confirmed by Nuclear Magnetic Resonance (NMR).

Keywords: Synthesis, AA-type monomer, Bio-based, Isosorbide, 4,4'-biphenol.

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[2] Gandini A, Macromolecules, **41**, 9491–9504, (2008).

Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – SRSN04

Synthesis, biological evaluation and molecular docking studies of novel benzopyrimidinone derivatives as potential anti tyrosinase agents

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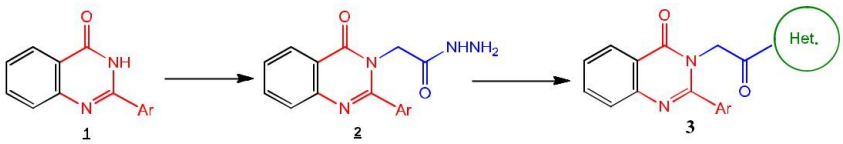
Abstract :

Heterocyclic chemistry constitutes an essential branch of organic chemistry and widely known to display an array of biological properties [1]. On the other hand, benzopyrimidinone derivatives have been recognized as important heterocyclic compounds due to their biological activities such as cytotoxic [2], antiviral [3] and antifungal. In view of the above mentioned facts, we have designed and synthesized some new benzopyrimidinone derivatives **3** through the combination of benzopyrimidinone moiety **1** with different pharmacophores such as pyrrole, pyrazole and pyrrolidinedione. Structures of all synthesized compounds were established on the basis of spectroscopic methods including ^{1}H NMR, ^{13}C NMR and ES-HRMS. Hereby we are reporting for the first time the anti-tyrosinase activities of the newly synthesized compounds. Furthermore, the structure-activity relationship (SAR) was supported with the molecular docking analysis.

Keywords: benzopyrimidinones, synthesis, anti-tyrosinase activity, molecular docking.



Scheme 1: Synthetic pathway of the benzopyrimidinone derivatives **3**

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Comparative study of the chemical composition of the essential oils of a Mediterranean plant : Dittrichia viscosa

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Abstract :

Many plants of Tunisian flora are currently exploited in the industry for the quality of their essential oils. [1] In the context of the valorization of these plants, our choice fell on a Mediterranean plant of the genus Dittrichia: D. viscosa. The objectives were : 1/ to extract the essential oils by hydrodistillation from the various organs of the plant : (leaves, flowers and the aerial parts), 2 to determine the chemical composition of the extracted essential oils and 3 to compare these compositions with those of the essential oils extracted from the same species of plant presented in the literature.

Comparative results showed that the essential oils of D. viscosa growing in Tunisia are very rich in oxygenated sesquiterpenes, while those extracted from the species harvested in Turkey are richer in oxygenated monoterpenes. On the other hand, the nature and the quantity of the majority of the identified compounds depend on the region where the plant was collected (Turkey, Algeria, Italy, France or Tunisia), as well as the climate, the harvest period without forgetting the operating conditions of the extraction.

Keywords : Dittrichia viscosa, essential oil, hydrodistillation, oxygenated sesquiterpenes.

[1] W. Aidi Wannes and B. Marzouk, Research progress of Tunisian medicinal plants used for acute diabetes, J. Acute Dis., 5, 357-363 (2016).

Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – SRSN06

Synthesis and characterization of benzo[*c*]phenanthrene and phenanthrene derivatives

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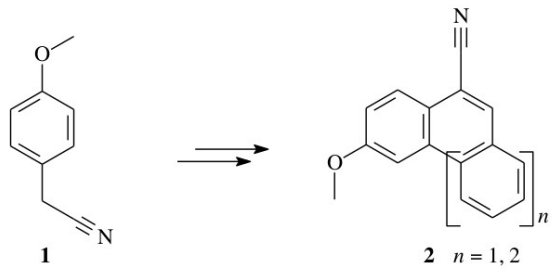
Abstract :

Polycyclic aromatic hydrocarbons (PAHs) are organic compounds consisting of several fused aromatic rings. Due to their π-conjugated electronic system they have attracted attentive in many fields, and were found to be used in particular in electronic devices [1] and as sensors [2].

In our work, we have synthesized π-conjugated tri-and tetra-cyclic systems carrying different reactive chemical functions. This synthesis was carried out in two stages. Condensation of *p*-methoxyphenylacetonitrile **1** on appropriate aromatic aldehydes, which provided a series of α,β-unsaturated nitriles, followed by oxidative photocyclization which yielded benzo[*c*]phenanthrene and phenanthrene derivatives **2** (Scheme 1). The absorption properties of these derivatives were evaluated experimentally and a remarkable behavior has been noted.

Key words: Condensation, Photooxidation, Optical properties.



Scheme 1 : Synthesis of phenanthrene and benzo[c]phenanthrene derivatives.

[1] K. Kano, S. Negi, H. Kamo, T. Kitae, M. Yamaguchi, H. Okubo, M. Hirama, *Chem. Lett.* 27 (1998) 151-152.

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Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – SRSN07

Design, synthesis and molecular docking studies of novel pyrimidine derivatives

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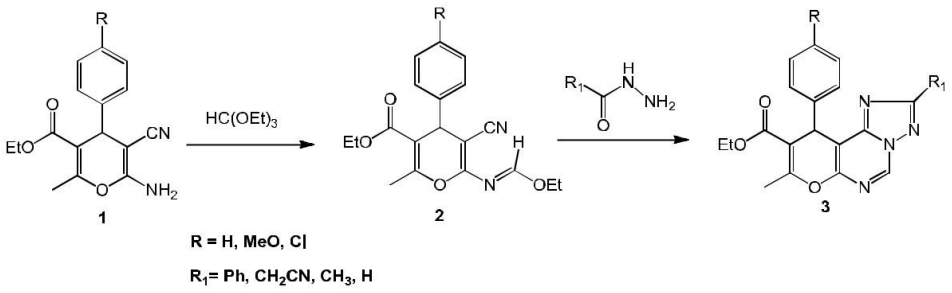
Abstract :

Heterocyclic chemistry has been constantly evolving for decades representing a very important class in organic chemistry. Thus, the synthesis of bioactive condensed pyrimidine derivatives is an important task in N-heterocyclic chemistry since they have been proven to be very interesting for the design of new molecular scaffolds for potential drugs with several pharmacological activities. Our work fits into this optical and aims to develop a convenient pathway for the synthesis of novel pyranotriazolopyrimidine **3** derivatives via the cyclocondensation reaction of α-functionalized iminoether **2**, with a series of hydrazides.

Structures of all synthesized compounds were established on the basis of spectroscopic methods including ^{1}H NMR, ^{13}C NMR and ES-HRMS.

Molecular docking analysis was performed to evaluate the inhibition potency of some novel compounds synthesized against the target protein, acetylcholinesterase (AChE), in order to screen for potential acetylcholinesterase inhibitors.

Key words: pyranotriazolopyrimidines, molecular docking, acetylcholinesterase.



Scheme 1: Synthetic pathway of compounds **3**

Faculté des Sciences de Monastir
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JDD 2019 – SRSN08

Synthesis And Spectroscopic Characterization Of A New Samarium Porphyrin Complexe

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Abstract :

We have prepared the monomeric lanthanide porphyrin complex [Sm^{III}(TTP)(acac)$(H_2O)_2$]. This species was characterized by UV-Visible, IR and 1H NMR techniques. The structure was confirmed using MALDI-TOF mass spectrometry.

The synthesis procedure used for the preparation of lanthanide complex were described by Wong et al., [1]. The meso-tetrakis(4-methylphenyl)porphyrin (H_2TTP) was dissolved in 1,2,4-trichlorobenzene (TCB) and the n-butyl lithium was added at 20 oC to yield lithium(4-methylphenyl) porphyrin complex [Li(TTP)]. Then the samarium(III) acetyl acetonate was added to the lithium (4-methylphenyl) porphyrin complex and the reaction was refluxed for 2 hours under a slow stream of high-purity nitrogen leading to the corresponding samarium(III) monoporphyrin species with the formula [Sm^{III}(TTP)(acac)$(H_2O)_2$].

The reaction mixture was purified by column chromatography using a neutral aluminum oxide to remove unreacted porphyrin. The UV-visible spectroscopy was used to follow up the reaction progression. Our synthetic compound was characterized by IR spectroscopy and the [Sm^{III}(TTP)(acac)$(H_2O)_2$] formula was confirmed par MALDI-TOF mass spectrometry.

Keywords: Lanthanide porphyrin complexes, UV-Visible, IR, 1H NMR, MALDI-TOF spectrometry.

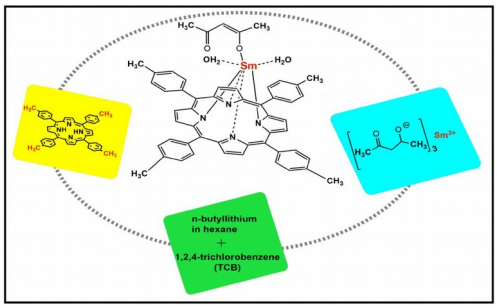

Figure 1 : Synthesis of the monomeric samarium porphyrin complex

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École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – SRSN09

Chemical composition, nutritional value and biological evaluation of Tunisian Okra (*Abelmoschus esculentus* L.)

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b. Laboratory of Bioresources: Integrative Biology and Exploiting, Higher Institute of Biotechnology of Monastir, University of Monastir, Tunisia.

c. Centro de Investigação de Montanha (CIMO), Instituto Politécnico de Bragança, Campus de Santa Apolónia, 5300-253 Bragança, Portugal.

d. Dipartimento di Farmacia, via Bonanno 6, Università di Pisa, 56126 Pisa, Italy

e. Centro Interdipartimentale di Ricerca "Nutraceutica e Alimentazione per laSalute" NutraFood, Università di Pisa, Italy.

Abstract :

Nutritional, and aroma volatile profiles, soluble carbohydrates and phenolic components of Tunisian okra pods (*Abelmoschus esculentus*) have been characterized. The chemical composition of Tunisian *A.esculentus* as well as its *in vitro* antioxidant, cytotoxicity and α-amylase and α-glucosidase inhibition activities were carefully evaluated. The approximate composition revealed that carbohydrates are the most abundant macronutrients (12.02g/100g fw) followed by proteins (4.77g/100 fw). In addition, okra pods were rich in organic acids (1.85g/100g fw), tocopherols (0.72g/100g fw) and chlorophylls (1.08g/100g fw). Volatile profile showed that oxygenated monoterpenes, sesquiterpene hydrocarbons and phenylpropanoids were the main essential class of volatile components in okra pods. Phenolic compounds were also investigated. Okra have shown good antioxidant activities, a significant cytotoxic potential against four cancer human cell lines, relevant inhibitory effect against α-amylase and α-glucosidase enzymes and interesting analgesic activity. These results highlight the efficacy health benefits of Tunisian *A.esculentus* as a potential source of nutriments and bioactive components.

Key words: *Abelmoschus esculentus* : Nutritional value ; Antidabetic activity ; Antiproliferative activity ; Analgesic activity.

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École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – SRSN10

Synthesis and characterization of a new chromium phosphate $NaNiCr(PO_4)_2$

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Abstract:

The present work reports the synthesis, X-ray structure and investigation by IR and Raman spectroscopies of a new chromium phosphate $NaNiCr(PO_4)_2$. This compound crystallizes with the unit cell parameters: a = 10.394(1) Å; b = 13.027(1) Å; c = 6.395(1) Å of the orthorhombic space group Imma. Its structure, belonging to the **α**-$CrPO_4$ type, features a three-dimensional $[NiCr(PO_4)_2]^-$**∞** anionic framework with interesting tunnels where the Na^+ ions are located (figure 1). This framework consists of two building blocks: (1) sheets parallel to the (b,c) plane and constructed by $M(2)_2O_{10}$ (M = 0.437 Cr^{3+} + 0.563 Ni^{2+}) binuclear units, corner-linked by PO_4 tetrahedra, and (2) chains running parallel to the b axis,

formed by M1O6 octahedra, alternating with PO4 tetrahedra knowing that M1O6 (M = 0.627 Cr^{3+} + 0.373 Ni^{2+}).

The IR spectrum is typical of a monophosphate and gives clear evidence of the occurrence of two crystallograpically distinct phosphorus sites. The results of refinements by the Rietveld method confirm the octahedral environment of the Cr^{3+} ions. The magnetic properties will be discussed shortly.

Key words: Phosphate de Chrome, DRX, IR, Raman.

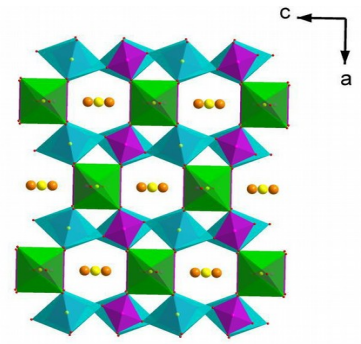

Figure 1: A projection along the [010] direction of the $NaNiCr(PO_4)_2$ structure.

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M. Hidouri, B. Lajmi, A. Driss et M. B. Amara, J. Chem. Cryst. 34 (2004) 10.

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JDD 2019 – SRSN11

Catalytic etherification of alcohols under green conditions

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Abstract:

Chemists was very passionate about in the area of green chemistry which are increasingly to design a careful planning of chemical synthesis and molecular design to reduce adverse consequences [1]. In this context, we present the solventless etherification of alcohols in environmentally conditions in the presence of Fe(SO4)3.5H2O as a catalyst. The use of simple, cheap, and readily available iron (III) sulfate as a catalyst makes this protocol highly attractive and environmentally benign that meet the principles of green chemistry [2]. Thus, all the structures were confirmed by spectroscopic data.

Key words: green chemistry, etherification, environmentally, catalyst, iron (III) sulfate.

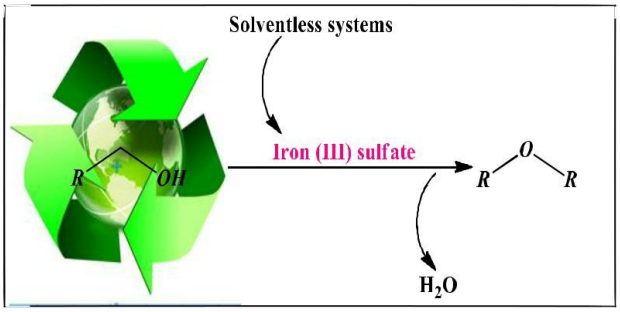

Figure 1

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JDD 2019 – SRSN12

Water dynamics in a mesopourous bioactive glass studied by NMR relaxometry

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Abstract :

Two CaO-SiO2-P2O5 materials have been compared: both have the same chemical composition but they have been made with different methods – standard or microfluidic techniques -, inducing different textural properties (surface areas, porous volume, mesoporous arrangement).

NMR is known for being particularly well suited for studying fluids embedded in mesostructured porous materials because, in addition of being non-invasive and relatively fast, it allows the characterization of molecules dynamics. In this study, we used NMR relaxometry, which consists in measuring spin relaxation times as a function of the measurement frequency (or equivalently of the static magnetic field B0), in order to determine the dynamics of water molecules embedded in the MBGs. The low field domain (10kHz-10MHz proton Larmor frequency) was investigated with measurements done with a fast field-cycling relaxometer and the socalled dispersion curves (longitudinal relaxation rate as a function of the measurement frequency) were analyzed in order to have additional insights on the motion of confined water.

The frequency dependence of the proton relaxation rate in MBGs was first studied by comparing the relaxation dispersion detected in HOD (residual proton of heavy water) with that in H2O, the proton low-frequency relaxation is thus shown to be mainly due to intramolecular dipolar interactions. Secondly, dispersion curves were recorded as a function of the filling degree and analyzed in the frame of the two-phase fast exchange model: tiny differences in the dynamical behavior of the water inside the two MBGs (exchange timescale, hydration layers) could be evidenced.

Key word : Confined water, NMR relaxometry, Bioactive glass.

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JDD 2019 – SRSN13

Characterization and antioxidant activities of extracted polysaccharides from *Foeniculum vulgare* seeds

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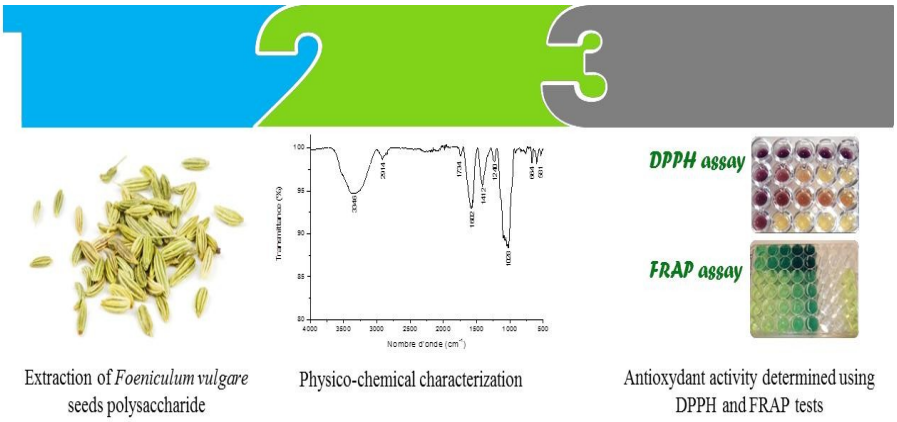
Abstract :

Foeniculum vulgare seeds are commonly used for food, flavoring, fragrance and medical fields; they are also known to be used as a household remedies since antiquity. In this work, polysaccharides from *Foeniculum vulgare* (FPS) seeds were extracted by water extraction. The polysaccharide fraction was characterized by Fourier Transform Infrared Spectroscopy analysis and Size Exclusion Chromatography (SEC/MALS/VD/DRI). Then, the physico-chemical and antioxidantof optimized FPS were studied, and the total sugar and galacturonic acid content were 61.2% and 57.5%, respectively. In addition, FTIR analysis confirmed the presence of uronic acids. Finally, the results indicated that FPS presents strong antioxidant activities *in vitro* in DPPH and FRAP.

Keywords: Foeniculum vulgare, polysaccharides, physicochemical characterization, antioxydantproperties.



Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – SRSN14

Synthesis and chiroptical properties of a new helicene

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Abstract :

Helicenes are inherently chiral molecules made-up of *ortho*-fused aromatic or heteroaromatic nuclei, displaying a nonplanar π-electron system [1]. These organic molecules show exceptionally intense chiroptical properties, such as a high optical rotation and very strong electronic circular dichroism (ECD). Consequently, helicenes and their derivatives have attracted considerable interest in a variety of fields: liquid crystals, sensors, molecular recognition[2] and electronic devices [3].

A new helically chiral hexacyclic helicene, bearing suitable functional groups at well defined positions, has been prepared through a four-step photochemical approach involving mild experimental conditions. Optical resolution of the racemic helicene has been accomplished affording enantiomers (+)-**1** and (-)-**1** in high optical purity, and their chiroptical properties were experimentally examined. Other optical properties such as UV-vis and photoluminescence have been also examined and an emission in the visible region was observed.

Key words: Helicenes, Chirality, Photochemical approach.

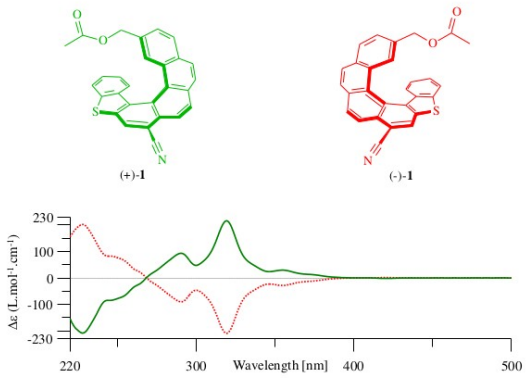

Figure: Electronic circular dichroism (ECD) spectra of (+)-**1** and (-)-**1** in CH_2Cl_2.

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[2] K. Kano, S. Negi, H. Kamo, T. Kitae, M. Yamaguchi, H. Okubo, M. Hirama, *Chem. Lett.* 27 (1998) 151-152,

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Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – SRSN15

New functional benzo[*ghi*]perylenes : Synthesis and photophysical properties

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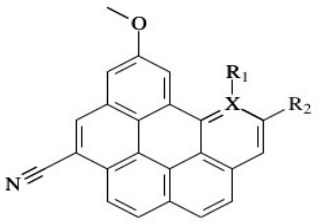
Abstract

Polycyclic aromatic hydrocarbons have been investigated for a variety of applications including organic field-effect transistors (OFETs), organic light emitting diodes (OLEDs), organic photovoltaics (OPVs), and so on [1-2]. The benzo[*ghi*]perylene and its derivatives are well known as polycyclic aromatic hydrocarbons formed by 6-membered rings, and are mainly focused as electro-conductive and photo-sensitive materials. In our work, new benzo[*ghi*]perylene derivatives (Fig.1) have been successfully synthesized *via* a photochemical approach. The optical band gap of these benzo[*ghi*]perylens, determined from the absorption onsets, was found to be less then 2.9 eV. The energy levels for highest occupied molecular orbital (E_{HOMO}) were also determined experimentally from their cyclic voltammograms to be −5.56, -5.36, -5.50 and −5.29 eV, respectively. The relatively large band gap and low E_{HOMO} levels imply that these materials have high stability against photo-degradation, and may be promising candidates for stable hole-transporting materials.

Key words: Coupling, photooxidation, Perylenes, Optical properties.



R_1 = OCH_3, $C_3H_5O_2$
R_2 = H, OCH_3
X = H, N

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JDD 2019 – SRSN16

Green synthesis of thiazolines and oxazolines under metal-free and solvent - free conditions

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Abstract :

Far from the use of toxic solvents, expensive catalyst, hard conditions, here we describe a new and soft method to access to thiazolines and oxazolines that are important scaffolds present in a great number of natural products[1,2]. This straightforward approach allows high conversion for a broad range of nitriles and an easy isolation of the desired products.

Keywords : Green synthesis , thiazolines, oxazolines, sealed tube.

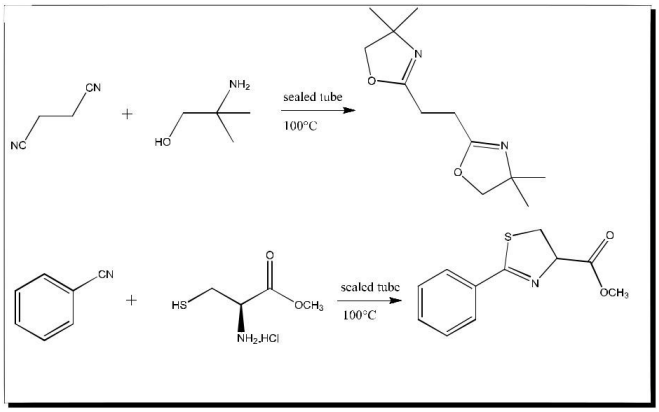

Figure 1 : Synthesis of oxazolines and thiazolines

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JDD 2019 – SRSN17

DFT study on 1,3-dipolar cycloaddition reaction of azomethine ylides with thiazolidine derivatives

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Abstract :

Density functional theory (DFT) at B3LYP/6-31G(d,p), is performed to enlighten the experimentally observed high regio- and stereoselectivity in the multicomponent 1,3-dipolar cycloaddition of azomethine ylides **1**, generated in situ from isatin derivatives and 1,2,3,4 tetrahydroisoquinoline, with *(Z)*-5-arylidene-1,3-thiazolidine-2,4-dione **2**. The regiochemistry of the reaction have been explained on the basis of transition state stabilities, where the results are in agreement with the experimental observations. The lengths of the C-C bonds directly involved in the cycloaddition reaction and HOMO /LUMO energies of **1** and dipolarophile **2** indicates that the reaction proceed along asynchronous concerted process.

Keywords: DFT, 1,3-dipolar cycloaddition, spiro[pyrrolo[1,2-a]isoquinoline-oxindole.

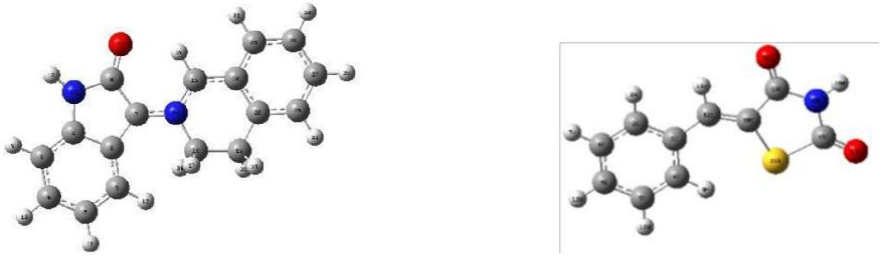

Figure 1: Structures of azomethine ylides **1** and dipolarophile **2**.

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JDD 2019 – SRSN18

Optimization of the performances of an existing API skimmer to enhance de-oiling of Petroleum production water

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Abstract :

In petroleum industry huge volume of water are produced daily, with a complex composition and traces of oil that must be separated from water before discharge. The most common equipment used for this purpose are skimmers. Production waters volumes are continuously increasing with the age of the oilfield and very often treatment equipment are not adequate any more to water volumes and composition. In the case of API-skimmers the upgrade is particularly complicated.

An original approach based on stock's law is applied in this work to upgrade the design of an existing API-skimmer according to the volume of wastewater to be de-oiled and characteristics of oil/water mixture, the addition of plates on the separator tank was investigated. The added plates will allow the treatment of more important volume of wastewater and will provide a longer path for the oil droplets to travel to the top of the separator so small droplets can coalesce and form larger droplets.

Diagnosis results shows that the existing API-skimmer is not adapted to the volume of water to be treated, calculation were confirmed with analytical results. The number and positions of plates required to suit to water volume and to eliminate smaller water droplets was also defined.

Keywords: Petroleum production water, oil-water separation, Conventional skimmer, corrugated plates, stock's law.

Microélectronique et Circuits Intégrés

Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – MECI01

Design and Analysis of on-membrane micro-heater for in-situ thermal annealing: COMSOL Multiphysics simulations.

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Abstract:

In the recent few years, on-chip thermal annealing has received widespread attention in the recovery of semiconductor based components from radiation induced defects [1-3]. Our previous works demonstrated a reliable in-situ thermal annealing of metal-oxide-semiconductor field-effect transistors (MOSFETs) after high gamma dose irradiation [4]; although the used Micro-Electro-Mechanical System (MEMS) based on Tungsten on-membrane micro-heater requires some improvement in term of efficiency and uniformity of thermal distribution. In this work, we use static and transient 3D COMSOL Multiphysics simulations in order to improve the thermal distribution over the membrane and study the time response of the micro-heater. The special interest in our case is to guarantee in-situ and uniform thermal annealing, over a specified circuit area, with high temperature around 900°C.

Mots-clés: MOSFETs, MEMS, Annealing, Radiation.

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Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – MECI02

An efficient Face Recognition Method Using PCA and CNN

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Abstract :

Face recognition is significant research and one of the actual challenging tasks in computer vision, where different methods have been proposed during the last years. Particularly, Convolutional Neural Networks (CNNs) have achieved outstanding performances in the field of face recognition. In this current study, we propose a face recognition method, which is based on Principal Component Analysis (PCA) and CNN under varying illumination. In our method, PCA is utilized to reduce the size of data. Then, we use CNN architecture as a classifier for face recognition. The experiments have been implemented with Extended-Yale B dataset. The experimental results verify the effectiveness of our approach, which attains good recognition accuracy. Thus, it achieves an important acceleration of the classification and lower memory consumption due to the use of the dimensionality reduction method.

Keywords : Recognition face, data reduction , PCA, CNN.

Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – MECI03

Approche de reconfiguration dynamique partielle pour un estimateur de mouvement à taille de blocs variable

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Résumé :

Le caractère dynamique devient actuellement un critère de performance dans un système sur puce SoC. Il s'agit des architectures dynamiquement et partiellement reconfigurables(DPR) dont le principe de base est d'adapter la structure du matériel au type d'application à charger et cela pendant l'exécution. À ce jour, la mise en œuvre des mécanismes de reconfiguration matérielle a principalement concernée les aspects calculatoires de ces architectures. Dans cette optique, l'estimation de mouvement à taille de blocs variable (VBSME: Variable Block Size Motion Estimation) se base sur la segmentation du Macro-Blocs (MB) de taille 16×16 en 16 MB de taille 4×4. Suite à cette segmentation, la norme H.264 définit 7 modes d'inter-prédiction possible. L'objectif principal de ce papier est de proposer une nouvelle architecture reconfigurable dynamiquement et partiellement d'estimation de mouvement en se basant sur la taille de la fenêtre de recherche et le type de la vidéo. L'implémentation de cette proposition conduit à une architecture exploitant le parallélisme massif des données tout en réduisant le temps de calcul et l'énergie consommée. Les résultats de simulation montrent que l'architecture proposée permet de garantir un gain au niveau de puissance consommée 54mW et au niveau de coût matériel utilisé.

Mots-clés : Reconfiguration Dynamique Partielle (RDP), VBSME, H.264.

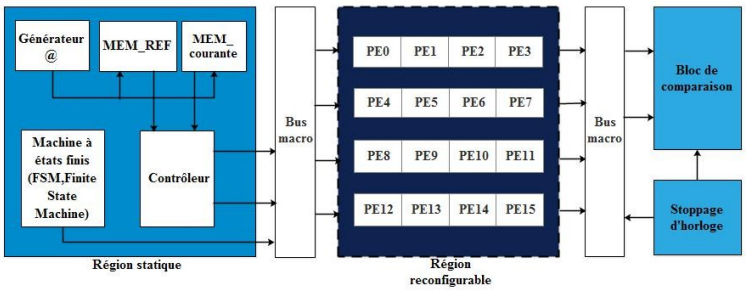

Figure 1 : Architecture d'un estimateur de mouvement reconfigurable

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Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – MECI04

Design of a control unit of M-sequence GPR signals

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Abstract :

The system Ground Penetrating Radar (GPR) is a special radar system that is used to detect objects buried in the ground or any another dielectric material and estimate their depths. GPR is an electromagnetic investigation method. When a signal is emitted via an antenna into the structure under investigation, a reflected signal caused by changes in material properties is recorded.

The main objective of this study is to design of a control unit of GPR system based on a M-sequence generator using an FPGA. The role of this block is to estimate the time delay between the transmitted and reflected signals.

Mots-clés : GPR, M-sequence, pseudo-random generator, control unit, non-destructive technique.

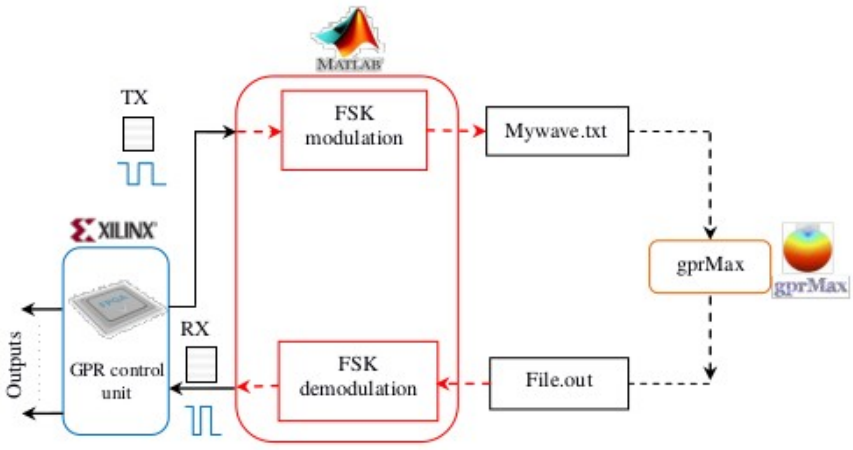

Figure 1 : Operating diagram.

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JDD 2019 – MECI05

Learning in memristor through modulation of weight dependent STDP

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Abstract :

Artificial synapses are critical units in neuromorphic systems. It is acknowledged that memristor is frequently implemented as artificial synapse due to its tunable resistance, simple structure, low power operation, and high-density integration. In this work, we present a simple and flexible memristor model that can be used to emulate a biological synapse. It is capable of supporting essential functions of biological synapses, such as potentiation and depression of synaptic weight. Then, we prove the capability of this memristor to simulate the spike timing dependent plasticity (STDP) and present simulated results that agree well with biological results. These results explore an interesting behavior that could be implemented in neuromorphic systems adequate for CNN, ANN …

Mots-clés : Memristor, artificial synapse, synaptic plasticity STDP, neural network.

Faculté des Sciences de Monastir
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JDD 2019 – MECI06

An Adaptable and Pipelined Accelerator for Deep Convolutional Neural Networks.

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Abstract :

In this project, an adaptable accelerator architecture for convolutional neural networks with an AXI Stream interface is implemented on a PYNQ-Z1 card [1]. This accelerator is adaptable for different convolution sizes (3x3, 5x5 and 7x7) and maximum pooling (2x2, 3x3) with a different stride. The advantage of the presented architecture is flexibility and adaptability. It can be easily adapted to a wide variety of deep learning models that also require different settings, without the need for a new design.

Mots-clés : Deep learning, CNN, FPGA, PYNQ-Z1, TensorFlow.

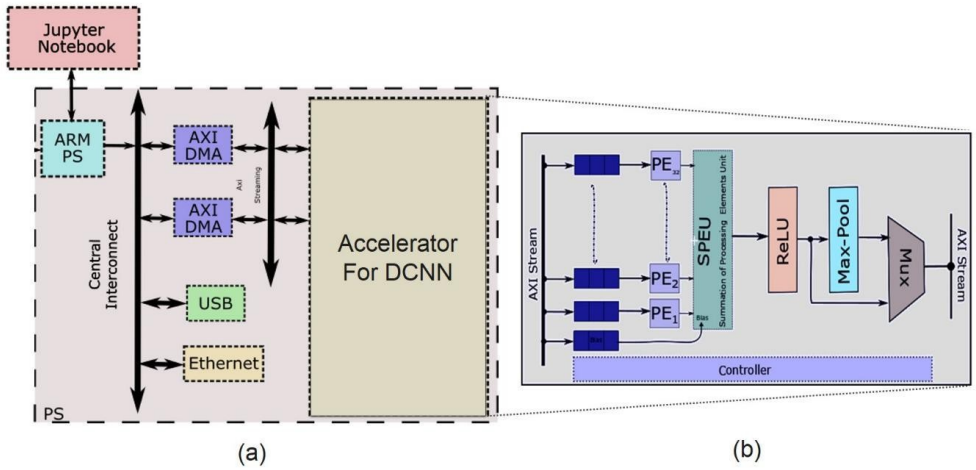

Figure 1: (a) Accelerator overlay diagram (PYNQ – Z1), (b) Hardware accelerator architecture.

[1] http://www.pynq.io.

[2] Y. LeCun, Y. Bengio, and G. Hinton, Deep learning, Nature, vol. 521, no. 7553, pp. 436444, 2015.

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JDD 2019 – MECI07

Effects of electromagnetic disturbances on the performance of quantum cloning machines

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Abstract :

The ability to copy information is fundamental for many processes in distributing and dealing with data. The cloning of quantum information is seriously restricted by the laws of quantum mechanics. This limitation is known today as the non-cloning theorem, guarantees absolute security of quantum key distribution in quantum cryptography. The implication is that an arbitrary quantum state cannot be copied perfectly, but only approximately or probabilistically. In order to characterize the quality of a cloning device, the fidelity it has been used. However V.Buzek and M.Hillery first investigated an universal quantum cloning machine (UQCM) for qubits produces copies of equal quality for all possible input states, with a fidelity being $^5/_6 \approx 0.833$. Since then, quantum cloning has attracted a vast amount of research and experimental implementations. Other quantum cloners have been conceived, such as phase-covariant cloning machine (PCCM), it clones only subsets of states for which we have some a priori information, called equatorial states, can be cloned with a higher fidelity up to the 0.854. In the present paper, we investigate how the magnetic field environment coupled to auxiliary qubits, required at the preparation stage of copying as a perturbation of the cloning process, modifies an output fidelity of the cloner. There are various types of quantum cloning machines dedicated to cloning often very specific and special classes of states, but we focus our attention of UQCM and PCCM. Results have been discussed using both the quality and the relative entropy. Much attention has been paid to the magnetic field-related decoherence of ancillary qubits before preparation effect on spin states at the input of the cloning machines. An attempt to explain the impact of this decoherence on the performance of the quantum cloning machines will be presented.

Mots-clés: Quantum cloning machine, Fidelity, Relative entropy, Magnetic field environment.

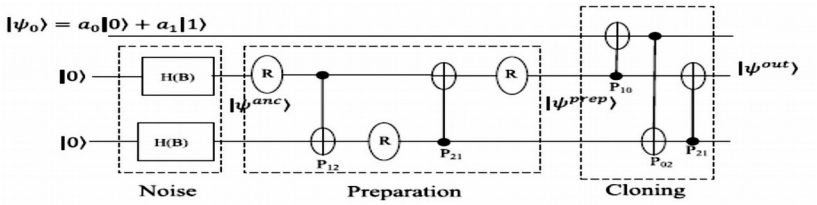

Figure 1 : Scheme of the Buzek–Hillery quantum copying machine. Noise resulting from the magnetic field environment is modeled by means of H(B) operators at the input of preparation circuit

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JDD 2019 – MECI08

Proposed Inverse-Raised-Cosine profile for next-generation orbital angular momentum system

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Abstract:

Enhanced performance of novel few-mode fiber (FMF) profile is proposed and designed to achieve larger separation between supported vector modes (≈2.9 × 10^{-4}), which ensures improved transmission performances compared to standard inverse-parabolic graded-index (IPGI) fibers. We apply a modified/adapted version of the inverse-raised-cosine (IRC) function, to the refractive index profile of the fiber, and optimize the design parameters in order to accommodate appropriate transmission of orbital angular momentum modes. A numerically study of the key characteristics and performance metrics of the proposed IRC fiber is performed over standard C + L ITU-T bands. Our modal analysis shows large separation between supported vector modes enabling low crosstalk between channels, enhanced purity in OAM modes, large resistivity to intrinsic crosstalk, increased tolerance to fiber imperfections and perturbations. Differential group delay and chromatic dispersion of the proposed fiber are also evaluated/analyzed and compared to IPGI fiber. Moreover, our investigation of the effective areas and the non-linearity coefficients of the propagating modes shows high similarity that leads to deal samely with most channels. The obtained results confirm that the proposed profile is a promising candidate for next-generation FMF-enabled orbital angular momentum transmission system.

Index Terms: Space division multiplexing, Optical few mode fiber design, orbital angular momentum.

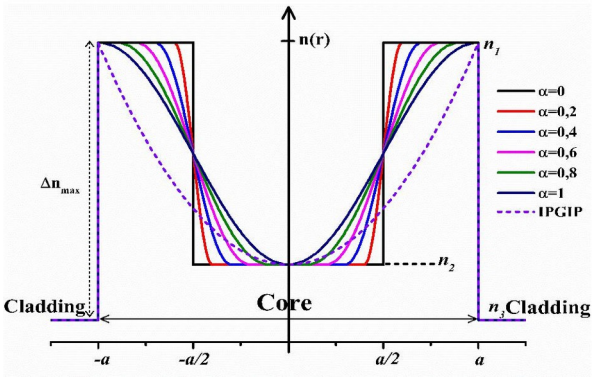

Figure 1: Refractive index profile of IRC for different values of α and that of standard IPGI (N=-4).

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JDD 2019 – MECI09

Dynamic and Real-time implementation of Edge and Corner detectors

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Abstract :

Computer Vision is an Artificial Intelligence (AI) discipline whose objective is to allow a machine to learn and understand what it sees when it is connected to one or more cameras. With the emergence of the increasingly powerful processors nowadays, it becomes practical to incorporate computer vision algorithms into Embedded Systems, in order to analyze their environments through video inputs. Likewise, Microelectronics advances provide new tools and devices each year making it possible to design more and more efficient artificial vision systems that meets the imposed constraints. All the elements are thus gathered to make the artificial computer vision one of the most promising, even unifying scientific challenges of nowadays. Among these all advances, designing and implementation using the dynamic criterion remains the most powerful technique in the hardware exploitation meaning. These are dynamically and partially reconfigurable architectures (DPR) whose basic principle is to adapt, at runtime, the hardware structure to be loaded. The focus of this paper is to design and implement a real-time Edges and Corners detectors on ZedBoard SoC (coupled with camera via FMC card) using the dynamic criterion in a Co-design architecture. That is to say that the proposed architecture process input video in a real-time manner based on hardware accelerators, which are Fast Corners and Sobel algorithms. The high synchronization between processing system and programmable logic unit's shows, in simulation results, the robustness of the proposed architecture in terms of operating frequency, power consumption, and hardware cost.

Mots-clés : AI, Computer Vision, DPR, ZedBoard SoC.

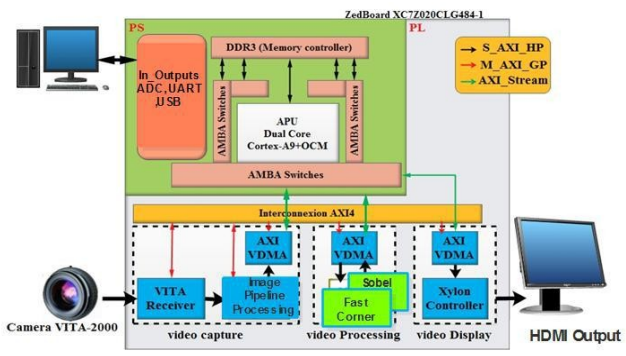

Figure 1: Partial and Dynamic Reconfigurable architecture of Edges and Corners detectors

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JDD 2019 – MECI10

A hybrid approach for MRI brain image classification

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Abstract :

The Magnetic Resonance Imaging (MRI) field has attracted recently considerable attention in the medical engineering community for its importance in medical applications and since it represents a non-invasive diagnostic technique. With the aim to detect correctly the unhealthy brain in MRI scanning, an automatic Computer-Aided Diagnosis (CAD) system is presented in this paper. The proposed system used Discrete Wavelet Transform (DWT) and Bag-of- Words (BoW) to extract image features. Support vector machine (SVM) was exploited in classification step. We employed 256x256 images from three datasets (DS-66, DS-160, DS- 255) provided by Harvard Medical School, in order to evaluate our method. 10*k-fold stratified Cross Validation (CV) technique was applied to validate the system performance.

The Accuracy reached respectively 100%, 100%, and 99.61% for DS-66, DS-160, and DS- 255 datasets. The overall computation time is about 0.027 s for each MR image. A comparative study with several works showed efficiency and robustness of our scheme.

Keywords: MRI, Brain Tumor, Classification, DWT, BoW

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JDD 2019 – MECI11

A new high-performance current comparator structure using WTA circuit.

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Abstract :

A New circuit "Winner Take All" based current comparator is introduced in this paper. Winner Take All (WTA) is designed, modified, and exploited as a comparator with reduced supply voltage, delay, differential resolution, and power consumption.

The proposed circuit exhibits superior performance compared to other previously reported works. The workability of the proposed comparator has been verified through ELDO simulations based on 0.18µm TSMC process. It achieves an enhanced conversion frequency (2G), low power consumption (0.07mW), a low resolution (6nA), and low propagation delay (0.62ns) from a low supply voltage (1V). The proposed comparator is very useful and attractive for low power and high-speed applications.

Keywords: low-voltage, Winner Take All, low-power, current mode , current comparator.

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JDD 2019 – MECI12

Gate shape impact on self-heating in sub-100 nm bulk MOSFET transistor

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Abstract :

A numerical analysis of heat transfer in metal-oxide-semiconductor-field-effect transistor (MOSFET) has been investigated. This thermal simulation module is based on the solution of the coupled heat flow, Poisson, and Current Continuity Equations, which is developed for the benefit of computational efficiency. Several gate shapes are used to study their effect on the maximum temperature of the device. Some comparison have made among partially insulated field-effect transistors (PiFET) under channel (PUC) and under source and drain (PUSD). A significant reduction in temperature is achieved in the new structures, suggesting that changing the gate shape can mitigate the self-heating effect.

Mots-clés : self-heating, MOSFET transistor, Finite element method, PUC-PiFET, PUSD-PiFET.

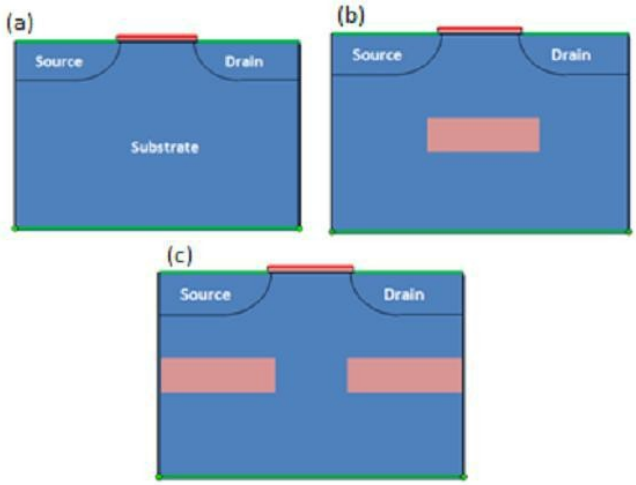

Figure 1 : Schematic geometry of bulk MOSFET (a), PUC-PiFET (b), and PUSD-PiFET (c)

Matériaux et Environnement

Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – ME01

Synthesis and characterization of [cobalt (II)/ethylenediamine and diethylenetriamine–cellulose] complexes as antibacterial agents The relationship between the geometry of matter and color

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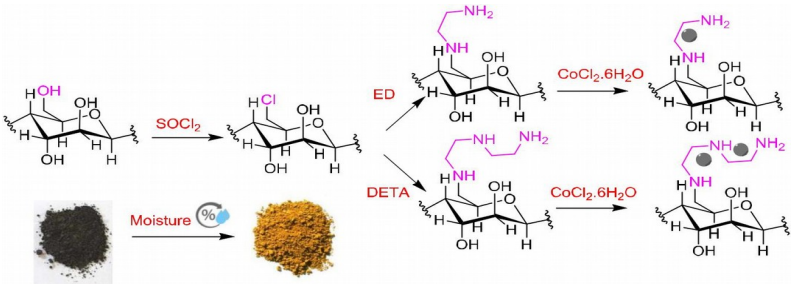
Abstract :

Ethylenediamine and diethylenetriamine grafted cellulosic fibers (ED/DETA–cellulose) were synthesized in two steps. The first step dealt with the preparation of 6-chlorodeoxycellulose (6-CDC) according to the method described by Tashiro and Shimura [1]. The second step was conducted by the reaction of (CDC) with (ED) and (DETA), subsequently the Co (II) complexes were prepared by condensation method [2]. The performance of the modified materials was characterized by FTIR, UV-Visible, TGA and SEM. Furthermore, the change of color of both complexes (materials), from green to yellow due to moisture, can be explained by the presence of a relationship between the geometry of matter and color, according to crystal field theory.

The synthesized complexes show an interesting activity against the human potent pathogenic bacterial strain *Listeria Monocytogenes*.

Keywords : cellulose, cobalt, crystal field theory, antibacterial activity.



Sheme 1 : Multi steps of prossesing [cobalt (II)/ethylenediamine anddiethylenetriamine–cellulose] complexes.

[1] T. Tashiro, Y. Shimura, Removal of mercuric ions by systems based on cellulosederivatives, J. Appl. Polym. Sci. **27**, 747-756(1982),

[2] L. Chaabane, H. Chahdoura, W. Moslah, M. Snoussi, E. Beyou, M. Lahcini, N. Srairi-Abid, M.H. Baouab. Appl. Organomet. Chem.,2019. DOI: 10.1002/aoc.4860.

Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – ME02

Hydrodistillation residues for heavy metal removal: Novel concept for waste reuse

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Abstract :

In the context of proposing a cleaner production process which aims to valorize by-products, the present study concerns a new concept of waste reuse, namely hydrodistillation residues, for the removal of heavy metals from aqueous solutions. As is known, the extraction of essential oils by the conventional extraction process requires large quantities of plant material and subsequently generates a huge stock of agricultural waste which generally remains unexploited. The idea of this study is the valorization of this abundant biomass in the purification of contaminated water. This proposed process proceeds without physical or chemical modification of the adsorbent produced. In addition to its advantage of being, clean, free and natural, this biosorbent BCH has high absorption capacities. The usage of the residues from the hydrodistillation process of *Centaurea nicaeensis* plant as a potential candidate for the biosorption of copper and zinc ions has been investigated providing a comprehensive analysis of the kinetics and equilibrium aspects to confirm the nature of adsorption mechanisms. The experiments were carried out as a function of pH, temperature, adsorbent dosage, initial metal ions concentration. In order to achieve the maximum retention, a mathematical optimization of the process parameters was performed using the Minitab statistical software with response surface methodology RSM-CCD. Under the optimal conditions obtained, the Removal (%) of metal ions could reach 82.12% and 92.02% for the zinc and copper respectively. The best fit of experimental data was achieved with the pseudo-first order kinetic model and the existence of a diffusion mechanism has been proven. The Langmuir monolayer adsorption capacities of 0,212 and 0,386 mmol.g^{-1} were obtained for zinc and copper cations, respectively. Sips isotherm gave the best fit to equilibrium data with higher (R^2= 98.91% and 99.26%) and lower SSE values (2.10 10^{-4} and 1.37 10-3) for Zn and Cu, respectively. Compared to commercial biochar's adsorption capacity, and with regard to the BET surface area, BCH (with BET surface =0.76 m^2.g-1) is nearly thirty times higher in retention capacity of copper (0.508 $mmol_{Cu}$ / m^2_{BCH}) than BCS (0.175 $mmol_{Cu}$ / m^2_{BCS}) and more than ten times better in retention capacity of zinc (0.279 $mmol_{Zn}$ / m^2_{BCH}) than BCS (0.243 $mmol_{Zn}$ / m^2_{BCS}) which presents a BET surface equal to 26.3 $m^2.g^{-1}$.

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JDD 2019 – ME03

Fonctionnalisation à base de structures organiques conjuguées des supports textiles : Développement d'un marqueur textile fluorescent

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Abstract :

L'objectif de ce travail est de développer un nouveau marqueur fluorescent. Pour faire, un matériau conjugué a été appliqué par diverses techniques (imprégnation, utilisation d'une résine, greffage) sur un fil textile 100% coton. Le support textile ainsi modifié a été caractérisé afin de mettre en évidence son caractère fluorescent qui sera exploité pour marquer et identifier un produit et par conséquent détecter les articles contrefaits ; et afin de contrôler les performances d'un tel traitement et sa répercussion sur les propriétés mécaniques du support textile.

Ainsi on a pu démontrer que l'imprégnation du fil dans un bain contenant une résine acrylique, le matériau conjugué et un absorbeur d'UV qu'est le TIO_2 permet d'obtenir un support textile fluorescent sous UV, qui résiste bien au lavage (45 min à 40°C) et à la lumière (1700 minutes suite à une exposition aux UV), tout en conservant au mieux sa résistance mécanique. Pour améliorer la permanence et la stabilité de l'effet fluorescent, on a procédé à la modification chimique du matériau conjugué de départ et ce afin de pouvoir le greffer chimiquement sur le support textile en coton. On a ainsi obtenu que pour une concentration du matériau conjugué modifié de $8\ 10^{-5}$ mol/ L et pour une réaction de greffage qui se fait à 80°C et à pH=9 pendant 4 heures, la fluorescence a résisté à 45 min de Lavage et à 12 heures d'exposition aux UV.

Mots-clés : structure textile, contrefaçon, polymères conjugués, fluorescence.

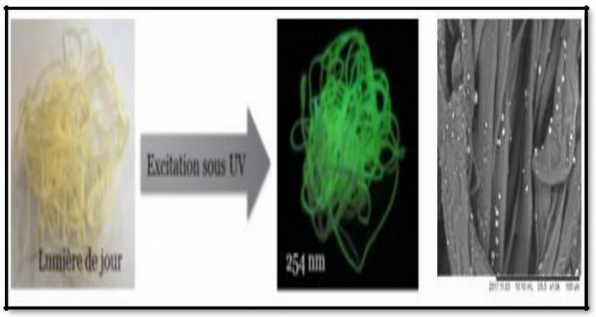

Figure 1 : Exposition du support textile fluorescent sous lampe UV.

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JDD 2019 – ME04

A new chemosensor material based on Tetrazole for the detection of heavy metal ions

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Abstract :

Chemosensors are molecules of the abiotic nature able to selectively and reversibly react with the analyte to produce a measurable signal with a real-time response (usually in less than several seconds). The general principle of operation of chemosensors is based on the phenomenon of coordination.

This communication covers an important area of the modern chemistry, namely, the detection of heavy metal ions using optical chemosensor. Thus, the importance of this method is in the toxicity of the metal ion. In fact, heavy metals are significant environmental pollutants and their toxicity is a problem of increasing significance for ecological, evolutionary, nutritional and environmental reasons [1].

The most commonly found heavy metals in waste water include arsenic, cadmium, chromium, copper, lead, nickel, and zinc, all of which cause risks for human health and the environment [2].

In fact, we developed a simple self-chemical, optical sensor for the sensing of the metal ions. In fact, the development of this type of sensor was based on the covalent attachment of Tetrazole-functionalized material with the metal ions. Monitoring was accomplished via UV– absorption spectroscopy. The response of polymer towards Cr^{2+}, Ni^{2+} and Zn^{2+} cations was studied and the results showed a good sensitivity upon addition of various metal ions.

Keywords: sensor; Tetrazole; semi-conducting polymer; Absorbance.

[1] Jaishankar, Monisha, et al. "Toxicity, mechanism and health effects of some heavy metals." Interdisciplinary toxicology ,7.2 ,60-72 (2014).

[2] Lambert, R. J. W. "Susceptibility testing: inoculum size dependency of inhibition using the Colworth MIC technique." Journal of applied microbiology 89.2 ,275-279 (2000).

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École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – ME05

Identification and Assessment of intense African dust events and Contribution to PM10 concentration in Tunisia

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Abstract :

Our study focuses both qualitatively and quantitatively on the assessment of the Contribution of the Saharan dust events to the PM10 concentration in three Tunisian sites. We Apply a current method following EC guidelines for the demonstration and subtraction of PM10 excess attributable to natural sources under the Directive 2008/50/EC. The maps and Backtrajectories used in this study have revealed coherence between the African Saharan origins, the dust transport and the intrusion during the intense Saharan dust event of 16th November, 2018.

This study shows a frequent exceedance of the average daily value of the PM10 concentration. For instance, a value of 1190µg/m^3 is measured in Gabes. This value is reduced to 160µg/m^{3}after subtracting the contribution of Saharan dust. These contributions can reach 88% of the daily PM10 measured values. After the elimination of Saharan dust contribution, the daily PM10 concentration has remained higher by 55% compared to the limit value. The daily anthropogenic PM10 concentration remained higher compared to the limit value.

A comparison between the PM10 diurnal evolutions of a Saharan dust day against a non-Saharan dust day shows the presence of one maximum out side the rush hours and the human activities during the event. However, two maxima have been registered during the two rush hour periods on a non-Saharan day, showing mainly the contribution of anthropogenic effects. Since Tunisia is close to the African Sahara, it is frequently affected by the Saharan dust outbreak as well as the anthropogenic sources.

Keywords: PM10, Regional background concentration,Saharan dust, Mediterranean.

Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – ME06

Modification of Cyano PPV via « click Chemistry » optoelectronic study

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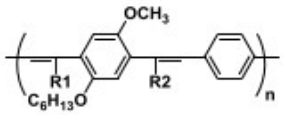
Abstract :

Organic electronics has become the most promising field following the discovery of the electroluminescence of poly (p-phenylenevinylene) (PPV). In fact, considerable progress has been made in the molecular engineering of π-conjugated polymers and their use as active components in various optoelectronic devices. Currently, semiconductor polymers find a promoting field of application in the field of chemical sonsors. In fact, our work falls within this framework, we synthesized and characterized 2 materials derived from PPV (CN-PPV and Tet-PPV). CN-PPV was prepared via the Knoevenagel polycondensation. Tet-PPV is the first tetrazole-modified PPV and was elaborated by modification of CN groups of synthesized precursor polymer (CN-PPV) using a click chemistry reaction. Indeed, the choice of functionalization of the PPV derivative by tetrazole is based on its particular complexation properties and interesting optical and electrical characteristics.



If R1, R2 :CN= **CN-PPV**
If R1 :CN et R2 : Tétrazole = **Tet-PPV**

The structural, thermal and photophysical properties of the polymers were investigated and some structure-property correlations were established depending on conjugated system nature. The obtained results showed a significant effect on the solid-state morphology and electronic properties. The absorption study demonstrated as well that the incorporation of the tetrazole units in Tet-PPV considerably decreased in the optical gap and promotes the π-π interactions between the conjugated systems in the solid state. The HOMO and LUMO levels determined by cyclic voltammetry show that the polymer Tet-PPV is a *p*-type semiconductor. The complexation study of the two polymers shows that the cyno-polymer CN-PPV has a sensitivity towards Pd2 + ions. However, the polymer containing tetrazole groups has good sensitivity for Pd2+ and Mg2+ ions. This behavior is attributed to the incorporation of the tetrazole groups into the macromolecular backbone.

Key words: Optical sensor, Semiconductor polymer, PPV, Optical property.

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JDD 2019 – ME07

Study of ethanol flux adsorbed by activated carbon

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Abstract :
In adsorption studies by microporous solids, the microporous structure of an adsorbent material is a key element for the implementation of all applications. The quantitative description of the pore structure in terms of pore size distribution (PSD) plays a very important role in the kinetic study of the adsorption of a gas by microporous solids.
In this paper, we propose a study based on the flow of the material quantity through a closed surface, which shows that the adsorption of a gas by a microporous solid passes through two stages: adsorption within micropores and mesopores, adsorption within macropores and on the lateral surface. The study allowed us to show the existence of two types of interaction forces between the adsorbate molecules and the adsorbent, each type of forces corresponds to one of the stages. The first type of force corresponds to a volume filling (adsorption in micropores and mesopores). The second corresponds to a multilayer adsorption in the macropores and on the lateral surface. These results justify the existence of two most common used models: Dubinin-Astakov (in the case of microporous filling) and Brunauer, Emmet and Teller (BET) (in the case of multilayer adsorption).

Keywords: Adsorption, Microporous solids, Flow, Interaction potential.

Matériaux et Nanostructures : Élaboration et Caractérisations

Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – MNEC01

MOF-199 thin film converted from copper(II) hydroxide nanoparticles at room temperature

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Abstract:

The processing of Metal organic frameworks (MOFs) as thin films is a topic of pronounced technological importance [1]. In fact, MOFs are a promising class of porous nanostructured materials constructed from metal ions and organic linkers [2]. The preparation of microporous thin films of these materials adds to their applicability as sensor coatings, membranes and catalysis [2]. In these circumstances, many innovative synthetic strategies for MOF thin film have been recently reported including layer-by-layer deposition on solid substrates.

In this work, we have studied the effect of EtOH/ H2O volume ratio of the precursor solution on morphology and homgeneity of MOF-199 thin film, prepared from. copper(II) hydroxide nanoparticule via layer by layer growth method. The structural and morphological studies of obtained film were characterized using ATR-FTIR(IR), Fourier X-ray diffraction (XRD) and optical microscopy. We showed that the lower EtOH/ H2O volume ratio prometed the deprotonation of H3btc in the conversion solution leading to large crystals

Keywords : Copper hydroxide, MOFs, conversion

[1] H. Furukawa , Cordova. KE, O'Keeffe .M, Yaghi. OM, Science, 341, 1230444 (2013)

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Faculté des Sciences de Monastir
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JDD 2019 – MNEC02

Electrical and optical characterization of silicon nanowires for photovoltaic applications

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Abstract :

This work presents analysis of the electrical and optical characteristics of silicon nanowires samples developed by the chemical etching method (Ag-ACVE). The main aim of this work is to characterize the surface species of the silicon (SiNWs) by Fourier transform infrated (FTIR) in reflection measurement mode. In this study, we also discussed the significant enhancement in the peak intensities in Raman spectra of SiNWs.Our results have confirmed that FTIR, Raman measurements demonstrated here are important methods for characterizing interface defects in SiNWs. Moreover,SiNWs were also characterized using current-voltage(I-V) andcapacitance-voltage(C-V) measurements at room temperature.Electrical parameters such as series resistance (Rs) ,ideality factor (n), barrier height (Φb) and doping concentration atoms (NA) were investigated. Overall, I-V and C-V plots of the SiNWs were closed to what was predicted in the literature.

Keywords: Silicon nanowire, FTIR, Raman, I-V, C-V.

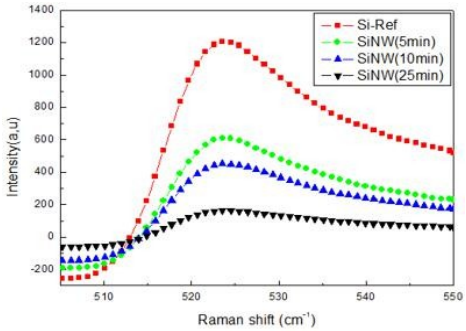

Figure 1 :Raman spectra of SiNWs measured at room temperature with the power 30mW.

[1] Ferrari, A. C., Piscanec, S., Hofmann, S., Cantoro, M., Ducati, C., & Robertson, J.Raman spectroscopy of silicon nanowires: Phonon confinement and anharmonic phonon processes. AIP Conference Proceedings , 685, 507-510 (2003).

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JDD 2019 – MNEC03

Effects of rare earth elements on structural, electrical and optical properties of 0.975KNN-0.025NBT ceramics

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Abstract

The Effect of Lanthanides Ln3+: Er, Eu, Dy, Nd ions incorporation on structure, microstructure, dielectric and photoluminescence properties of lead-free 0.975 K1/2Na1/2NbO3 -0.025Na1/2Bi1/2TiO3 (NBT) ceramic prepared via solid state reaction were investigated. XRD analyses evidenced the symmetry biphasic "orthorhombic Amm2 + monoclinic Pm" with great percent of Amm2 symmetry. SEM measurement shows ceramics possessing better compositional homogeneity and finer grains. Different Raman intensity arising to the deformed octahedral symmetry caused by the increased disorder of the A and B sites respectively. The relaxor –like characteristics and good dielectric proprieties has been obtained for KNNBT:Er and KNNBT:Nd (εr = 24882, εr = 39398, respectively at TC and 1KHz). New dielectric anomaly at room temperature for KNNBT:Eu and KNNBT:Dy (εr = 1113 at 311 K, εr = 3928 at 327 K) were detected. Photoluminescence shows that the introduction of RE3+ ions in the 0.975KNN-0.025NBT host lattice shows different light emissions over the wavelength range from visible to near infrared region. These overall properties show that Ln3+ doped 0.975KNN-0.025NBT ceramics have great potential in multifunctional optoelectronic application.

Keywords: solid state reaction; ceramics; dielectric proprieties; photoluminescence.

Faculté des Sciences de Monastir
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JDD 2019 – MNEC04

GINA's Photo-Electrical Properties for Optoelectronic and Photovoltaic Applications

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Abstract :

GaInNAs so called GINA has been grown on GaAs substrate by molecular beam epitaxy. This work aims to reveal physical properties of this quaternary via photocurrent (PC) and photoluminescence (PL) techniques. PL spectrum has reached the telecommunication wavelengths 1.3-1.55 µm and it has shown an asymmetric line shape of PL intensity near band edge emission. This signature may be referred to the non-uniform distribution of N atoms in the host matrix and to the alloy fluctuations. In addition, PC measurement was performed by showing a small contribution of GINA (compared to GaAs) to the photogenerated current. The latter may be related to the short diffusion length of the minority carriers and the high defect density due to N incorporation. This problem can be remedied by thermal annealing to minimize the omnipresent defects in dilute III-V nitrides. This makes GaInNAs a promoted material for photovoltaics.

Mots-clés: GaInNAs, Photoluminescence, Telecommunication wavelengths, Photocurrent.

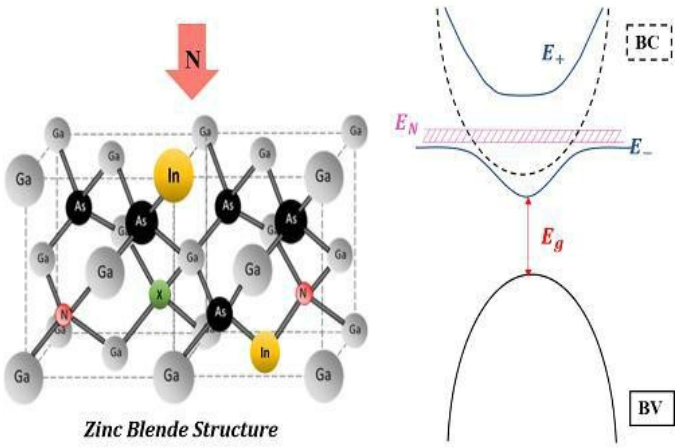

Figure 1 : Bandgap shrinkage after nitrogen incorporation into InGaAs ternary

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JDD 2019 – MNEC05

Critical behavior around the paramagnetic-ferromagnetic phase transition and estimation of the spontaneous magnetization through magnetic entropy change in $La_{0.7}Sr_{0.3}Mn_{0.9}Cu_{0.1}O_3$

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Abstract :

$La_{0.7}Sr_{0.3}Mn_{0.9}Cu_{0.1}O_3$ ceramics was synthesized via the sol–gel reaction method. Structural, magnetic and magnetocaloric properties have been investigated. X-ray diffraction displays that our compound crystallizes in the rhombohedral structure with the $R^{-}(3\ )$ c space group. Magnetic measurements indicated the presence of a second order phase transition. According to hysteresis cycles, for our studied sample, at 10 K a typical soft FM behavior with a low coercive field was observed. Through various approaches such as modified Arrott plot (MAP), Kouvel-Fisher (KF) method and critical isotherm analysis, the critical parameters (β, γ, and δ) as well as the Curie temperature T_C have been determined. The critical exponents values for our sample (β=0.489±0.003 with T_C=323.41K±0.23, γ=1.014±0.020 with T_C=324.32K±0.48 and δ= 3.074) are found to be close to the mean-field theory, indicating the existence of long range ferromagnetic coupling in our system. The reliability of these critical parameters was confirmed by both the universal scaling hypothesis and the Widom scaling relation. Additionally, to estimate the spontaneous magnetization $M_S(T)$, we use a process depend on the analysis of the magnetic entropy change (- S_M). A satisfactory accord was found between the values of the spontaneous magnetization determined from the entropy change ((-S_M) vs. M_2) and those obtained from the extrapolation from the Arrott curves ($\mu_0 H/M$ vs.M^2).

Mots-clés : Critical behavior ; mean-field theory ; spontaneous magnetization ; Model of Hamad.

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JDD 2019 – MNEC06

Effect of Fe Doping on the Structural, Magnetic and Magnetocaloric Properties in $La_{0.6}Ba_{0.2}Sr_{0.2}MnO_3$

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Abstract:

In this paper, we investigate the effect of iron doping at the Mn site on the structural, magnetic and magnetocaloric properties of La0.6Ba0.2Sr0.2Mn1-xFexO3 (0< x< 0.06) samples. Our compounds are prepared using the solid state reaction method at high temperature. The X-ray diffraction pattern refined by the Rietveld method showed that all samples crystallize in the rhombohedral system with R 3c space group. Magnetic measurements have shown that our samples undergo a FM-PM transition around the Curie temperature (Tc). The Curie temperature Tc decreases with Fe content from 349K for x = 0 to 249K for x = 0.06. The change of the maximum values of the magnetic entropy were found to be 2.43 $JKg^{-1}K^{-1}$, 2.16 $Jkg^{-1}K^{-1}$ and 1.65 $Jkg^{-1}K^{-1}$ under a magnetic field change of 5T for x =0, 0.03, and 0.06 respectively. The relative cooling power (RCP) values vary between 245.36 and 302.02 Jkg^{-1} this makes our samples a suitable candidates for magnetic refrigeration applications.

Mots-clés : manganite, Magnetic entropy change, Magnetocaloric effect, magnetic refrigeration.

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JDD 2019 – MNEC07

Copper-doped lanthanum manganite $La_{0.65}Ce_{0.05}Sr_{0.3}Mn_{1-x}Cu_xO_3$ influence on Structural, Magnetic and Magnetocaloric Effect

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Abstract :

Bulk nanocrystalline samples of $La_{0.65}Ce_{0.05}Sr_{0.3}Mn_{1-x}Cu_xO_3$ ($0 \leq x \leq 0.15$) manganites are prepared by the sol–gel based Pechini method. The effect of the substitution for *Mn* with *Cu* upon the structural and magnetic properties has been investigated by means of X-ray diffraction (*XRD*), Raman spectroscopy and dc magnetization measurements. The structural parameters obtained using Rietveld refinement of *XRD* data which showed perovskite structure having rhombohedral (*R-3c*) symmetry without any detectable impurity phase. The analysis of the crystallographic data suggested a relationship between a distortion of the MnO_6 octahedron and the reduction in the Curie temperature, T_C. Paramagnetic to Ferromagnetic phase transition at T_C, is observed. The experimental results confirm that *Mn*-site substitution with *Cu* destroys the *FM* interaction in $La_{0.65}Ce_{0.05}Sr_{0.3}Mn_{1-x}Cu_xO_3$ matrix The maximum magnetic entropy change is found to decrease with increasing of *Cu* content from 4.43 $J.kg^{-1}$ K^{-1} for x = 0 to 3.03 $J.kg^{-1}$ K^{-1} for x = 0.15 upon 5T applied field change.

Mots-clés : Perovskite manganite, Pechini sol – gel method, X-ray diffraction, Raman spectroscopy, magnetocaloric effects.

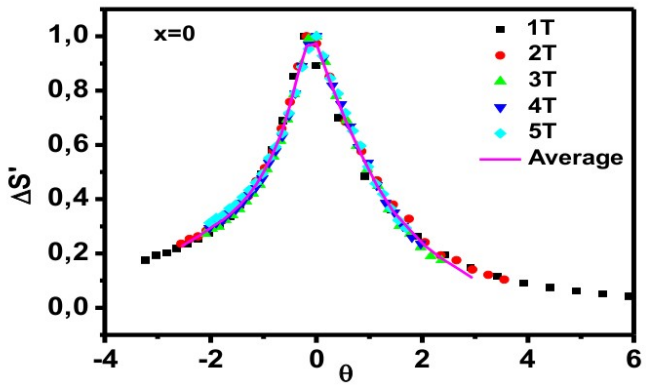

Figure 1 : Normalized S_M versus rescaled temperature θ for $La_{0.65}Ce_{0.05}Sr_{0.3}Mn_{1-x}CuxO_3$, the solid line is the average curve.

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JDD 2019 – MNEC08

Electrical properties of $Ba_{0.97}La_{0.02}TiO_3$ ceramics at room temperature

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Abstract :

We report here the electrical properties of $Ba_{0.97}La_{0.02}TiO_3$ ceramics prepared by the molten salt method. The X-ray diffraction pattern of the sample at room temperature showed a single perovskite phase having a tetragonal structure with a P4/mmm space group. The electrical properties were studied by complex impedance spectroscopy in the frequency range (1-10^7Hz) at room temperature. The real and imaginary parts of the impedance decreased with the increase of frequencies. The Warburg element explains the complex impedance plot with a single impedance semicircle for this compound, identified at high and medium frequencies, followed by a linear low frequency section.

Mots-clés : Molten salt, Perovskite, Warburg element.

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JDD 2019 – MNEC09

Room temperature magnetocaloric effect and critical behavior in $La_{0.67}Ca_{0.23}Sr_{0.1}Mn_{0.98}Ni_{0.02}O_3$ oxide

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Abstract :

The structural, magnetic and magnetocaloric properties of nano-crystalline manganite are investigated systematically. The compound is elaborated based on Pechini sol-gel method and then annealed at 1000 °C for 24 h. X-ray powder diffraction shows that, the sample crystallizes in a rhombohedral structure with space group. A magnetization versus temperature study shows that the compound exhibits a second-order magnetic transition from a ferromagnetic to a paramagnetic state at a Curie temperature = 263 K 296 K. To evaluate the magnetic entropy change we measure the magnetization as a function of temperature and magnetic field. At ambient temperature, we find that sample has a very important magnetocaloric effect (MCE). In a magnetic field variation of 5 T, this MCE is explained by a maximum of magnetic entropy change and a big RCP values at 4.92 and 145 J / kg, respectively, around room temperature (296 K), which give the possibility of technologic application in magnetic refrigeration area. In addition, we find an admirable estimate of the magnetic entropy change, which is based on the Landau theory. Finally, we use the magnetic field dependence of to determine the critical exponents of the system and we find that β=0.39, γ=1.35, and δ=4.43, are very close to those predicted to the 3D-Heisenberg model. These results indicate that the present compound is one of candidate materials for magnetic refrigerators near room temperature.

Mots-clés: Magnetocaloric effect, Sol-gel mehod, Entropy change, 3D Heisenberg model.

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JDD 2019 – MNEC10

Overview on electrets material for electrostatic energy harvesting

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Abstract:

During the last years, electrets, stable electrically charged dielectrics [1], have seen a growing interest particularly as initial voltage source for electrostatic transducers for energy harvesting systems, schematized in figure 1. Consequently, different works have investigated the characterization of electrets and charges injection technics for their fabrication. We present in this paper an overview on the main used electrets for electrostatic harvesters and their characterization technics.

Key words: Dielectric materials, Electret, Charge injection, Electrostatic transduction

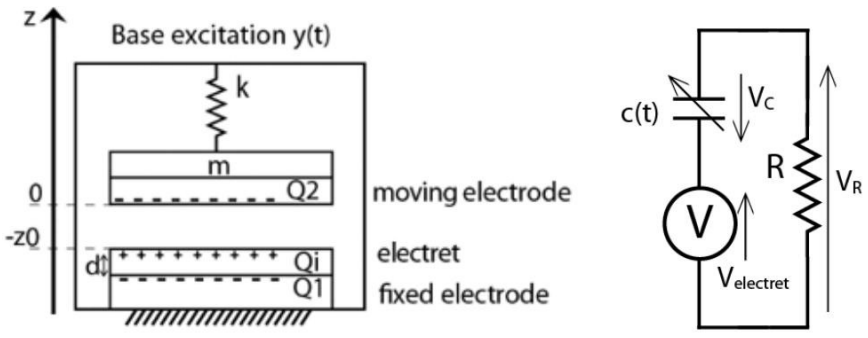

Figure 1: Schematic principle of electret-based electrostatic harvesting (left) electromechanical system (right) electrical modelization.

[1] S. Boisseau, G. Despesse, T. Ricart, E. Defay, and A. Sylvestre, "Cantilever-based electret energy harvesters," *Smart Materials and Structures*, vol. 20, no. 10, p. 105013, 2011.

Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – MNEC11

Temperature effect on GaN:Bi growth behavior

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Abstract :

Undoped GaN and diluted GaNBi alloys were grown on (0001) sapphire substrate by metalorganic vapor phase epitaxy (MOVPE) at 480°C, 510°C and 550°C. By using in-situ laser reflectometry, it is found that the increase of growth temperature did not almost affect the average value of reflectivity oscillations for the undoped GaN series. However, for the diluted GaNBi alloys, this temperature increase leads to a decrease in the relative reduction of the average value. Scanning electron microscopy (SEM) images gave a clear observation of the surface morphology. The energy dispersive X-ray (EDX) analysis showed that the diluted GaNBi alloys contain islands which are rich in Bi compared to the flat GaN surface, and distributed randomly on the GaN surface. The appearance of those structures could be responsible to the reduction of the reflectivity oscillations average value. The growth temperature increase leads to a decrease in the density of the islands with an increase in their size. Moreover, the surface morphology between islands is improved justifying then the surfactant effect of bismuth and the results of in-situ reflectometry.

Mots-clés : MOVPE, GaN, Bismuth, SEM.

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JDD 2019 – MNEC12

Numerical simulation for determining optoelectronic properties of strained $GaN_xAs_{1-x-y}Bi_y$ using Pikus-Bir theory

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Abstract :

The ***k.p*** and Pikus-Bir theories were adopted in the investigation of strained $GaN_xAs_{1-x-y}Bi_y/GaAs$ optoelectronic properties. This study was performed at room temperature in terms of band gap , spin-orbit splitting Δ_{so} and interbands transition energies. The incorporation of a small N or Bi content affects the strain types and induces a large variation in the properties of these alloys. As results, we note essentially that a little nitrogen influence in Δ_{so} energy was found compering with that of bismuth. It is also proved that *GaNAsBi* alloys have the potential to cover a wide spectral range from near-to mid-infrared with flexible control of the band gap and spin-orbit splitting as a function of N and Bi contents. The CHSH Auger and intervalence band absorption (IVBA) suppression ($\Delta_{so}>E_g$) is possible over a wide range of band gaps raising the additional possibility of highly efficient GaAs-based lasers operating in the mid-infrared.

Keywords:

GaNAsBi/GaAs structures; k.p method; Pikus-Bir theory; optoelectronic properties; Strain.

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JDD 2019 – MNEC13

Fluorescence sensor based on 3-mercaptoprponic acid capped CdTe/ZnSe QDs for detection of Ag^{+} ions in aqueous solution

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Abstract:

Quantum dots (QD) of the II-IV family have attracted considerable interest due to their size-dependent chemical, optical and physical properties that allow their direct application in lasers, semiconductor lighting, solar cells and biomedical domains (in vivo and in vitro imaging). In this study, an easy method was introduced in the preparation of CdTe QDs covered by a shell (CdTeZnSe) surrounded by a 3MPA legend to be applied as a new optical nano-sensor for the detection of Ag ions in aqueous solutions. The CdTeZnSe QDs prepared have been characterized using different analytical techniques, in particular the X-ray diffraction (XRD) of the CdTe shows that the nanocrystals have the zinc blend structure. After the growth of the ZnSe layer at the periphery of the CdTe core, the diffraction peaks move to the standard position of the ZnS blind structure. This result proves the formation of the core / shell structure and indicates the diffusion of Zn2 ions in the core of the CdTe system, which results in a modification of the parameters of the crystal lattice of the nanocrystals of the CdTe system. Transmission electron microscopy (TEM) analyzes show spherical CdTeZnSe with an average diameter of about 4mm. It was found that the fluorescence intensity of CdTeZnSe at 640 NM (excitation at 410 NM). QDs were selectively deactivated in the presence of traces of Ag ions relative to different metal ions. In other words, a simple, very sensitive, selective and fast analytical approach has been used for the detection of Ag ions in the (0-12) $\times$ 10^{-4} µM concentration range with a detection limit of 2,91 $\times$ 10^{-4} µM and quantification limit 8.83 $\times$ 10^{-4} µM.

Keyword: CdTe quantum dot, Core shell, detection.

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JDD 2019 – MNEC14

Synthèse et caractérisation des Quantum Dots ZnSeS dopé Manganèse

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Abstract :

Depuis quelques années, les QDs ternaires connaissent un développement exponentiel grâce à leur photoluminescence qui peut être contrôlée par leur taille et également par leur composition. Ils ont attiré l'attention, non seulement pour les études fondamentales, mais également pour leurs applications potentielles dans les diodes électroluminescentes, le marquage biomédical, les cellules solaires et la photocatalyse. Le dopage des nanocristaux ZnSeS par des cations de métaux de transition comme Mn2+ permet de doter les QDs de nouvelles fonctionnalités par modulation des propriétés électroniques et optiques et donc d'avoir de nouvelles applications (magnétisme, dispositifs électroluminescents, capteurs, lasers, sondes pour l'imagerie de fluorescence, …). Dans la présente étude, la synthèse en milieu aqueux, la caractérisation et les propriétés optiques des QDs ternaires ZnSeS, ZnSeS dopé par le Manganèse et les QDs cœur/ coquille ZnSeS:Mn/ZnS sont présentées. Différents paramètres de synthèse tels que le ligand, le pH du milieu réactionnel et le pourcentage de dopant ont été modifiés. Le dopage des QDs ZnSeS par le Mn a permis un fort déplacement de Stokes et d'éviter tout recouvrement entre l'absorption UV-visible et la fluorescence, surtout lorsque les nanocristaux sont utilisés à forte concentration. Typiquement, le dopage par Mn2+ génère une émission vers 590 nm (transition 4T1 → 6A1 de l'ion Mn2+) alors que le matériau non dopé émet à environ 480 nm. Les diagrammes de diffraction des rayons X (DRX) des QDs ZnSeS sont présentés, les analyses en microscopie électronique à transmission (MET) montrent que les QDs ZnSeS :Mn sont sphériques d'un diamètre moyen d'environ 2.5 nm. Les spectres de photoluminescence (PL) des échantillons (ZnSeS, ZnSeS :Mn, ZnSeS :Mn/ZnS) ont été enregistrés à différents stades de la croissance des nanoparticules afin d'optimiser leurs propriétés optiques en ajustant les paramètres de synthèse. Pour le pourcentage de Mn=10%, le spectre PL des ZnSeS :Mn QD présente une bande d'émission centrée à 580 nm. Après l'introduction de la coque de ZnS, un légère décalage rouge du pic de PL est observé et l'émission de PL est située autour de 585 nm, ce qui confirme la formation de nanocristaux ZnSeS:Mn/ZnS. Ces QDs présentent aussi une photostabilité même pendant 3h sous irradiation d'une lampe solaire ainsi que sous irradiation d'une lampe Hg-Xe d'intensité égale à 50 mW/cm2. On observe une augmentation de l'intensité de photoluminescence, ce qui indique que ces nanoparticules sont stables.

Mots-clés : Nanoparticules, dopage, fluorescence, déplacement de stokes , photostabilite

Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – MNEC15

Study optical properties of the perovskite $Ba_{0.96}Nd_{0.0267}Ti_{(1-x)}W_xO_3$ceramic synthesized using Molten Salt Method

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Abstract :

The Ba 0.96 Nd 0.0267 Ti (1-x) W x O 3 (BNTx) ceramic with a single phase tetragonal structure was synthesized by the Molten Salt method. Raman spectra, absorption spectra (Vis-NIR), photoluminescence spectra (PL) in the temperature range from 10- 300K were used to investigate the correlations between the crystal structure and the optical properties of BNTx ceramics. Raman analyses indicated that the W +6 ions are incorporated sufficiently into in BNTx lattice. The optical absorption spectra were recorded in the wavelength ranges of 400- 1000nm. The emission spectra exhibited three prominent peaks located at 880, 1058 and 1340 nm corresponding to the $^4F_{3/2} -> {}^4I_{9/2,11/2,13/2}$ transition levels, respectively. It also, showed a decrease in the intensity of emission spectra following the addition of W 6+ ions. This decrease is due to the slight changes in the crystal environment around Nd 3+ and the nonradiative energy transfer.The temperature-dependent PL emission spectra of the BNT x (x=0.00 and x=0.05), we notice that the PL intensity gradually decreased with increasing the temperature from 10 to 300K. This decrease is due to the temperature-dependence of the electron-phonon interaction.

Mots-clés : Perovskite; Raman; Photoluminescence; Optical properties; Energy transfer; Rare-earth.

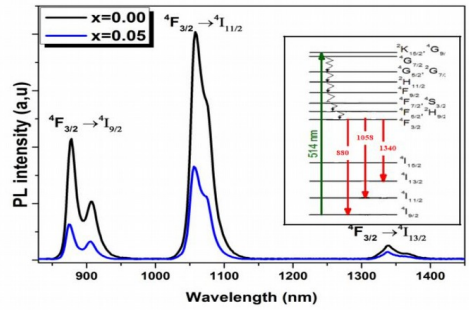

Figure 1 : Emission spectra of the $Ba_{0.97}Nd_{0.0267}Ti_{(1-x)}W_xO_3$ ceramics excited at 514nm at room temperature. Inset Schematic energy level scheme of Nd^{3+} ions in $Ba_{0.97}Nd_{0.0267}Ti_{(1-x)}W_xO_3$ (x=0.00 and x=0.05).

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JDD 2019 – MNEC16

Electrical properties and percolation model in $La_{0.75}Ca_{0.25-x}Na_xMnO_3$ for x= 0 and 0.05 type manganites

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Abstract :

In this communication, $La_{0.75}Ca_{0.25-x}Na_xMnO_3$ (x= 0 and 0.05) samples were synthesized by Flux method and their structural and electrical properties had been systematically undertaken. X-ray diffraction of our samples showed an orthorhombic structure with Pbnm space group. Furthermore, to get a better understanding of the electrical properties, the resistivity ρ (T) as a function of temperature was measured by a standard four-probe method. The maximum resistivity values decreased and the insulator-metal transition temperature (T_{M-SC}) shifted to a higher temperature with increasing magnetic field. At low-temperature region ($T < T_{M-SC}$), ρ was fitted by the equation $\rho(T) = \rho_0 + \rho_2 T^2 + \rho_{4.5} T^{4.5}$ which indicates that the transport mechanism is governed by a combination of electron-electron, electron– magnon and electron-phonon scattering processes. Also, at high-temperature ($T > T_{M-SC}$) region the transport mechanism was explained using the adiabatic small-polaron hopping and the variable-range hopping models. Then, to get into insight into the change in the resistivity plots, in entire temperature, ρ (T) was fitted by the percolation model. Interestingly, we note that the activation energy (Ea) decreased with increasing Na^+ content which indicates the enhancement of the double exchange (DE) interaction.

Mots-clés: percolation theory, metal-insulator transition, small polaron hopping

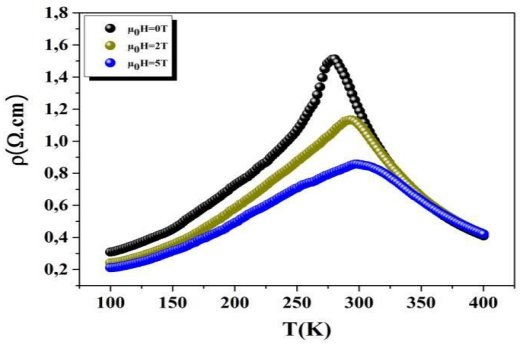

Figure 1: Electrical resistivity ρ (T) as function of temperature for $La_{0.75}Ca_{0.20}Na_{0.05}MnO_3$

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JDD 2019 – MNEC17

Comparative study on structural and optical properties of GaN grown on (100) and (113) GaAs substrates

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Abstract:

The growth of cubic GaN layers on (001) and (113) oriented GaAs substrates were investigated by metal organic vapor phase epitaxy (MOVPE). The growth of low temperature GaN nucleation layers (500-550 °C) was in-situ monitored by laser reflectometry (LR). The simulation of experimental reflectivity curves, by using an optical model which includes both time-dependent growth rate and surface roughness profiles, shows differences between growth kinetics depending on substrate orientation. Thus, growth anisotropy was observed. The effect of high temperature (750-900 °C) GaN sublayers grown on 130 nm thick GaN buffer layer deposited on (113) GaAs substrate at low temperature (550 °C) was analyzed. The GaN sublayers were ex situ characterized by scanning electron microscope (SEM), high resolution X-ray diffraction (HRXRD) and room temperature cathodoluminescence (RT-CL). Based on comparative study between structural and optical qualities of GaN layers grown on the two substrate orientations, we conclude that the crystalline structure strongly depends on both temperature and substrate orientation. The SEM micrographs and $2\theta/\omega$ spectra showed that the oriented GaAs promotes the alignment of cubic GaN (113) columns at a growth temperature close to 850°C. For this temperature, the RT-CL spectra exhibited only cubic GaN emission (3.23eV) for the two orientations (001) and (113) of GaAs substrate.

Mots-clés : MOVPE, c-GaN(113), GaAs(113) substrate, HRXRD, Cathodoluminescence.

Faculté des Sciences de Monastir
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JDD 2019 – MNEC18

Thermal expansion contribution to the temperature dependence of the band gap in InGaAs and GaAsBi alloys

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Abstract :

Photoluminescence (PL) and photoreflectance (PR) measurements have been used to determine the band gap energy of $In_xGa_{1-x}As$ and $GaAs_{1-x}Bi_x$ alloys. The temperature dependence of optical transitions in the temperature ranging from 12 to 300 K were investigated. Three theoretical models (Varshni, Viňa, and Pässler) were used to fit the experimental points. The results show that the temperature dependence of the fundamental gap energy, E_g (T), is attributed to the sum of two contributions: the thermal expansion (TE) and the electron-phonon interaction (EPI). For InGaAs with different In concentrations (x=0, 0.08, 0.16 and 0.37), the contribution to the EPI of the longitudinal optical (LO) phonon increases, relatively to the longitudinal acoustical (LA) phonon, with increasing In concentration. In the low temperature range, the small decrease in the optical transition energy is explicated by the competition between the two contributions (TE and EPI). At high temperatures, the linear decrease of gap energy is explained essentially by the EPI. Additionally, we have estimated the thermal expansion coefficient of GaAsBi with different Bi concentration (x=0.013, 0.037 and 0.048). The results show a slowly decrease in the TE with temperature and Bi composition. This effect is considered to play an important role in the reduction of the temperature dependence of the band gap energy of GaAsBi alloys. GaAsBi alloys are important materials for the fabrication of temperature insensitive optical devices.

Mots-clés : InGaAs/ GaAs structures, GaAsBi/ GaAs structures, energy gap, thermal expansion, electron-phonon interaction.

Études des milieux réactifs et ionisés

Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – EMRI01

Magnetocaloric Effect in Ni doping Manganite near Room Temperature

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Abstract :

In this paper, we showed the effect of Ni doping on the physical properties of $La_{0.8}Na_{0.2}Mn_{1-x}Ni_xO_3$ perovskite manganites. All the compounds crystallized in the rhombohedral structure with space group. Magnetic studies, M(T), showed a Ferromagnetic (FM) – Paramagnetic R3c (PM) phase transition around the Curie temperature (TC). The several values were found to be 297 K, 275K and 257 K for x = 0, 0.03 and 0.06, respectively. A monotonous decrease in TC was achieved with the increase of Nickel content. This decrease can be related to the weakness of the Mn^{3+}-O-Mn^{4+} double exchange (DE) mechanism. The magnetocaloric effect (MCE) has been estimated through the calculation of the magnetic entropy change as a function of temperature at different applied magnetic field. The highest values of the magnetic entropy change $-\Delta S_M^{max}$ at 5T applied magnetic field were found to decrease from 4.5± 0.1 J. kg^{-1}. $K^{-1}$to 3.7±0.1 J. kg^{-1}. K^{-1} for x = 0 and 0.06, respectively, with Ni doping.

Mots-clés : Manganite, Sol-Gel, Magnetic entropy change, magnetocaloric effect.

Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – EMRI02

Exploration of large amplitude motions in the Ca^+Ar_2 complex

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Abstract :

We present a theoretical study of the ground electronic state potential of the Ca^+Ar_2 complex and of its photoabsorption spectra, simulated at temperatures ranging between 20 and 220 K. These calculations exploit a Monte-Carlo (MC) method based on a one -electron pseudo-potential approach, a MC random walk is used to select a series of geometries that are representative of ground-state Ca^+Ar_2 clusters at temperature T. A pairwise additive potential fitted to coupled cluster ab initio points, is used to model the Ca^+Ar_2 complex, where Ar-Ar and Ca^+-Ar interactions are described by the Lennard Jones and Tang-Toennies potential, respectively. The Ca^+-Ar_2 complex has previously been found to exhibit quasi-linear or linear minimum energy geometry, with an additional bent local minimum [J.Velasquez, K.N.Kirschner, J.E.Reddic and M.A.Duncan, Chem.Phys. Lett. 343, 613 (2001)]. In the present work, the geometry of Ca^+Ar_2 is found to be bent (C_{2v} symmetry). The one electron pseudo-potential model explains these conclusions and is able to account almost quantitatively for the binding energy of the second Ar atom. Trends in binding energies De, bond lengths and bond angles are discussed. Analysis of the spectrum establishes that the complex is bent, where a structural transition to the linear geometry is found at T=100K. Additionally, the results are presented and discussed in terms of orbital hybridization, combined with the success of our potential model; the expectation that these complexes are all physically bound is confirmed.

Mots-clés : photoabsorption spectra, One-electron Pseudopotential Model, MonteCarlo method, Bent Ca^+Ar_2

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JDD 2019 – EMRI03

One-electron pseudo-potential investigation of Na(3s) Xe_n and Na(3p) Xe_n Clusters

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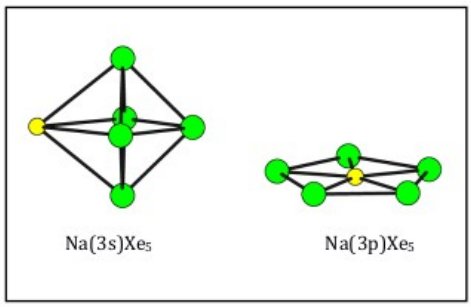
Abstract :

We present a quantum-classical determination of stable isomers of NaXen clusters with both an electronic 3s ground state and 3p excited state of the sodium atom. The Na atom is perturbed by xenon atoms in NaXen clusters. The energy of the system is described using additive potentials with VNa-Xe and VXe-Xe representing the pair interactions. The electronic structure of the alkali valence electron in the environment of the rare gas atoms is determined via a procedure close to the ab initio methodology involving e-Na+ and e-Xe semi-local pseudo-potentials complemented by core polarization operators. The geometry optimization is carried out via the basin-hopping method of Wales et al1. The present study confirms that for the 3s ground state, the sodium atom remains weakly bound to the surface of the xenon clusters, while for the 3p excited state, the small NaXen clusters tend to form ring-type planar geometries.

Mots-clés : Clusters, Structures, Pseudo-Potential method, Basin-Hopping method



[1] D. J. Wales and J. P. K. Doyle. J. Phys. Chem. A 101- 5111 (1997).

Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – EMRI04

Ab-initio calculations of the electronic structure of the BaX (X=Rb, Cs) molecules, with and without spin-orbit effect

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Abstract :

An *ab initio* approach based on the effective core potentials ECP, core polarization potentials CPP with three valence electrons and multireference configuration interaction MRCI level of calculation, is used to determine the adiabatic potential energy curves, the spectroscopic constants and the permanent and transition electric dipole moments of the lowest doublet and quartet electronic states of BaAlk (Alk=Rb, Cs) molecules. These states are dissociating into the first six asymptotic limits of the alkali—alkaline earth molecules, BaAlk. Only the ground state has been studied in the literature [1] for both molecules and the comparison with the available results has shown a very good agreement. Both relativistic and nonrelativistic calculations are presented, which allows us to determine the influence of Spin-orbit coupling.

Mots-clés : Clusters, Structures, Pseudo-Potential method, Basin-Hopping method

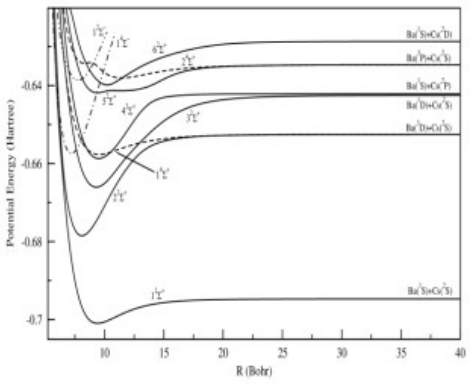

Figure 1 : . Potential energy curves for $^2\Sigma^+$(solid lines) and $^4\Sigma^+$ (dashed lines) states of BaCs.

[1] Gou, D.; Kuang, X.; Gao, Y.; Huo, D. *Theoretical study on the ground state of the polar alkali metal-barium molecules: Potential energy curve and permanent dipole moment.* J. Chem. Phys. 2015,142, 034308.

Matériaux pour l'énergie solaire

Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – MES01

$MAPbBr_3$ Perovskite Solar Cells via two-step deposition process

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Abstract :

Photovoltaic cells based on hybrid organic-inorganic perovskite materials are currently the most competitive emerging technologies and promising in the field of photovoltaics. In this work, simple structures of the type: ITO / PEDOT: PSS / $MAPbBr_3$ are developed using a two-step method based on the transformation of PbBr2 into perovskite MAPbBr3 after dipping in a MABr solution. By dip-coating time study we have demonstrated that for dip-coating time of 10min we have showed an improvement in the structural, optical and electrical properties in hybrid perovskite film. The optical absorption intensity has been increased. The intensity of photoluminescence (PL) emission has been decreased, which indicating an efficient charge transfer. Similarly, the structural properties are improved. We have also demonstrated that the increase in annealing time have induced the enhancement of perovskite properties. In conclusion, the perovskite solar cell elaborated with a "dip-coating" time and an annealing time for 10 min, exhibited the highest power conversion efficiency of 4.8%, with a short circuit current density of 16.16 mA.cm−2, an open circuit voltage of 0.84 V, and a fill factor value of 35.50.

Keywords : Hybrid inorganic-organic perovskite; $MAPbBr_3$; Dip-coating Method ; annealing time ; Optical ; sturctural ; electrical properties

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JDD 2019 – MES02

Enhanced optical and electrical properties in ternary hybrid structure for photovoltaic application

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Abstract :
The use of ternary blend is currently being pursued to enhance the different properties of bulk heterojunction solar cells by expanding the spectral range of light absorption [1]. we report a ternary hybrid structure containing one donor polymer poly[N- 9'-heptadecanyl-2,7-carbazole-alt-5,5-(4,7-di-2-thienyl-2 ',1',3'-benzothiadiazole] (PCDTBT) and two acceptor materials[6,6]-Phenyl-C71-butyric acid methyl ester (PC71BM) and graphene oxide (GO). However optical, electrical and dialectical properties of ternary hybrid structures based on PCDTBT:PC71BM:Grapheneoxide nanocomposite were reported. The effect of addition PC71BM into PCDTBT:GO bulk heterojunction (BHJ) was discussed. Emission optical spectrum of PCDTBT:PC71BM nanocomposites show a quenching in photoluminescence intensity due to charge or energy transfer at the interface between the donor and the acceptor of electrons. The electrical parameters such as the ideality factors (n) the barrier height (ϕb) and the series resistance (Rs) were calculated. Indeed, the Charge transport was evaluated by space charge limited conduction mechanism. The dielectrical behavior show a strong effect of addition graphene layers which increase the trap state density (Nss). Moreover, a relaxation peak appeared in the imaginary parts of impedance (Z'') in the range of (ms) indicating a dipolar relaxation type. There results were comparable to those P3HT:PCBM:GO ternary blend in literature[2] . This work indicates that ternary blend have the potential to surpass the performance of binary blend after further devices engineering and optimization [3].

Keywords: Ternery hybrid structure ; bulk heterojunction; PCDTBT:PC71BM; Graphene oxide, electrical properties.

[1] LU, Luyao, XU, Tao, CHEN, Wei, *et al.* Ternary blend polymer solar cells with enhanced power conversion efficiency. *Nature Photonics*, 2014, vol. 8, no 9, p. 716.
[2] LIU, Zhiyong, HE, Dawei, WANG, Yongsheng, et al. Graphene doping of P3HT: PCBM photovoltaic devices. Synthetic Metals, 2010, vol. 160, no 9-10, p. 1036-1039.
[3] LEFRANÇOIS, Aurélie, LUSZCZYNSKA, Beata, PEPIN-DONAT, Brigitte, et al. Enhanced charge separation in ternary P3HT/PCBM/CuInS 2 nanocrystals hybrid solar cells. Scientific reports, 2015, vol. 5, p. 7768.

Électrochimie et catalyse

Faculté des Sciences de Monastir
École doctorale Matériaux, Dispositifs et Microsystèmes
JDD 2019 – EC01

Dapsone electrochemical biosensor based on molecular imprinted graphene oxide modified glassy carbon electrode

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Abstract

A novel electrochemical biosensor, based on molecular imprinted polyaniline film matrix prepared on reduced graphene oxide (RGO) and gold nanoparticles (AuNPs) modified glassy carbon electrode (GCE). The developed sensor was used for convenient and selective detection of dapsone (DDS), which plays the role of the template. The resulting imprinted sensor was characterized by Scanning Electron Microscopy (SEM), UV-Vis, Fourier transform infrared spectroscopy (FT-IR) and electrochemical methods. Throughout this study various analytical parameters, such as pH value, concentration of monomer and template, incubation time and electro-polymerization cycles were investigated and optimized. The modified surface exhibited excellent electrochemical response and was able to detect dapsone (pH=3) by electrochemical impedance spectroscopy (EIS). Under the optimized conditions, the peak current of dapsone was linear to its concentration in the range of 1.0 x 10-7M - 1.0 x 10-3M with a low detection limit of 6.8x10-7 M. The sensor showed high selectivity for dapsone in the presence of some interferences according to the specific recognition nature of the synthesized material. Results indicated that this method possessed excellent potential applications in different urine and serum samples with acceptable recovery rates.

Keywords: Dapsone, gold nanoparticles, molecular imprinted, polyaniline, reduced graphene oxide.

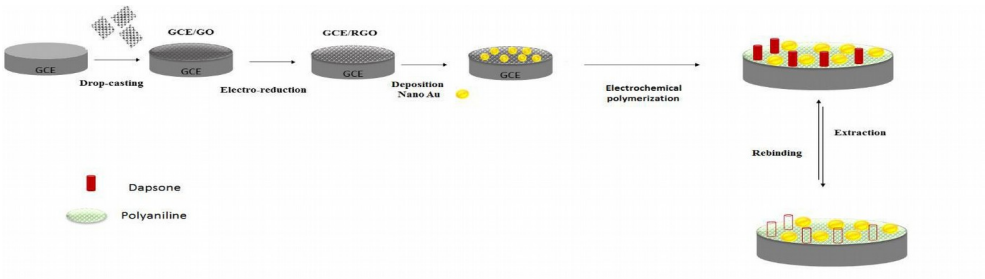

Figure: Schematic of the MIP sensor preparation for the detection of dapsone.

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JDD 2019 – EC02

Molecularly Imprinted Electrochemical Sensor for Dopamine Detection

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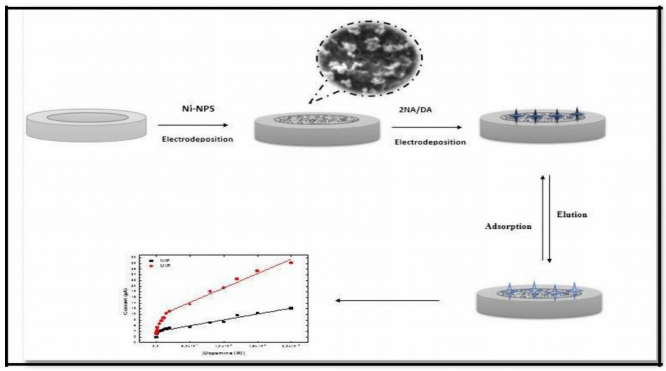
Abstract:
Dopamine (DA) plays a significant role in the function of the central nervous, renal and hormonal system as an important neurotransmitter. So, it is important to develop sensitive sensor for the determination of dopamine without interference. In this report we have developed an electrochemical sensor based on molecular imprinted poly-2-nitroaniline membrane onto nickel nanoparticles (Ni-NPs) modified glassy carbon (GC) electrode for dopamine (DA) detection. Electrochemical measurements such as cyclic voltammetry (CV) and differential pulse voltammetry (DPV) were employed to characterize the analytical performances of the sensor.
Under optimized conditions; the number of cycles for the electropolymerization, the scan rate and the pH, the prepared CV/Ni-NPs/2NA-MIPs electrode has a sensitivity of 0.121 A / mol.L^{-1} defined over a linear range from 0 to 2.10^{-4} M of dopamine.

Keywords: Molecularly Imprinted Polymer, Poly-2-nitroaniline, Dopamine.



Schematic illustrations of the fabrication procedure for the CV/Ni-NPs/2NA-MIPs imprinted layer.

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Elaboration and characterization of a nanofibrillated cellulose modified electrode for the detection of amino acids

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Abstract

In this work, a modified glassy carbon electrode with anionic cellulose nanofibers (NFC -) was developed. Cellulose fibers from Ammophila arenaria were fibrillated into nano-sized fibrils throughout the TEMPO oxidation chemical pretreatment. Then the mixture is subjected to mechanical disintegration by homogenizer.
NFC - layer was deposited on a carbon glassy electrode (CGE) by simple adsorption. The characterization of this modified electrode was performed by cyclic voltammetry (CV) and was subsequently verified by differential pulse voltammetry (DPV) in the presence of Fe(CN) 6-3/-4 as a redox probe. The modified electrode was used for the detection of amino acids by differential pulse voltammetry in a phosphate buffer solution (pH = 7). As a result, the modified electrode with nanofibrillated cellulose exhibited reproducible response, high sensitivity and good stability for aminos acids.

Mots-clés : Chemically Nanofibrillated cellulose modified CGE, polysaccharides, detection, amino acids,