UNIVERSITE DE MONASTIR

Ecole Doctorale
Matériaux, Dispositifs et Microsystèmes
ED 08FSM01

FACULTE DES SCIENCES DE MONASTIR

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BIENVENUE aux JDD 2020

Journées des Doctorants 2020

Deuxième édition

20 & 21 Décembre 2021

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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 aux Journées des Doctorants «JDD 2020» qui se tient à la Faculté des Sciences de Monastir. Nous remercions l'ensemble des participants et le comité scientifique, sans eux l'organisation des JDD 2020 n'aurait pas été possible. Nous remercions particulièrement le Professeur *Mohamed Mongi Ben Salem,* Doyen de la Faculté des Sciences de Monastir et Monsieur *Jalel Memmi,* 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

Dr. Koussai Lazaar

Le Directeur de l'École Doctorale

Pr. Abdelaziz Bouazizi

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Professeur Mohamed Mehdi CHEHIMI
(ITODYS – UMR 7182, Université Paris Est)

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Titre de la conférence :
Spectroscopie de photoélectrons X (XPS).
Principes de base et quelques applications

Professeur Christophe RAMSEYER
(LCE - UMR 6249, Université de Franche-Comté)

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Titre de la conférence :
La simulation numérique au service de la santé

Professeur Kamel BESBES
(CRMN, Technopôle Sousse)

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Titre de la conférence :
Accès aux technologies spatiales à travers les nanosatellites

Spectroscopie de photoelectrons X (XPS). Principes de base et quelques applications

Mohamed Mehdi Chehimi

Directeur de Recherche au CNRS,
Editeur en Chef Exécutif de Chemistry Africa
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La spectroscopie de photoélectrons X (X-ray photelectron spectroscopy, XPS ; ou electron spectroscopy for chemical analysis, ESCA) est la technique d'analyse chimique de surface la plus employée de nos jours pour étudier la chimie de surface des matériaux solides (qui ne subliment pas) comme les métaux, alliages, céramiques, complexes organo-métalliques, catalyseurs, polymères et leurs (nano)composites pour ne citer que ceux-là.
La technique XPS permet de suivre toutes les transformations chimiques de surface : oxydo-réduction, greffage de molécules, chimisorption, échanges ioniques, croissance de polymères et immobilisation de protéines, ainsi que d'autres réactions d'intérêt comme la formation de carbures ou de nitrures.
Elle permet de détecter, dans une profondeur de 2 à 10 nm, tous les éléments et leurs états chimiques (sauf l'hydrogène et l'hélium) ce qui lui a valu d'être nommée « la RMN de la classification périodique des éléments » ! En outre, en raison de cette spécificité de l'analyse chimique de surface ; elle avait valu à Kai Siegbahn le Prix Nobel de Physique en 1981. Depuis, cette technique n'a cessé d'évoluer.

Dans ce séminaire, nous aborderons les principes de base de la technique XPS et montrerons quelques-unes de ses applications en catalyse hétérogène, croissance de revêtements polymères multicouches ou texturés, nanocomposites (argile-polymère), criminalistique (révélation d'empreintes digitales latentes)... Si le temps le permet, nous parlerons également de quelques rares cas de dégradation de matériaux en cours d'analyse, sous l'effet des rayons X.

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La simulation numérique au service de la santé

Pr. Christophe Ramseyer

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Université de Franche-Comté
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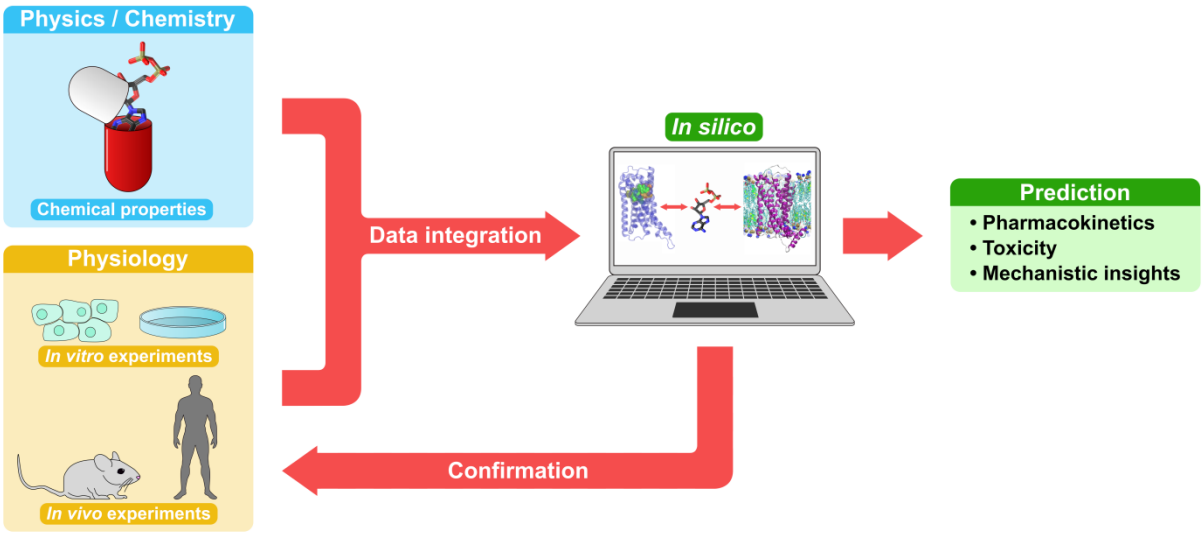
Les simulations numériques à l'échelle moléculaire sont depuis très longtemps utilisées pour étudier les propriétés physiques et chimiques des matériaux solides. Les mêmes techniques de simulation comme la dynamique moléculaire classique, les calculs de chimie quantique et le docking sont également utilisés dans les sciences du vivant et notamment en médecine et pharmacologie. Au cours de ce séminaire, nous montrerons que les physiciens et les chimistes peuvent apporter un regard nouveau notamment en cancérologie. Plusieurs exemples issus des travaux de recherche menés par le Prof. C. Ramseyer seront présentés pour illustrer les avantages et les inconvénients des simulations numériques dites « in-silico » par rapport aux expériences « in vitro » et « in vivo » menées traditionnellement en médecine et pharmacie.



THEMATIQUES

Modélisation et Calcul Théorique «MCT»

Molecular structure, electronic and docking studies of carboxylic acids based on 1-benzofuran

Abir SAGAAMA[a*], Olfa NOUREDDINE[a], Silvia Antonia Brandan[b], Anna Jarczyk- Jędryka[c], Henryk T.FLAKUS[c], Noureddine ISSAOUI[a]

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Abstract :

In the present work, experimental and theoretical analysis of 1-benzofuran-2-carboxylic acid (2BF) and 1-benzofuran-3-carboxylic acid (3BF) have been reported using B3LYP/6-311++G(d,p) method. The theoretical geometrical parameters have been compared with experimental data, intermolecular interaction such as hydrogen bond (H-bond) and Van der Waals interactions (VDW) have been investigated with the help of reduced density gradient (RDG). Molecular stability of 2BF and 3BF resulting from electronic exchange and hyper-conjugative interactions is analyzed via natural bond orbital analysis (NBO). The molecular electrostatic potential (MEPs) predict the chemical reactivity and indentifies the nucleophilic and electrophilic attack, which responsible for the H-bonds interaction. Using Time-Dependent DFT approach, the UV-Vis spectrums were obtained in order to determine the electronic transitions in the title compounds. The anticancer and antimicrobial activities of the both molecules were examined by using molecular docking package (iGEMDOCK).

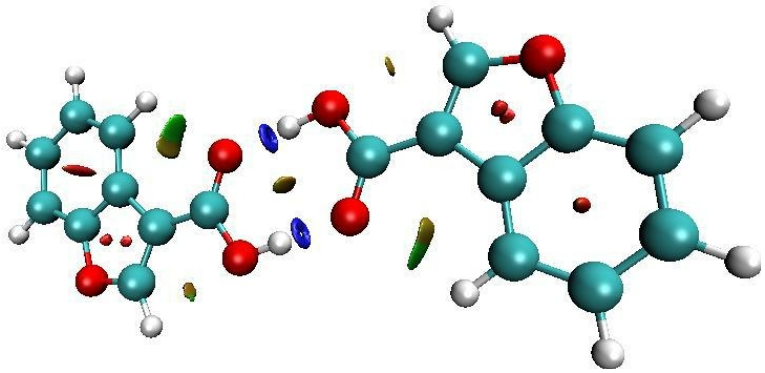

Figure 1 : Visualization of various inter and intramolecular interactions in 3BF dimer using Multiwfn and VMD programs.

keywords: DFT approach, H-Bond, NBO, MEP, Molecular docking.

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JDD 2020 – OMCT02

Vibrational description of the LiAr molecule in its $X^2\sigma^+$ and $A^2\Pi$ electronic states in the framework of an algebraic model

Insaf Sboui[a*], Marwa Slama[a] , Mounir Ben El Hadj Rhouma[a]

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Abstract :

In this work, the vibrational energy levels, the kinetic energy and the potential energy of the LiAr molecule in its $X^2\sigma^+$ and $A^2\Pi$ electronic states are studied using the Morse potential and so(2,1) spectrum generating algebra approach. An algorithm for the recursive evaluation of expectation value of

$$Z^q=\left(e^{-\alpha\left(r-r_e\right)}\right)^q$$

for a given state of Li($X^2\sigma^+$)Ar and Li($A^2\Pi$)Ar are proposed. As an application closed-form estimations for the value $r>\square_n$ of Li($X^2\sigma^+$)Ar and Li($A^2\Pi$)Ar were derived by means of Jensen's inequality. This allows us to obtain several inequalities relating the radial expectation values $r>\square_n$ of Li($X^2\sigma^+$)Ar and Li($A^2\Pi$)Ar at the logarithme of the expectation values of $Z^q=\left(e^{-\alpha\left(r-r_e\right)}\right)^q$. These obtained outcomes are compared to the published results, both theoretical and experimental, and show a good agreement.

Keywords: Bound states, Coulomb field, Hydrogen spectrum, Symmetries

Experimental and DFT calculations for 2-(3,4-dihydroxyphenyl) ethanaminium nitrate: molecular structure, non-covalent interactions, chemical reactivity and biological activity analysis

Mouna Medimagh, Noureddine ISSAOUI, Sofian Gatfaoui, Omar Al-Dossary, Aleksandr S. Kazachenko, Houda Marouani, Marek.J. Wojcik

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Abstract :
In the present study, a theoretical and experimental studies of the structural and electronic proprieties of 2-(3,4-dihydroxyphenyl) ethanaminium nitrate (abbreviated as 2DOPN) was performed. The density functional theory (DFT) has been employed including the B3LYP functional with 6-311++G(d, p) basic set to obtain the stable structure of the title compound. The intra and intermolecular interactions that exist within our molecule are analyzed by different methods namely the topological analysis AIM and the reduced gradient of the density (RDG). These approaches make it possible to characterize the hydrogen-bond interactions. The NBO analysis was used to investigate the electronic charge transfer into the molecule. In addition, the chemical reactivity of 2DOPN was discussed in terms of molecular electrostatic surfaces potential (MESP) and the frontier molecular orbitals (FMOs). To determine the biological activity of 2DOPN, molecular docking calculations were carried out. This method supports the partnership between theoretical and pharmaceutical researchers to discover new drugs to fight against Parkinson disease.

Keywords: AIM, chemical reactivity, DFT, hydrogen-bonds, FMOs, NBO, RDG .

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JDD 2020 – OMCT04

Numerical modeling of intersubband optical properties in ZnSe/ZnS core-shell quantum dot.

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Abstract:
We have performed theoretical calculations of the optical properties in a core-shell shape ZnSe/ZnS quantum dot (CSQD). We have used a numerical method which is based on a combination of coordinate transformation and the finite difference method. We have evaluated the linear, non-linear and the total absorption coefficients between the first excited state and the ground state for electron as a function of photon energy with different values of incident optical intensity and different dimensions of CSQD. The linear, non-linear and total refractive index changes are also investigated.

Keywords: ZnSe/ZnS, Core-shell, Coordinate transformation, Absorption coefficients, Refractive index changes.

A computational, structural and electronic investigation with molecular docking studies on 4-phenylpiperazine-1-ium dihydrogen phosphate

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Abstract:
Structural, electronic and topological evaluation of the hybrid material "4-Phenylpiperazine-1-ium dihydrogen phosphate" (4PPHP) has been undertaken by using quantum chemical calculations via the density functional theory. The optimized structure of 4PPHP were determined by Becke's three parameter hybrid functional with Lee-Yang-Parr correlation functional LYP (B3LYP) theory with the 6-311++G** basis set. Intra-molecular and intermolecular interactions were analyzed by the reduced density gradient (RDG), natural bond orbital (NBO) and topological AIM analysis. The intermolecular interactions of crystal of 4PPHP were analyzed using fingerprint plots of Hirshfeld surface. The molecular electrostatic potential (MEP) and the electronic properties (HOMO and LUMO) were also computed. Finally, the biological activities of 4PPHP were investigated by using molecular docking analysis. The studied compound have a great effect in the treatment of Parkinson and Schizophrenia diseases.

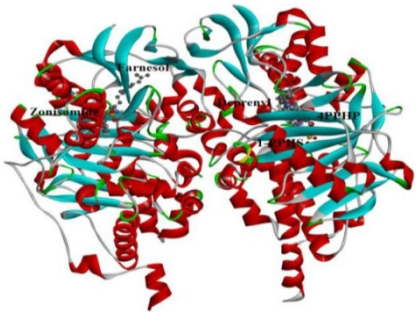

Figure 1: Amarrage moléculaire de la protéine MAOB avec les ligands Zonisamide, Deprenyl, Farnesol, 1-PPHS et 4PPHP.

Keywords: Density Functional Theory; inhibitor activity; RDG; NBO; electronic properties.

Intermolecular interactions in an equimolar methanol-water mixture as studied by neutron scattering and DFT calculations

Sahbi Trabelsi[a] ,Mouadh Tlili[a], Hafedh Abdelmoulahi[a], Salah Bouazizi[a], Salah Nasr[a], Miguel A. González[b], Marie-Claire Bellissent-Funel[c], Jacques Darpentigny[c].

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c. Laboratoire Léon Brillouin, CEA, CNRS, Université Paris-Saclay, CEA Saclay, 91191 Gif-sur-Yvette, France.

Abstract:
A detailed analysis of methanol water (MeW) liquid structure at 298 K and atmospheric pressure is performed using neutron scattering and Density Functional Theory (DFT) calculations. New neutron scattering data at large scattering wave vectors were explored to determine the structure factor , the molecular form factor and the intermolecular pair correlation function . To describe the local order of the mixture, a large variety of hydrogen-bonded possible clusters has been optimized using DFT calculation with the 6-311++ G(d, p) basis.

Key words: Neutron scattering; H-bond; DFT calculation.

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JDD 2020 – PMCT01

Thermodynamic study of the phase equilibria in the Ga-Sb-Bi compounds

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Abstract:
GaSbBi alloys have recently attracted great attention, due to their properties of band-gap reduction and spin-orbit splitting. The incorporation of Bi into antimonide based III-V semiconductors is very attractive for the development of new optoelectronic devices working in the mid-infrared range (2–5 μm). However, due to its large size, Bi does not readily incorporate into GaSb and the epitaxy of GaSbBi alloys thus very challenging. In the context of a comprehensive investigation of their thermodynamic and thermal properties, the behaviour in phase diagram is here studied. This work presents the thermodynamic investigation of the Ga-Sb-Bi alloys. Predicting of phase equilibria in Ga-Sb-Bi system requires the knowledge of the thermodynamic parameters of simple elements and constituent binairies Ga-Sb, Ga-Bi, Sb-Bi forming the ternary alloy. On the basis of these parameters, the Ga-Sb-Bi ternary system phase diagrams are calculated according to CALPHAD methode, using Pandat software. Such results like the isothermal sections at different temperatures, liquidus projection and vertical sections are evaluated.

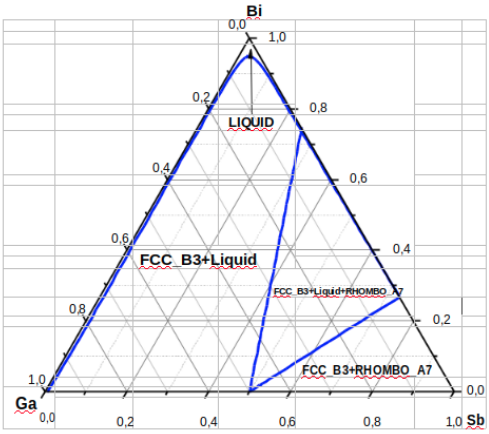

Figure 1 : Calculated isothermal section of Ga-Sb-Bi ternary system at 400°C .

Keywords: Ga-Sb-Bi ternary system, CALPHAD, phase diagram, isotherm section, liquidus projection.

Enhanced mid-infrared emission by energy transfer in Er3+/Yb3+ and Nd3+/Pr3+ co-doped zinc tellurite glass

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Abstract :

A study of the broadband near-infrared emission in zinc-tellurite glasses for improving the efficiency of a Silicon (Si) solar cell has been studied. A series of glasses with the nominal molar composition 70TeO2-30ZnO- wEr2O3-xYbO3- yNd2O3-zPr6O11, single doped with Pr3+, Nd3+,Yb3+Er3+ ions, co-doped with Pr3+/Nd3+, Er3+/Yb3+ ions and quadric-doped with Pr3+/Nd3+/Yb3+/Er3+ were prepared using melt quenching technique. Their optical absorption and luminescence measurements techniques were investigated at room temperature. The influence of RE ions concentration on the line- shape and intensity of electron transition has been analyzed. Based on above absorption and excited emission spectra, the Praseodymium ions has a strong sensitivity in the field of high energy (350-650 nm).

Under the excitation of 488 nm laser, an ultra-broadband emission from 900 to 1150 nm was found owing to the perfect overlapping of emission bands from Er3+, Yb3+ and Pr3+. This glass can efficiently transfer the high energy part of the solar spectrum into near infrared light close to 1000 nm based on the frequency conversion mechanism.

Keywords: rare-earth ions, broadband around 1.0 µm, Si solar cells.

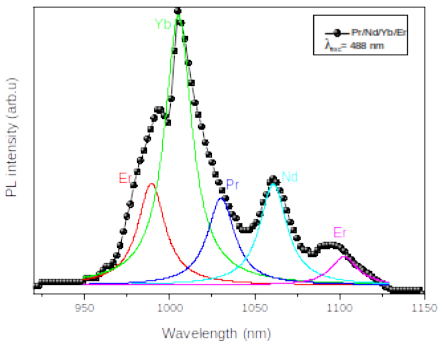

Figure 1: NIR emission spectra of tellurite glasses under 488 nm laser excitation

Experimental and theoretical investigation of new anthracene grafted oligophenylene for optoelectronic applications

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Abstract :

Photo-physical properties of a new synthesized anthracene-oligophenylene (OMPA-ANTH) were investigated using optical absorption, steady state and transient photoluminescence spectroscopies. As well as, electronic properties were theoretically investigated using Density Functional Theory (DFT) and TD-DFT methodologies. The grafting of anthracene into the backbone of the oligomer induce a great change into the electrochemical and the photo-physical properties of the OMPA synthesized oligomer. Indeed, the optical band gap decrease dramatically from 3.2 eV for unmodified OMPA oligomer to 2.5 eV for the anthracene modified one. Computational analysis shows that a great change occurred into the frontier orbitals HOMO and LUMO and in the electronic parameters under the chemical grafting of anthracene into the [4-(methoxyphenyl)acetonitrile] (MPA) unit.

Keywords: 4-(methoxyphenyl)acetonitrile, Anthracene, Optical properties, DFT

Modeling by statistical physics and interpretation of the adsorption of odorants thiols on the OR2M3 human olfactory receptor

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Abstract :
In this work, a statistical physics treatment was used to study the adsorption of two odors 3-mercapto-2-methylbutan-1-ol and 3-mercapto-2-methylpentan-1-ole on the human olfactory receptor OR2M3. A physicochemical and thermodynamic investigation of the adsorption of the two odorous thiols allows us to obtain steric and energetic characterizations of these adsorption systems. The single-layer model with identical and independent sites is the most suitable model for this description. Indeed, the numerical values of the three parameters resulting from the adjustment of the response curves (Rm, N, C1/2) are used to characterize the anchoring and the orientation of the odorous molecules on the surface of the adsorbent. By applying statistical physics and a numerical method we have determined the interactions energies between the two odorants and the human odor receptor throw the adsorption energy distributions (AED). For thermodynamics, we followed the evolution of the entropy to study the disorder of the adsorption systems.

Keywords: Adsorption; olfaction; adsorption energie distribution (AED), entropy.

Isomers in organic semiconducting dumbbell-shaped molecules for cell solar application: A computational and experimental investigation

Chaima Mahmoudi*[a,b], Ibrahim Bulut [a], Jiang Jing [c], Sadiara Fall [c], Benoît Heinrich [d], Stéphane Méry [d], Thomas Heiser [c], Patrick Lévêque [c], Emilie Steveler [e], Mustapha Majdoub[b], Nicolas Leclerc [a]

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b. 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.
c. Laboratoire ICube, UMR 7357-CNRS, Université de Strasbourg,
d. Institut de Physique et de Chimie des Matériaux de Strasbourg (IPCMS), UMR 7504-CNRS, Université de Strasbourg,
e. Laboratoire ICube, UMR 7357-CNRS, INSA Strasbourg.

Abstract :
Recently, some publications have reported the study of the regioisomers resulting from the ortho or para linkage between the SBF unit and the conjugated backbone. Thus, Bulut et al. reported the two regioisomers with the SBF used as end-capper, while Yang *et al*. implemented the SBF unit as a conjugated bridge between two perylene diimide (PDI) units. in this context, the solid-state structures and opto-electronic properties are significantly change from one isomer to the other, resulting in device performance that varies substantially. Finally, very few examples have been reported studying the influence of the different isomeric structures on the solid-state structures and optoelectronic properties of more or less fused extended conjugated chemical molecules. Two new dumbbell-shaped molecules based on two solubilizing and structuring triazatruxene (TAT) units linked by a central chromophore were synthesized and studied. The central chromophore was an electro-deficient fluorene-malononitrile (FM) unit, that can be functionalized symmetrically on two different positions, giving rise to two positional isomers, called TAT-pFM and TAT-mFM, when the TATs are connected to the 2,7- and 3,6-positions, respectively. The two isomers exhibited different electronic conjugation pathways that drastically affect their absorption properties and energy levels. Moreover, while TAT-pFM was organized in a stable 3D mesomorphic structure from room-temperature to the melting point, TAT-mFM remained crystalline and decomposed before melting. Finally, despite a lower hole mobility, the TAT-mFM exhibited the highest Power Conversion Efficiency (PCE) of about 2% in organic solar cells.

Keywords: Triazatruxane, Regioisomeres, Semi-conductor, Cell solar

Modeling and interpretation based on statistical physics treatment of adsorption of gram-negative bacteria onto nanostructured silicon carbide

Kouira Oumaima, Bayouth Sonia et Abdelmottaleb Ben Lamine

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Abstract :
Récemment les études décrivant l'adsorption des bactéries à la surface des nanostructures de carbure de silicium (SiC) sont très limitées. Le SiC semble être complètement inerte vis-à-vis des systèmes biologiques. Il peut interagir avec des cellules vivantes lorsqu'elles sont des nanostructures. En effet l'étude des interactions entres les nanostructures de carbure de silicium et les organismes vivants présente un grand intérêt. Ceci nous a encouragé à étudier l'adsorption de la bactérie Gram-négative Pseudomonas Putida sur la surface des nanostructures de SiC, en utilisant la modélisation par la physique statistique des isothermes d'adsorption expérimentales de cette bactérie [1]. Pour cette enquête, le modèle de Hill a été choisi comme un modèle adéquat qui présente une bonne corrélation avec les isothermes expérimentales de l'adsorption des bactéries sur les nanostructures de SiC (NRSiC et le NFSiC). Le modèle triple couche à une seule énergie a été choisi comme un modèle adéquat qui présente une bonne corrélation avec les isothermes expérimentales de l'adsorption de la bactérie sur le µmSiC. Trois paramètres du chaque modèle sont ajusté à savoir le nombre de particules par site n, la quantité adsorbée à la saturation Q_{sat} et la concentration à demi-saturation $C_{1/2}$. Les résultats montrent que l'adsorption des bactéries est important seulement pour les nanostructures NRSiC et NFSiC, par contre elle est faible pour le µmSiC, elle dépend du pH du milieu, de la morphologie et de la texture du SiC. De plus nous avons déterminé les énergies d'adsorption, à partir du paramètre $C_{1/2}$, reflétant un processus de physisorption.

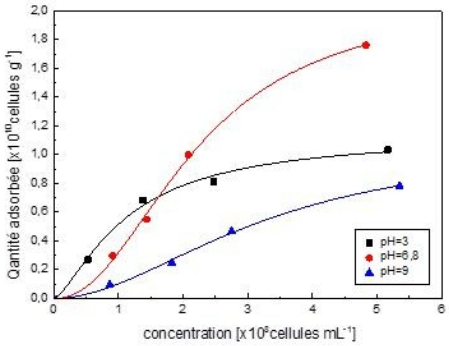

Figure 1: Fitted adsorption isotherms of bacteria gram-negative on NFSiC by HILL model in statistical physics

Mots-clés: adsorption, bacteria, gram-negative, silicon carbide, modeling

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Electronic properties of ZroS and ZrOSe mono and bi-layers using ab-initio calculations

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Abstract

We have investigated the structural and electronic properties of the ZrOS and ZrOTe mono and bi-layers, using Density Functional Theory (DFT) as implemented in VASP. In this framework, exchange and correlation were approximated using either LDA of Ceperley and Alder or GGA of Perdew-Burke-Ernzerhof, with a plane wave cutoff of 500 eV and a 12 × 12 × 1 k-point mesh. Similar parameters were applied for HSE and GW calculations that were conducted to achieve accurate values for the bandgap. By calculating their total energy, we have revealed that our monolayers and bilayers are firmly stable. We show that their electronic bandgaps, as obtained with GGA, range between 0.5 and 1.30 eV, which are promising candidates for electronic devices as field-effect transistors, photodetectors, and other optoelectronics.

Keywords: DFT, VASP, 2D materials, ZrOS, ZrOTe

Effect of dielectric matrix and optical intensity on linear and third-order nonlinear optical properties of CdS/ZnSe core/shell QD-Matrix

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Abstract

In this research, the effective mass approximation (E.M.A) and the compact density matrix approach have been used to compute the energy eigenvalues, the linear, third-order nonlinear and total absorption coefficient and refractive index changes of CdS/ZnSe core/shell spherical quantum dots (CSSQD) surrounded by three different matrices. The influence of the geometrical factor (core to shell radii ratio), dielectric matrix and the optical intensity on the transition energy and linear and nonlinear optical properties have been analyzed. Our numerical results demonstrated that the total absorption coefficient and refractive index changes are strongly affected by the dielectric environment and incident optical intensity. These findings offer the possibility of tuning the resonant peaks and transition energy by using the combined effect of the spatial confinement, the dielectric mismatch between the dot and the surrounding medium and the effect of high optical intensity. We believe that, our results have been turned out to be a powerful tool to explore various optoelectronic properties of semiconductor nanostructures.

Keywords: Nonlinear optic, Effective mass approximation, Core/shell quantum dot, dielectric matrices.

Matériaux: Élaboration et Caractérisations «MEC»

Nitridation of InAs/GaAs self-assembled quantum dots: experimental study

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Abstract :
The effect of time nitridation on the properties of InAs quantum dots (QDs) grown on GaAs substrate by molecular beam epitaxy (MBE) has been studied by X-Ray Photoelectron Spectroscopy (XPS) and Photoluminescence (PL) techniques. XPS is used to determine the species created at the surface. In fact, we focused our attention on the N1s and In3d XPS spectra. At low temperature region, power dependent analysis of the PL intensity reveals a conventional power law close to one, in agreement with the type II nature of the emission. The analysis of PL spectra exibit that the emission wavelength increases further by increasing the time nitridation in the InAs QDs. Our results displayed a significant improvement of the crystalline quality and enhancement of the optical properties for InAs QDs grown after nitridation.

Keywords: Nitridation, X-ray photoelectron spectroscopy (XPS), Photoluminescence (PL).

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Simulation of in situ time-reflectance during high temperature growth of GaN by MOVPE on GaAs (110) substrate

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Abstract :

The effect of high temperature GaN growth by metal-organic vapor phase epitaxy (MOVPE) on GaAs (110) substrate was investigated. We used an optical model which incorporate time-dependent growth rate and time-dependent surface roughness to simulate the in situ reflectance-time during MOVPE of GaN layers. The main goal was to give a quantitative study of the contribution of Ga diffusion from GaAs substrate in the early stages of high temperature GaN growth and its effect on kinetic growth. Surface roughness and growth rate profiles was suggested to give good simulations. From the best simulations of time-reflectance traces we deduced the optical constants and both profiles of growth rate and surface roughness during high temperature GaN growth. The results showed a relatively high initial growth rate compared to their limit value reached at steady state of GaN growth. The initial growth rate as found to depending on growth temperature while the limit value is almost independent on growth temperature. The increase of surface roughness is more enhanced at high growth temperature. This quantitative study gives measurements of Ga diffusion coefficient in GaN at different growth temperature and its thermal activation energy which is close to 0.35 eV. Ex situ analyses by UV-Visible (200-900 nm) reflectance and atomic force microscopy (AFM) were correlated with the output simulations.

Keywords: time- reflectance, MOVPE, GaN, GaAs (110) substrate, Ga diffusion.

Thermal decomposition effects on GaN films

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Abstract:
We studied the partial decomposition of GaN films, grown on silicon nitride (SiN) treated c-sapphire substrates in an atmospheric pressure metal organic vapor phase epitaxy (AP-MOVPE) vertical reactor. We investigated a series of annealed GaN layers. An as grown sample was cut up into five pieces; one piece was taken as reference and the remaining four pieces have undergone one, two, three and four temperature rise-fall. The thermal decomposition process was effectuated at 1170 °C under pure N_2 in MOVPE reactor at atmospheric pressure. Scanning electron micrographs showed a change of the surface morphology after annealing. In fact, as grown sample presented a relatively smooth and flat surface while the annealed ones showed a flat surface with the appearance of nanostructures. Increasing the temperature rise-fall times led to variations of the grains density and size. This surface morphology change can be attributed to an elastic relaxation of GaN films do to the formation of those nanograins. We proved then that this annealing process can be used to get grainy GaN films. The optical properties of the decomposed films were then studied by using the cathodoluminescence (CL) technique. CL results showed a relaxation of the annealed GaN compressive strain which led to an improvement of the decomposed GaN films optical quality compared to the un-annealed one. X-ray GaN rocking curve scans were also treated to be sure that the annealing process did not destroy the layers crystalline quality.

Key words: MOVPE, GaN, annealing, grains.

SOL-GEL METHOD SYNTHESIS AND CHARACTERIZATION OF NEW CHROMIUM PHOSPHATE BELONGING TO α-$CrPO_4$ type STRUCTURE"

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Abstract:
This work is a part of systematic investigation of ternary chromium phosphates belonging to the K_3PO_4-$M_3(PO_4)_2$-$CrPO_4$ systems where M is a divalent cation. It describes the synthesis and the structural characterization of a new phosphate $KCoCr_2(PO_4)_3$. This compound crystallizes in the orthorhombic system with the space group Imma and the cell parameters *a* = 10.494(5) Å;*b* = 13.231(3) Å and *c* = 6.484(6) Å. Its structure (Fig. 1) closely resembles to those of α-$CrPO_4$ type, which consists of a 3D framework of$Cr(1)O_6$ and $M(2)O_6$[M(2) = 0,5 Co + 0,5 Cr] octahedra, and PO_4tetrahedra. The $Cr(1)O_6$ octahedra are isolated from each other whereas each pair of $M(2)O_6$ share one edge to form $M(2)_2O_{10}$ bioctahedra. These two types of structural units are linked directly though common corners and by means of PO_4 tetrahedra, via corner- and edge-sharing. The resulting 3D skeleton forms interesting tunnels which propagate infinitely along the [100] and [010] directions, where the K^+ ions occupy two distinct sites. The IR and Raman spectra are typical of a monophosphate and give clear evidence of the occurrence of two crystallograpically distinct phosphorus sites. The UV-vis spectrum confirms the octahedral environment of the Cr^{3+} ions.

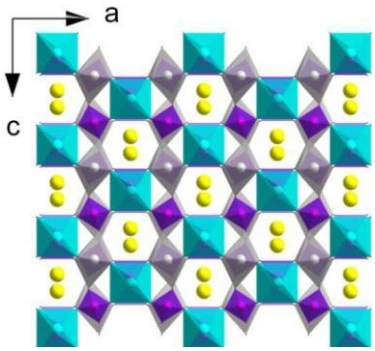

Figure 1: *A projection along the [010] direction of the $KCoCr_2(PO_4)_3$ structure.*

Key words: Sol-gel Synthesis**,** Chromium phosphate, IR, Raman, UV-vis,

Etude de cycle d'adsorption: conception des différents cycles, modélisation, calcul de rendement énergétique et interprétation par la physique statistique

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Abstract:
In this work, the adsorption isotherms of the carbon dioxide onto highly porous activated carbon have been fitted by advanced statistical physics models to give reasonable interpretations of the adsorption process. Fitted physicochemical parameters values have been deducted by means of the best fitting model. To describe the adsorption process, the fitting results showed that the CO_2 molecules formed only one layer on the modified activated carbon (MAC). These molecules have been mainly docked with a parallel position on adsorbent receptor sites with adsorption energies varying from 7.16 kJ/mol to 8.24 kJ/mol. These values reflected a physisorption process. The calculated internal energy values suggested the spontaneity and the exothermicity of the CO_2 adsorption process onto. As application, the enthalpy function is utilized and calculated to perform the thermodynamic evaluation of CO_2 adsorption cycle in a cooling system and to calculate the coefficient of performance (COP) as a function of the regeneration temperature. This parameter was found to be in the interval [0.09–0.19] corresponding to a regeneration temperature varying from 303 K to 343 K.

Key words: Carbon dioxide adsorption, Modified activated carbon, Cooling system, Coefficient of performance COP, Statistical physics model.

Growth of a-plane GaN epi-layers on r-plane sapphire substrates with optimization of high growth temperature

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Abstract :

The effect of high growth temperature, ranging from 1040 °C to 1120 °C, on the properties of a-plane GaN layers grown by MOCVD on r-plane Al2O3 substrates was investigated. The growth process was in-situ monitored by Laser Reflectometry. Ex-situ analyses, such as scanning electron microscopy (SEM), high-resolution X-ray diffraction (HRXRD), and low-temperature photoluminescence (PL) studies were then carried out and showed a strong dependence on growth temperature. Structural results showed that the increase of growth temperature promotes the three-dimensional (3D) growth mode and the alignment of GaN columns toward the $(11\bar{2}0)$ preferred orientation. Indeed, the almost fully oriented layer was found to be grown at 1090 °C. The optical measurement revealed that all LT-PL spectra were dominated by the 3.41 eV emission, commonly attributed to the excitons bound to basal plane stacking faults, along with well-known donor-acceptor pair emission located around 3.28 eV. Where a decrease in PL intensity of the emission band at 3.41 eV accompanied by a slightly blue shift, was observed while increasing growth temperature. This behavior is attributed to the strain effect.

Keywords: GaN, MOCVD, Al_2O_3, non-polar, HRXRD, PL.

Investigation of In-rich InGaAs by structural, morphological, and optical techniques

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4. *Nanophotonics Research and Application Center, Cumhuriyet University, 58140, Sivas, Turkey.*
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Abstract :
The epitaxial layer of InGaAs on InP substrate was grown by Metal-Organic Vapor Phase Epitaxy for 65% of Indium content. SEM-EDX and XRD measurements were performed to evaluate the indium composition, the crystalline quality and the dislocation density within the hetero-structure. The room temperature photoluminescence proved the operation of InGaAs in the Short Wavelength Infra-Red (SWIR) range. The temperature dependence of photoluminescence from 10 K to 300 K demonstrates an S-shaped form at lower temperatures identified as red-blue-red shift. This anomalous photoluminescence behavior was quantitatively reproduced by Localized State Ensemble model where the localization degree is estimated to be 4.8 meV. We referred the localization phenomenon to the clusters of indium atoms because of the high indium concentration and the potential fluctuation due to the inhomogeneous distribution of indium.

Keywords: InGaAs/InP, Localized State Ensemble (LSE), Photoluminescence, SEM-EDX, XRD.

Conduction mechanisms study in CaCu 2.8 N i0.2 Ti 4 O 12 ceramics sintered at different temperatures

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Abstract :
CaCu 2.8 Ni 0.2 Ti 4 O 12 ceramics were prepared via the solid-state reaction. The pellets were sintering at 1050 ° C and 1100 ° C for 24h. The X-ray diffraction (XRD) exhibits the crystallization of all the samples in the cubic structure with Im 3 space group. The scanning electronic microscope (SEM) analysis show the growth of grain size by increasing sintering temperature from 1.66 to 18.58 µm. The conductivity analysis present a notable increase with the heating treatment. Both ac and dc electrical conductivity are fully examined as function of frequency and temperature. The ac conductivity discloses that correlated barrier hopping and non-overlapping small polaron tunneling models are the dominated conduction mechanisms existing in our compounds. By rising the sintering temperature the barrier height, above which jump the polarons or the electrons, tends to lower. The dc conductivity reveals that the conduction is achieved by the jump of polaron to the neighboring site and at variable distances.

Keywords: CCTO, sintering temperature, grains growth, ac conductivity, dc conductivity.

Effect of thickness on the Structural and optical properties of cubic GaN on GaAs (114) substrate by metalorganic vapor phase epitaxy

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Abstract:
In this work, we have investigated the influence of thickness on morphological, structural and optical properties of cubic GaN (c-GaN) films. We have grown a set of c-GaN layers on (114) GaAs substrates with thickness ranging from 0.15 to 1.5 µm by metalorganic vapor phase epitaxy (MOVPE) at 850 °C. Scanning electron microscopy (SEM), atomic force microscopy (AFM), high-resolution X-ray diffraction (HRXRD) and room temperature Cathodoluminescence (RT-CL) studies were carried out. Detailed morphological analyses using SEM and AFM reveal the film thickness dependence on the rate of crystallization. X- ray diffraction has shown that GaN films have a (002) preferential growth direction. RT-CL spectra showed only c-GaN (3.23 eV) emission.

Keys words: MOVPE, Cubic GaN, (114) GaAs substrate, Thickness.

The effect of Ni doping on the dielectric properties of La0.8Na0.2MnO3

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Abstract :
The manganite sample La0.8Na0.2Mn1-xNixO3 (x = 0.03 and 0.06) was synthesized by the sol-gel method. The effect of Ni doping on the structural and dielectric properties were investigated. These compounds crystallized in the rhombohedral structure with R3c space group. The dielectric response was studied by complex impedance spectroscopy in the frequency range (10 - 106 Hz). The ac conductivity values were fitted by Jonscher's law σ(ω) = σDC + Aωn. The existence of an electrical relaxation in these compounds was achieved by Complex impedance analysis. The dielectric constant and the dielectric loss decreased with the increase in Ni doping. The Normalized plot of modulus indicates that the dynamical processes are temperature independent.

Keywords: Manganite, Sol-Gel, Permittivity, Impedance spectroscopy.

The effect of defect induced_ localized centers on the luminescence mechanism in CsPbBr3 perovskite film investigated by steady state and time resolved photoluminescence spectroscopies

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Abstract :
Recently, a tremendous interest has been devoted to the studies of all inorganic perovskite materials (CsPbX3, X= Cl, Br and I) as single crystals, thin films and nanocrystals (NCs) due to their excellent photophysical properties[1] .Thus, CsPbBr3 is a very promising material for many optoelectronic devices[1]. Herein, optical properties of CsPbBr3 thin film, prepared by the solution processing method, are studied by mean of steady state and time resolved photoluminescence spectroscopies. The PL emission in CsPbBr3 film were suggested to arise from the recombination of free excitons and localized defects states induced mainly by halogen vacancies in the lattice. It has been observed that the PL decay time of the band edge emission in CsPbBr3 perovskite film is strongly dependent on the excitation power density. Our results revealed mixed monomolecular and bimolecular recombination mechanisms which were attributed to the competition of trapped and free carrier recombination.

Key words : Inorganic perovskite, Photoluminescence, defects, PL lifetime.

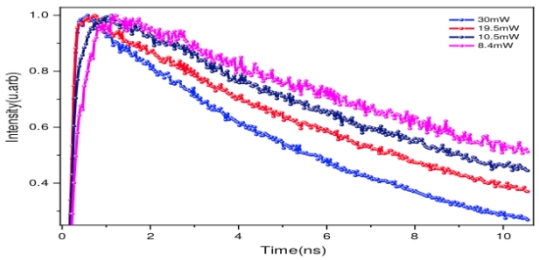

Figure 1: the excitation power dependent PL decay curves of the band edge emission

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Colloidal development and photocatalytic application of Mn doped ZnS nanocrystals

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Abstract:

Colloidal Semiconductor nanocrystals play a crucial role in separate fields such sensors [1] and photocatalysis [2]. In this work, Manganese-doped Zinc Sulfide nanocrystals with different Mn concentrations (4, 8 and 12%), were successfully prepared through colloidal method. The structural, functional and optical of the products were characterized by XRD, FTIR, TEM, UV-Visible and PL techniques. X-Ray diffraction studies revealed the formation of crystalline structures of ZnS and Mn doped ZnS with two crystalline phases, cubic and hexagonal. The calculation of the average size of ZnS nanocrystals by the Debye Scherrer relation gave nanometric size values between 2 and 3 nm. The FTIR spectroscopy allowed us to highlight the functionalization of the surface of nanocrystals synthesized by an organic molecule (TGA: Thioglycolic acid).The optical band gap was increased from 3.75 to 3.92eV with increasing Mn dopant concentrations [3]. The PL of ZnS nanocrystals exhibit emission in the range of 410-490 nm. The addition of Mn2+ reveal a very high intensity in the same energy range except that there appears an emission band around 580 nm (2.13eV) connected to the 4 1→ 6 1 transition of the Mn 2+ ion with low surface defect density. The photocatalytic activity of undoped ZnS shows better efficiency than doping with manganese, which shows that doping with manganese has a retarding effect for the photocatalytic degradation of Methyl Orange dye in water.

Keywords: Mn doped ZnS; Nanocrystals; Photocatalysis; Photodegradation.

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The effect of copper doping on the optical and electrical properties of nickel oxide thin films deposited by spin coating technique

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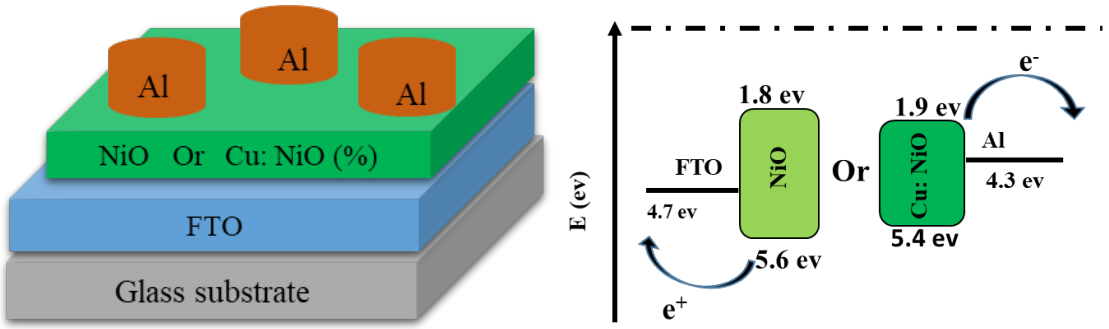
Abstract:
In this work, we have synthesized and successfully prepared the nickel oxide and the copper doped nickel oxide thin films by spin coating. We have investigated the effect of copper doping on the optical and electrical properties of nickel oxide thin films. The energy band gap values reduced with increase in copper concentration which indicate that copper doped nickel oxide (Cu: NiO) is suitable for optoelectronic application. The average transmission of the copper doped nickel oxide film is decreased in the visible wavelength range from 95 % to 75 %. This decrease can be attributed to the increase in the scattering of the incident light resulting from the increase in surface roughness of copper doped nickel oxide film. The PL response shows an increase of intensity with the increase of copper concentration that linked to the increase of defect levels and confirms the incorporation of Cu^{2+} in the nickel oxide film. The electrical properties of the FTO/NiO/Al and FTO/Cu: NiO (5%, 10%)/Al structures device showed that charge mobility and electrical conductivity were improved with copper doping. These result indicates that copper is an excellent dopant for NiO.



Effects of Thermal Annealing on the Optical Properties of GaAsBi/GaAs quantum dots

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Abstract :
Photoluminescence (PL) spectroscopy was used to investigate the effects of thermal annealing on GaAsBi/GaAs quantum dot (QD) structures grown by metalorganic vapor phase epitaxy. The PL spectra exhibit a well-defined doublet-like QD peak attributed to a bimodal size distribution of small and large GaAsBi QDs. After thermal annealing, the PL spectra from the GaAsBi QDs show a reduction of the localized state density and showed significant increases in the intensity with annealing temperature. The annealing process is suspected to have reduced the number of nonradiative recombination centers. In particular, after annealing at 650 °C, the emission of small QDs shifts to the lower energy side and the large QDs increases the intensity. This reduction in energy is largely related to changes in the QD shape and size, especially changes in the aspect ratio (height/width) that result from annealing.

The effects of Nd and Er elements on structural, electrical and optical properties of 0.975KNN-0.025NBT ceramics

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Abstract :
The Effects of Nd and Er ions on structure, microstructure, dielectric and photoluminescence properties of lead-free 0.975 K1/2Na1/2NbO3 - 0.025Na1/2Bi1/2TiO3 (0.975KNN-0.025NBT) ceramics prepared via solid state reaction method were investigated. The XRD analyses evidenced the biphasic symmetry “orthorhombic Amm2 + monoclinic Pm” with great fraction of Amm2 symmetry. The SEM measurement revealed a good compositional homogeneity and fine grains size of ceramics. The Raman investigations confirm the introduction of RE3+ elements into the 0.975KNN-0.025NBT matrix by a clear presence of the mode at 107 cm-1 and the shift of υ1 and υ5 modes to the lower frequency. Continuation of existence of new dielectric anomaly T1 at room temperature for KNNBT:Er and KNNBT:Nd (εr = 2042 at 24 °C, εr = 2002 at 27 °C), clair presence and shift of depolarization anomaly to lower temperature have been obtained by dielectric measurement. The introduction of RE3+ ions in the 0.975KNN-0.025NBT host lattice shows characteristics emissions bands of Er and Nd in the infrared wavelength region. These overall properties show that Ln3+ doped 0.975KNN-0.025NBT ceramics have great potential in multifunctional applications.

Key words: solid state reaction, RE3+, dielectric proprieties, photoluminescence.

Microstructural, structural and dielectric analysis of $Na_{0.5}Bi_{0.5}Ti_0O_3$perovskite ceramic

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Abstract :
In this study, $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) lead-free ceramic was fabricated via the solid-state reaction. The structural and dielectric properties of our compound were investigated in detail. The X-ray diffraction (XRD) showed that our compound crystallized, at room temperature, in the rhombohedral structure with R3c space group, a_H=5.4829(1) Å, c_H = 13.5298(4) Å, V = 352.2456 (1) Å^3, exhibits an anti-phase, $a^-a^-a^-$ oxygen tilt system. The 3-dimensional overview of crystal structure of Na0.5Bi0.5-TiO3 is generated by using refined parameters. Homogeneously compacted microstructure with square shape grain morphology is observed in FESEM. The presence of different bonds has been confirmed from FT-IR analysis. Finally, to evaluate the dielectric behaviour, the dc conductivity curve was found to follow the Arrhenius plot and Jonscher's power law has been used to find different models of ac conductivity.

Synthèse, réactivité et substances naturelles «SRSN»

École doctorale Matériaux, Dispositifs et Microsystèmes
Journées des Doctorants, 20 & 21 Décembre 2021
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JDD 2020 – OSRSN01

Identification et quantification de triacylglycérols d'extraits de noyaux de la plante *Prunus armeniaca* L de TUNISIE par HPLC-APCI/MS.

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Abstract :
Les triacylglycérols (TAG) sont une source importante de lipides alimentaires qui constituent une partie essentielle d'une alimentation saine. Dans la présente recherche nous avons étudié la composition lipidique de quatre extraits de noyaux de la plante Prunus armeniaca L. Les TAGs ont été identifiés et quantifiés en utilisant une chromatographie solide-liquide couplée à une spectrométre de masse à ionisation chimique à pression atmosphérique (HPLC-APCI/MS). Des profils de

TAGs identiques dans les quatre extraits ont été obtenus. Au total, 26 TAG ont été identifiés, dont 18 n'avaient pas été signalés auparavant dans le noyau de P.armeniaca L.. Six diacylglycérols (DAGs) et 19 triacylglycérols (TAGs) ont été détectés dans tous les extraits avec la prédominance de LLO (1,2-linoleyl-3-olein), OOL (1,2-oleoyl-3-linoleoyl) et OOO (triolein), avec des pourcentages variant de 19-32,8%, 20,3-23,6% et 12,1-20,1%, respectivement. À ce jour, cela représente le plus grand nombre de TAG identifiés dans le noyau de *P.armeniaca* L..

Mots clés : *Prunus armeniaca* L; extraits; noyaux; TAGs ; HPLC-APCI/MS.

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Journées des Doctorants, 20 & 21 Décembre 2021
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JDD 2020 – OSRSN02

ELECTROPHILICITE AMBIDENTE DES 4 NITROBENZOCHALCOGENADIAZOLES : ETUDE CINETIQUE ET CORRELATIONS STRUCTURE-REACTIVITE

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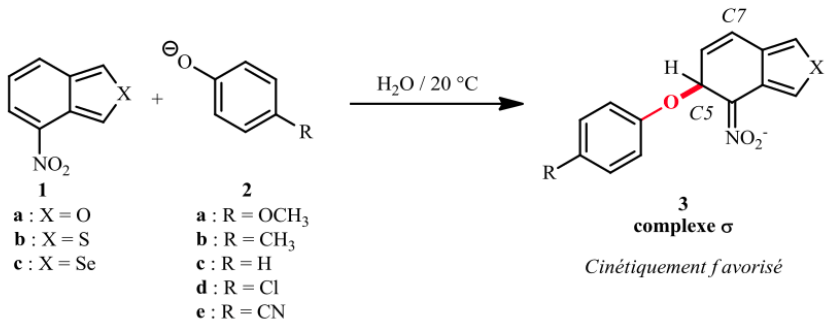
Abstract :
Récemment, les valeurs du paramètre d'électrophilie (E) selon l'approche de Mayr des 4-nitrobenzochalcogénadiazole 1a-c en position C-7 ont été mesurées sur la base de l'équation (1) et insérées au sein de l'échelle universelle E qui couvre actuellement plus de 32 unités.

$$\log k\ (20°C) = s\ (E + N) \qquad (1)$$

Dans ce contexte, l'objectif de ce travail était d'une part, l'étude cinétique de la réaction de couplage des 4-nitrobenzochalcogénadiazole 1a-c avec une série d'anions phénate 2a-e dans l'eau à 20 °C, ce qui impliquait une détermination de la valeur du paramètre de la réactivité C-5 de nos trois Electrophile et d'autre part le positionnement de sa réactivité carbonée dans l'échelle E de classification des électrophiles. Par ailleurs, l'effet de la basicité des anions phénate sera également discuté.



Mots-clés : équation de Mayr, 4-nitrobenzochalcogénadiazole, électrophilie, cinétique.

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École doctorale Matériaux, Dispositifs et Microsystèmes
Journées des Doctorants, 20 & 21 Décembre 2021
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JDD 2020 – OSRSN03

Synthesis, structural characterization and photophysical properties of 14-acétoxymethyl-7-cyano-thiahexahelicene

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Abstract :
Helicenes represent a fascinating class of polycyclic aromatic molecules in which a regular cylindrical helix is formed through an all-ortho annelation of aromatic or heteroaromatic rings[1]. The two structures are mirror images of one another, nonsuperimposable,and consequently considered chiral Functionalized [n]helicenes (n ≥ 6) exhibit a large optical stability and a strong resistance to isomerisation, which make them efficient as chiral catalysts [2] and ligands for asymmetric synthesis [3].
14-acethoxymethyl-7-cyano-thiaexahelicene has been prepared in racemic form through a short photochemical synthetic approach and its enantiomeric separation was studied and allowed to obtain (*P*)- and (*M*)-enantiomers in 100% ee and >98.5% ee, respectively. The optical rotatory dispersion and electronic circular dichroism (ECD) spectra of the resolved ones were measured. Other optical properties such as UV and photoluminescence as well as the electrochemical behavior were also examined in solutions

Key Words: Heck, , photophysical properties, HPLC, photocyclisation

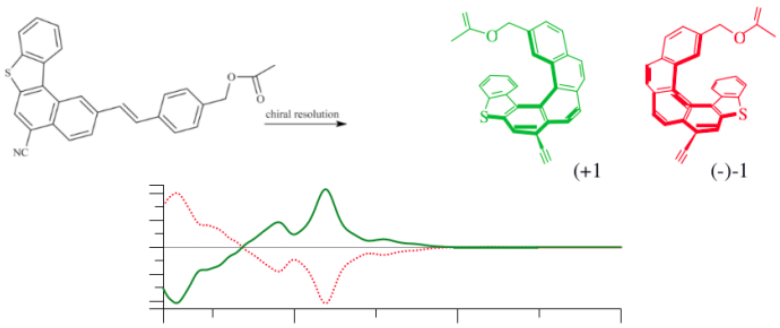

***Figure**: Electronic circular dichroism (ECD) spectra of (+)-**1** and (-)-**1** in CH_2Cl_2.*

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Effect of gamma irradiation on thermoluminescence characteristics of Cu+-Na+ ion-exchanged silicate glasses

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Abstract :

Thermoluminescence (TL) characteristics of gamma ray irradiated commercial silicate glasses ion-exchanged with copper have been studied in the temperature range 50-400 °C for doses ranging from 0.1 to 100 kGy. Ion-exchange route was performed at temperatures varying from 800 to 900 °C in a molten mixture of CuSO4 and NaSO4 with CuSO4 concentration between 1 and 60% for durations 30, 60 and 90 minutes. The glow curves of these glasses have exhibited a dosimetric peak at about 250°C attributed to intrinsic impurities which increases when increasing dose and two other TL peaks that were showing up after the ion-exchange and may be attributed to Cu+ and Cu2+. Results have shown an inhibition of TL which was due to the presence of larger concentration of CuSO4 and short duration of ion exchange. Dose response, linearity and sensitivity have been studied for different conditions of ion-exchange.

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JDD 2020 – OSRSN05

Interpretation of adsorption isotherms of Zn^{2+}, Ni^{2+}, Cd^{2+} and Cu^{2+} ions on carbon-based adsorbents via physical modeling

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Abstract :
A theoretical physicochemical and thermodynamic investigation of the adsorption of heavy metals Zn^{2+}, Cd^{2+}, Ni^{2+}, and Cu^{2+} on carbon-based adsorbents was performed with statistical physics fundaments. Particularly, the experimental adsorption isotherms of heavy metal removal, at 30°C and pH 5, using adsorbents obtained from the pyrolysis of three biomasses (cauliflower cores, broccoli stalks, and coconut shell) were modelled and interpreted with a homogeneous statistical physics adsorption model. Calculations indicated that the heavy metal adsorption with these carbon-based materials was a multi-ionic process where several ions interact simultaneously with the same carboxylic functional group on the adsorbent surface. Adsorption capacities for these metal ions and adsorbents were correlated with electronegativity theory, which established that the adsorbate with the highest electronegativity was more readily adsorbed by the carboxylic functional groups available on the adsorbent surfaces. Also, the chemical compositions of biomass precursors explained achieved adsorption capacities for these metallic ions. The best adsorbent for heavy metal removal was obtained from cauliflower core biomass pyrolysis. Calculated adsorption energies for heavy metal removal could be associated with physisorption-type forces. Finally, the adsorption mechanism analysis was complemented with the determination of adsorption thermodynamic functions using the statistical physics.

Keywords: Adsorption, Heavy metals, Carbon-based adsorbents, Homogeneous statistical physics adsorption model, Carboxylic functional group.

Structural and dielectric study of Mg–Ag spinel ferrites

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Abstract:
In this paper, we investigated the structural and dielectric properties of $Mg_{0.94}Ag_{0.06}Fe_2O_4$ synthesized by the Sol-Gel (Pechini) route. The XRD refinement shows that our sample possesses metallic silver together with the cubic spinel phase. The electrical characterization was performed by complex impedance spectroscopy in the frequency range (100 Hz to 10^6Hz) at various temperatures (295-580 K). The conductance response was investigated on the basis of Jonscher universal power law: $G(\omega) = G_{DC} + A\omega^n$, where ω is the frequency and n is the exponent. From the DC-conductance data, it is found that our sample achieve metal- semiconductor transition. The impedance plane plot shows semicircle arcs at different temperatures and an electrical equivalent circuit has been proposed to explain the impedance results. The study of the normalization curves of impedance and electrical modulus showed a mismatch of both peaks, which suggests the presence of short-range motion of charge carriers.

Keywords: DRX; Dielectric properties; Spinel ferrites; conductance; impedance spectroscopy

Synthèse, détermination structurale et étude des propriétés d'un nouveau polyoxomolybdate hybride

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Résumé :
Un nouveau matériau hybride optique non linéaire à base de polyoxoselenomolybdate tridimensionnel (3D) de type Strandberg (C 6 H 14 N 2) 2 [Se 2 Mo 5 O 21].2.6 H 2 O a été obtenu avec la méthode de synthèse « voie douce » et caractérisé par spectroscopie infrarouge et ultraviolette, analyse thermogravimétrique et voltammétrie cyclique. L'étude cristallographique par diffraction des Rayon X sur monocristal, a montré que le composé synthétisé cristallise dans le système orthorhombique avec le groupe d'espace non centrosymétrique $P2_12_12_1$, ce qui donne en principe des propriétés optiques non linéaires. L'architecture supramoléculaire présente un arrangement périodique des anions de Strandberg [Se 2 Mo 5 O 21] 4 – reliés les uns aux autres par les molécules d'eau et les cations organiques de Dabconuim via des interactions des van der Waals et des liaisons hydrogène.

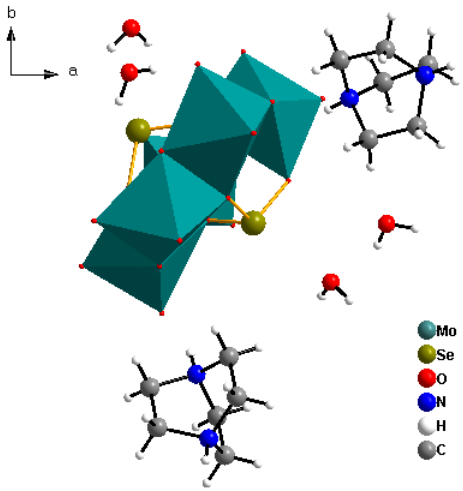

Figure 1: *Unité asymétrique du composé* $(C_6H_{14}N_2)_2[Se_2Mo_5O_{21}]\cdot 2.6H_2O$

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JDD 2020 – OSRSN08

Concentration et répartition du Cadmium dans le gisement des phosphates (Bassin Gafsa) et Essais de décadmiation

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Abstract :
La régularité de la répartition des métaux lourds dans le phosphate [1], entraîne également une grande contamination des sols et des plantes par ces métaux, des quantités qui dépassent des niveaux acceptables. Parmi ces métaux lourds, le cadmium, qui semble être l'élément le plus nocif et le plus toxique et représente aussi un grave danger pour la santé humaine et l'environnement [2]. Dans ce travail, nous avons prélevé des échantillons à partir de gisement de Jallabia et Nagues (Bassin de Gafsa-Metlaoui, sud-ouest de la Tunisie), des échantillons de ce gisement traité pour éliminer les impuretés. Ensuite, nous sommes passés à la diffraction des rayons X (DRX), aux analyses minéralogiques binoculaires, aux analyses chimiques et sous microscope polarisant. On utilise une méthode physique qui est basée surtout sur les propriétés physiques du cadmium et du phosphate, c'est la raison pour laquelle on a décidé d'utiliser la flottation. , Les manipulations de séparations densimétriques des phases pures par liqueurs denses, nous ont aidés à définir la répartition et les formes de présence du cadmium dans les phosphates du bassin de Gafsa. Le facteur principal, qui a été utilisé dans ces expériences, est la répartition inégale du cadmium dans les fractions densimétriques des phases pures de phosphate de quelques gisements du bassin de Gafsa. Dans notre cas, les expériences de flottation ont été faites sur le phosphate marchand et se sont basés sur la séparation sélective de la fraction lourde (ou se concentre le cadmium) de la fraction légère (de teneur basse en Cd). Cette méthode sélective a très bien marché sur le phosphate du bassin de Gafsa, où on a obtenue un surnageant avec une teneur de Cd arrivant jusqu'à 11ppm, et un plongeant de teneur minimale égale à 25 ppm.

Mots-clés : Phosphate, Cadmium, décadmiation.

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Variation of Sorption potential with the nature of the organophosphorus insecticide dimethoate in Tunisian agricultural soils

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Abstract :
The subject of this work falls within the general framework of the environmental impact of agricultural activities. Indeed, these activities are continuous sources of surface pollution which infiltrates through the soils at speeds and degrees which depend on the nature of the natural environment and the contaminant. The irreversible consequence of this infiltration is the degradation of the quality of the groundwater. The pesticide subject of this study is dimethoate whish is classified according to the food and agriculture organization of the United Nations (FAO) and the world health organization (WHO) as an insecticide dangerous to health. It is for this reason that this insecticide has been banned in French, Italian and Spanish orchards since 2016 .However, this insecticide still used by the farmers in Tunisian orchards. This study analyzed how the organic additives (xylene and cyclohexanone) in DMOc (Dimethoate commercial solution) and the physico-chemical properties of soils affected the DMO sorption. For that purpose two soils samples were collected from two different Tunisian regions: sandy soil (SS) and sandy loam soil (SLS) .The soils SS and SLS characterization was carried out by evaluating: the pH, the conductivity, the point of zero charge, the cation exchange capacity, the specific surface, the elementary composition....The experimental pesticide characterization was affected by infrared spectrum (IR) and spectrophotometer (UV) as well as its theoretical characterization which was realized by the density functional theory (DFT) stimulation. The sorption of DMOc and DMOp (Dimethoate pure solution) process was evaluated using the batch procedure. The adsorption isotherms data for the two pesticides were well described by the koble Corrigan model. The additives effect was evaluated and the results prove firstly, that a cooperative adsorption takes place between the different constituents of the commercial emulsion so that the pesticide is better fixed to the soil in the presence of the additives (DMOc) than in their absence (DMOp)and secondly that the cyclohexanone (additive) is the least well retained compound followed by dimethoate (active ingredient) then xylene (additive).

Keywords : Sorption, Insecticide, Soil, Dimethoate,

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Preparation and characterization of activated carbon from food waste by chemical activation H3PO4

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Abstract :
Activated carbon (AC) is widely used in the adsorption field thanks to its interesting properties (large specific surface area, chemical and structural composition).
The idea of this work consists of the recovery of industrial waste from the food industry for the preparation of activated carbon as an adsorbent material for environmental applications. Thus, chemical activated carbons were synthesized from a solid residue of a vegetable oil extraction industry H_3PO_4 as an activating agent. The optimization of various parameters (pyrolysis temperature, carbonization time, concentration of the activating agent) which have an influence on the process of synthesis of activated carbon was done.
To evaluate these physicochemical properties of the synthesized active carbons, different analyzes were done to determine their adsorbing capacity for the retention of certain phytosanitary products. Thus, the evaluation of iodine number (QI2), methylene blue number QMB, zero charge pH (pHzch) and surface functions by the Bohem method were done.
The results of this work show that a concentration of the activating agent H_3PO_4 at 5% associated with a pyrolysis temperature of 400 °C and a heating time of 120 min made it possible to develop the best AC in terms of yield: 38%. However, the best results in terms of iodine number (IQ2 = 979.70 - 999.64 mg / g) and methylene blue index (QMB=8.53 mg/g) are for a concentration of H_3PO_4 at 12.5%, temperature of 800 °C and a carbonization time of 180 min

Keywords: activated carbon, chemical activation, iodine number, methylene blue number.

Fractionnement et Efficacité insecticide de l'huile essentielle de la plante Criste marine contre un ravageur des denrées alimentaires stockées : *Tribolium castaneum*

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Résumé :
Dans le but de contribuer à la valorisation de la flore Tunisienne en vue d'identifier de nouvelles substances potentiellement intéressantes sur les plans biologiques et thérapeutiques, nous avons procédé à l'étude phytochimique de la plante criste marine (appelée aussi *Crithmum maritimum*) collectée de la falaise de Monastir. Cette plante est très employée en médecine traditionnelle grâce à ses diverses vertus.[1] L'analyse par CPG-FID et CPG/SM de l'huile essentielle extraite de ses feuilles a permis d'identifier 8 composés dont le dill apiole est le composé prédominant (94,1%). Par la suite, cette huile a été fractionnée sur une colonne de gel de silice en utilisant un mélange Hexane/Acétate d'éthyle de polarité croissante. Ainsi, cinq fractions de composition différentes ont été recueilles.
D'autre part, l'huile essentielle et ses fractions ont été évaluées pour leurs pouvoirs insecticides vis-à-vis d'un ravageur des denrées stockées « *Tribolium castaneum* » par les tests de répulsivité et de toxicité par contact. Les résultats obtenus ont montré que cette huile est très répulsive (93,33% après 2h) à une concentration de 0,02g/L. Quant aux fractions, nous avons constaté que la 5^{éme} fraction riche en dill apiole a manifesté l'activité relativement la plus élevée (96,66% après 2h) d'où l'importance du fractionnement pour localiser le ou les principes actif(s). L'évaluation de l'activité insecticide par le test de toxicité par contact de l'huile brute et de ses fractions a montré des résultats significatifs. Ceci indique que cette huile pourrait être utilisée comme matière première active dans la formulation d'un biopesticide alternatif aux insecticides de synthèse afin de protéger les aliments stockés contre cet insecte nuisible.

Mots-clés : Criste marine, huile essentielle, dill apiole, pouvoir insecticide, *Tribolium castaneum*.

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Extraction, physicochemical characterization and evaluation of anti-herpetic activity of polysaccharides from *Ficus carica L.*

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Abstract:
Because of the numerous secondary effects of conventional drugs of the herpes simplex virus 2 (HSV-2) and the growing phenomenon of resistance, the researchers turned to the natural kingdoms as a source of new drugs with anti-HSV-2 potential. Because the bioactive extracts of natural origin are less harmful and non-toxic than their synthetic counterparts. This study was designed to characterize the physicochemical properties of the polysaccharides isolated from *Ficus carica L.* and to evaluate its anti-herpetic activity. The different macromolecular characteristics of the extracted polysaccharides were determined by size exclusion chromatography combined with multi-angle laser light-scattering detection (SEC-MALLS), Fourier transform infrared spectroscopy (FTIR) analysis and nuclear magnetic resonance spectroscopy (^{1}H NMR and ^{13}C NMR). The monosaccharide composition of the extracted polysaccharides was performed by gas chromatography coupled with mass spectrometry (GC–MS). Moreover, the result of the antiviral activity against the herpes simplex virus 2 (HSV-2) showed that the tested polysaccharides exhibited strong activity which confirmed that the *Ficus carica L.* may comprise the natural raw materials for new anti-herpetic drug.

Keywords: Polysaccharides, SEC-MALLS, spectroscopic analysis, GC-MS, anti-herpetic activity

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SYNTHESE DES NOUVEAUX COMPLEXES A BASE DES TETRAZINE

Ons AMAMOU[a,b], Riadh EL ABED [a], Clève D. MBOYI [b], Julien ROGER [b], Jean-Cyrille HIERSO [b] et Taoufik BOUBAKER [a]

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b. Université de Bourgogne, Institut de Chimie Moléculaire, Organométalliques, Catalyse, Stéréochimie, UMR CNRS 6302, Av Alain Savary-BP 4787021078 Dijon Cedex, France ;

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Abstract :
Les 1,2,4,5-tétrazines présentent une chimie de coordination particulière, caractérisée par le phénomène de transfert de charge et par la capacité de ces ligands riches en hétéroatomes ponter les centres métalliques de diverses manières. Les conséquences structurelles du transfert d'électrons ainsi que la capacité de pontage métal-métal efficace et variable font des tétrazines de composants précieux des matériaux supramoléculaires.
Dans ce contexte, nous avons synthétisé et étudié de nouveaux ligands de tétrazine présentant une structure inédite de type pince-ponté et leurs complexes de coordination afin d'évaluer leur utilité comme composantes dans des assemblages moléculaires à réactivité multiélectronique.

Mots-clés : 1,2,4,5-tétrazine, Chimie de coordination, Matériaux supramoléculaires.

[1] W. Kaim, J. Coord. Chem. Rev., 2002, 230, 127.
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JDD 2020 – PSRSN02

Synthesis and characterization of new copper metalloporphyrin's complexes. Application as catalysts in the degradation and reduction of certain chemical pollutants

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Abstract:

The copper (II) meso-tetrakis(4-methoxyphenyl)porphyrin (CuTMPP) (Figure **1**) and the copper (II) meso-tetrakis(4-chlorophenyl)porphyrin (CuTClPP) (Figure **2**) are synthesized following Adler Longo method. These compounds have been characterized by UV-Vis, proton nuclear magnetic resonance H^1 NMR, MALDI-TOF mass spectrometry and IR spectroscopy. The authors must give here some results of these characterizations As an application, the complexes were used as a support for the catalytic reduction and degradation of 4-Nitrophenol (4-NP) with sodium borohydride ($NaBH_4$) in water to give 4-Aminophenol (4-AP) without the formation of byproducts. The same remark here: the authors must give some results such as: the yields of the degradation Unlike 4-NP, its reduced product 4-AP has a lower toxicity and is used in pharmaceutical industries for the manufacture of analgesic, antipyretic and other drugs.

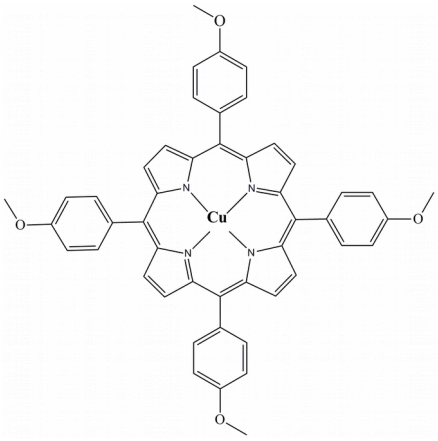

Figure 1: Structure of [Cu(TMPP)] (1)

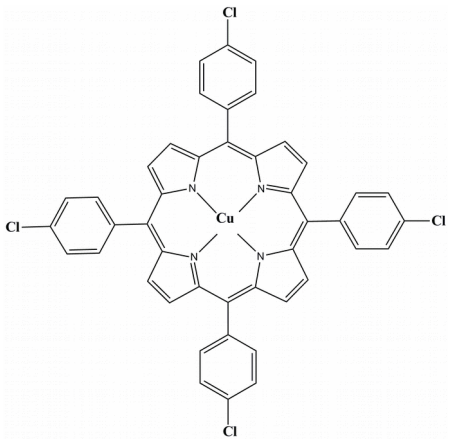

Figure 2: Structure of [Cu(TClPP)] (2)

Keywords: Copper(II)-porphyrin,MALDI-TOF, Reduction,Degradation, 4-Nitrophenol.

Rare Earths Effect on Structural, Electrical and Optical Properties of Na0.4K0.1Bi0.5TiO3 ceramics

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Abstract:
Lead-free Sodium Potassium Bismuth Titanate ((Na 0.4 K 0.1)Bi 0.5 TiO 3) ferroelectric ceramics doped with rare earth (RE: Ho, Pr, Nd, Er, Dy) elements are synthesized thru solid state reaction technique. Then, Electric, ferroelectric and optical performances were studied. The X-ray diffraction outcomes evinced that the RE-doped NKBT ceramics displayed a pure perovskite structure with R3c as a space group and the particle size varied between 45 and 58 nm. The ferroelectric properties of the pure $(Na_{0.4}K_{0.1})Bi_{0.5}TiO_3$ ceramics (P_r : 15.69µC/cm 2 , E c : 30Kv/cm) are somewhat higher than the values found for the doped elements, which is assigned to minimizing of the number of Bi lone pairs through the substitution of Bi with RE elements in the perovskite lattice. The incorporation of RE 3+ ions in the NKBT host lattice displayed different light emissions over the wavelength variety from visible to near infrared region. Strong green ($^4S_{3/2} \rightarrow {}^4I_{15/2}$) and red ($^5F_5 \rightarrow {}^5I_8$) Up Conversion luminescence were observed in the ceramics NKBT-Er and NKBT-Ho respectively, when excited with a 975 nm diode laser.

Keywords: Ceramics, Ferroelectric, Rare earth.

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JDD 2020 – PSRSN04

Synthesis and characterization of a novel alkali mixed magnesium-aluminum phosphate with a layered structure–$KMgAl(PO_4)_2$

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Abstract:
A novel phosphate compound potassium magnesium-aluminum double phosphate with chemical formula $KMgAl(PO_4)_2$ has been synthesized both by flux growth and sol-gel reaction. This compound have been characterized by X-ray diffraction, differential thermal analysis, vibrational spectroscopy and electronic structure calculations. $KMgAl(PO_4)_2$ crystallizes in the trigonal centrosymmetric space group P-3m1 (No. 164) with unit cell parameters a = b = 5.347(1) Å, c = 7.903(10)Å, γ= 120 °(Z = 1). The main characteristic of the crystal is the two-dimensional (2D) lamellar framework, with the K^+ cations located within the interlayer space. The Platelet morphology and chemical composition were revealed by the scanning electron microscopy–energy-dispersive X-ray spectroscopy analysis. The IR spectroscopy of $KMgAl(PO_4)_2$ confirmed the existence of a single PO_4 group in agreement with the structural study. A relatively large indirect band gap of 3.86 eV was determined.

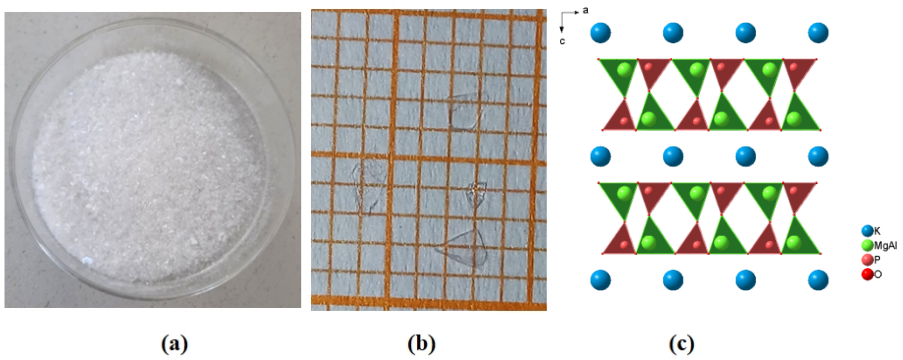

***Figure 1**: Photographs of $KMgAl(PO_4)_2$ samples: (a) single-crystalline, (b) individual platelet-shaped samples. (c) Projection of $KMgAl(PO_4)_2$ structure on the **a-c** plane showing the layered stacking along the b -axis.*

Keywords: Complex phosphates, Layered structure, Electronic structure, Optical properties.

Solid state synthesis and characterization of the $Na_2Co_2Cr_{0.75}Al_{0.25}(PO_4)_3$ phosphate materials

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Abstract :
This work is a part of a general study of alkali transition metal phosphates belonging to the A_3PO_4-$B_3(PO_4)_2$-$M^{III}PO_4$ systems (A: Alkali metal, B: divalent cation; M^{III} = trivalent transition metal) using solid state reaction, in a search of new materials with attractive physical and chemical properties. It reports the synthesis by solid state reaction of the $Na_2Co_2Cr_{1-x}Alx(PO_4)_3$ (x = 0; 0.25) compounds. Their investigation by X-ray diffraction showed that they crystallize in the monoclinic system with the space group *C2/c* and the cell parameters *a* = 11.7819 (6)Å; *b* =12.3623 (7)Å *c* = 6.4100(3)Å for x = 0 and *a* = 12.101(1) Å; *b* = 12.591 (1) Å *c* = 6.481(2) Å for x = 0.25. Their structure (fig. I.1) is built up by $M(1)O_6$ and $M(2)O_6$ octahedra linked by PO_4 tetrahedra forming 3D framework similar to those of Alluaudite type. This framework can be described in terms of [AlCr2(PO4)3] equivalent mixed layers stacked perpendicular to the [010] direction. One layer can be imzagined as made by infinite chains of edge-sharing octahedra with a sequence CrO_6–AlO_6–CrO_6 parallel to the [101] direction (Fig I.1). The morphology of the powders and their chemical compositions were determined by scanning electron microscopy (SEM) and energy- dispersive X-ray spectrometer (EDS). The IR and Raman spectra are typical of a monophosphate and give clear evidence of the occurence of two crystallograpically distinct phosphorus sites.

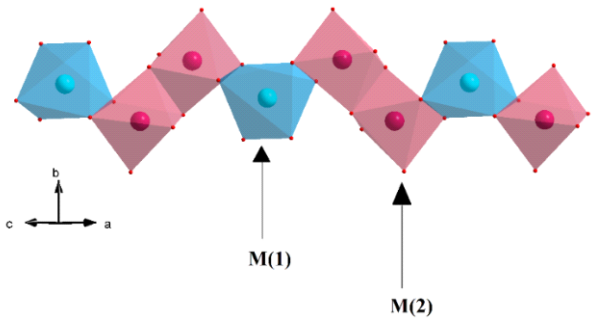

Figure 1: *Edge-sharing octahedra forming an infinite zigzag chain running along [101] in* $Na_2Co_2Cr_{0.75}Al_{0.25}(PO_4)_3$

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JDD 2020 – PSRSN06

Voltammetric Determination of Sulfamethoxazole at a Glassy Carbon Electrode Modified With a Multi-Walled Carbon Nanotubes

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Abstract :
Sulfamethoxazole is an antibiotic largely used as an efficient antimicrobial agents and one of the most effective sulfa medicines in the treatment of urinary infections. So, it is among the priority pollutants to be monitored in animal derived food products, as well as a wide variety of matrices, because their undesirable residues can remain and be incorporated into waters, soils, crops, animal tissues, and bio-fluids (milk and plasma). Classic electrode materials such as vitreous carbon and platinum have shown low electrocatalytic activity for the oxidation of sulfamethoxazole in water. Electrode surface modification by carbon nanotubes, characterized by high electrical conductivity and surface area, significant mechanical strength and good chemical stability, is used to overcome the slow kinetics of the sulfamethoxazole electrochemical oxidation reaction. In this work, we have investigated the effect of operating parameters on the electrochemical response of sulfamethoxazole in aqueous solution on a glassy carbon electrode modified with a multi-walled carbon nanotubes.

Keywords: Sulfamethoxazole, multi-walled carbon nanotubes, glassy carbon electrode, electrochemical oxidation.

SYNTHESIS AND SPECTROSCOPIC CHARACTERIZATION OF (OXO) (OCTAETHYLPORPHYRINATO) VANADIUM(IV) COMPLEX AND (OXO) (OCTACHLOROTETRAPHENYLPORPHYRINATO) VANADIUM(IV)

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b. Université J. Fourier, Département de Chimie Moléculaire, UMR CNRS 5250, ICMG – FR 2607, Laboratoire de Chimie Inorganique Rédox, BP 53, 38041 Grenoble Cedex 9, France

Abstract :
Porphyrins and metalloporphyrins have been studied in several research areas, especially because Porphyrins and metallopoprphyrins are involved in numerous biological functions such as the chlorophylls, hemoglobin, myoglobin and cytochromes P450 [1]. Recently, Vanadyl-porphyrins have attracted much attention due to their reported involvement in potent insulinomimetic activity and anti-HIV agents [2]. In this communication, we describe the synthesis of the new VanadylPorphyrins derivatives: (Oxo)(octachlorotetraphenylpoprphyrinato) vanadium(IV) with the formula [VIV(TPP-Cl8)(O)]and(Oxo) (octaethylphenylpoprphyrinato)vanadium(IV)[VIV(OEP)(O)]. These species were characterized by UV-vis, IR, 1H NMR spectroscopy and voltammetry cyclic. The single crystal X-ray data collection of the [VIV(TPP-Cl8)(O)] complex was performed on a Bruker APEXII CCD diffractometer.

Key-words : porphyrin, vanadylporphyrin,voltammetry cyclic

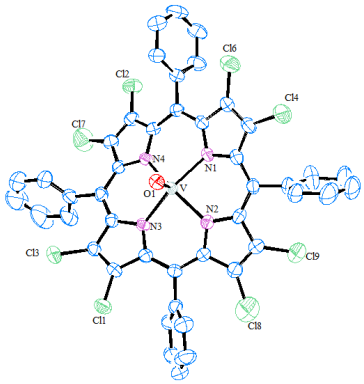

Figure 1 : ORTEP diagram of [VIV(TPP-Cl8)(O)].

[1] A. D. Adler, F. R. Longo, J. D. Finarelli, J. Goldmacher, J. Assourand L. Korsakoff, Org. Chem., 1967, 32,476.
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JDD 2020 – PSRSN08

Synthesis and photophysical properties of new heptacyclic helicene

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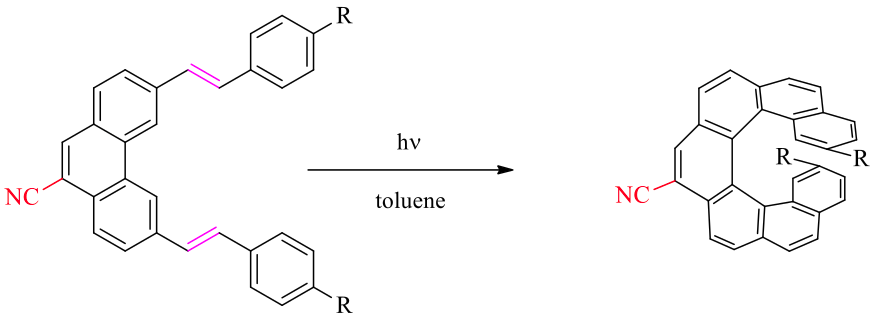
Abstract :

Helicenes represent a class of polyaromatic hydrocarbons consisting of orthoannellated benzene nuclei with a non-planar topology [1]. The helical structure of such molecules results from the repulsive interaction between terminal aromatic rings [2] making them inherently chiral despite the absence chiral centers. They have attracted much interest due to their unrivalled structural features [3]. These organic molecules present left- and right handed chiral helical structures of M and P configuration, respectively. In our work, new helically chiral heptacyclic compounds bearing suitable functional groups have been prepared, in a good overall yield, through a four-step sequence involving mild experimental conditions. The target polyfunctional [7]-helicenes showed a good solubility in common solvents and interesting optoelectronic properties. Their photophysiacal properties have been evaluated using UVevis absorption, the electrochemical band gap was less than 2.7 eV.

Key words: Condensation, Photooxidation, photophysical properties.



Scheme 1 : Synthesis of new heptacyclic helicenes.

[1] R. H. Martin, Die Helicene, Angew. Chem., 727-738(1974).
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Effect of Pressure Variation on the Composition Profiles from Wild Carrot (Daucus carota susbp. maritimus) Extracts using Supercritical Carbon Dioxide

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Abstract :
Herbal and plant remedies have been used for centuries and they possess a huge potential for future pharmaceutical therapies. Although, plant extracts, essential oils and their active molecules are widely studied by research groups around the world within the aim to strengthen Human immunity and to combat the resistance to herbal pathogens. Recently, the technology of supercritical fluid extraction is considered as one of the most potentially useful new methods suitable to obtain essential oils of better qualities [1-2]. Thus, the present study constitutes the first attempt to investigate the chemical composition of Daucus carota subsp. maritimus extracts using supercritical fluid technology (SFE) as a high quality and environmentally clean scientific method of extraction. The effect of pressure on the nature of extractable substances from wild carrot has been performed at a constant temperature of 50 °C and two different pressures (100 and 300 bar). The highest extraction yield (2.98%) was obtained at 50°C and 300 bar. The chemical compositions of the extracted essential oils were analyzed on the basis of gas chromatography coupled to mass spectroscopy (GC–MS). Consequently, geranyl acetate, β-bisabolene and elemicin have been identified as the major aroma in both extracts.

Keywords: Daucus carota subsp. maritimus, Essential oils, Supercritical fluid extraction, Geranyl acetate.

[1] A.M. Aliev, G.K. Radjabova, A.M. Musaev. Dynamics of supercritical extraction of biological active substances from the Juniperus communis var. saxatillis. J Supercrit Fluid, 102, 66–72 (2015).
[2] N. Aghel, Y. Yamini, A. Hadjiakhoondi, S.M. Pourmortazavi. Supercritical carbon dioxide extraction of Mentha pulegium L. essential oil. Talanta, 62, 407–411 (2004).

Chemical composition, antibacterial and antifungal activities of Plantago afra L. essential oil

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c. Department of Phytochemistry ICMR-National Institute of Traditional Medicine, Nehru Nagar-Belagavi, 590010, Karnataka, India.

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Abstract:
Essential oils have long been used traditionally as remedies against infections and commercialized because of their biological activities. Thus, the antimicrobial properties of essential oils are continuously investigated searching for potential candidates to overcome the problem of microbial drug resistance. The aim of this research is to investigate for the first time the chemical composition and the antimicrobial effects of Plantago afra L. (Black psyllium) essential oil. The aerial parts were collected from the north-western of Tunisia, extracted by hydrodistillation, and the resulting essential oil was analyzed using gas chromatography coupled with mass spectrometry. Antimicrobial activities were evaluated using the micro-well plate dilution assay for five bacterial strains: Escherichia coli (ATCC 8739), Salmonella enterica (CIP 8039), Pseudomonas aeruginosa (ATCC 9027), Staphylococcus aureus (ATCC 6538) and Bacillus subtilis (ATCC 6633) along with the yeast Candida albicans (ATCC 30031).
Analysis of the essential oil composition led to the identification of forty five components representing 92.4 % of the whole constituents. Thymol, 3-[4-(t-butyl) phenyl] furan-2,5-dione and palmitic acid, were identified as major components. The results of the biological testing showed a significant antimicrobial activity, especially against Candida albicans human pathogenic yeast (MIC=MFC=312.5 µg /mL). Thus, we suggest that Plantago afra could be effective as a source of natural antimicrobial agents.

Keywords: Plantago afra L., essential oil, chemical composition, antimicrobial activity.

Synthesis, characterization and X-Ray structure of a new decavanadate (C7H11N2)4 [H2V10O28]

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Abstract:
Polyoxometalates(POMs) are a class of molecular - defined inorganic metal oxide clusters formed from early transition metals in their highest oxidation states (V,Nb,Ta, Mo, W) and oxygen, which have been studied in various applications in different fields such as catalysis, energy storage, medicine, magnetism and electro chromic applications to name a few. In order to obtain new materials with novel structures and interesting properties, we report in this work for the first time the synthesis, characterizations, crystal structure of the novel decavanadate (C7H10N2) (C7H11N2)3[H3V10O28],crystallized in a monoclinic system, P-1 space group with the cell parameters : a = 9.8519 (11)Å ,a = 11.0820 (11) Å, c = 12.9098 (14) Å, β = 111.760 (1) ° and Z = 1.

Key words: Synthesis, Characterization, X-ray diffraction.

Zinc(II) triazole meso-arylsubstituted porphyrins for uv-visible chloride and bromide sensing

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Abstract:
Three novel triazole meso-arylporphyrins: H2(TAzP-HVP) (4a), H2(TAzP-HVP) (5b) and H2(TAzP-HVP) (4c) bearing the 3-methoxy-4-((1-phenyl-1H-1,2,3-triazol-4-yl)methoxy)phenyl) moiety (H-triazole derivative), the 4-((1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl)methoxy)-3-methoxyphenyl) moiety (chloro-triazole derivative) and the 4-((1-(4-iodinephenyl)-1H-1,2,3-triazol-4-yl)methoxy)-3-methoxyphenyl) moiety (iodine-triazole derivative), respectively, have been synthesized by the "click chemistry" approach using azide-alkyne couplings. The corresponding zinc(II) coordination compounds (5a-c) have also been prepared. All 4a-c and 5a-c porphyrin species were fully characterized by elementary analysis, ESI and MALDI-TOF mass spectrometry, IR, proton NMR, UV-visible, fluorescence and cyclic voltammetry. Both chloro-triazole and the iodine-triazole zinc(II) derivatives [Zn(TAzP-ClVP)] (5b) and [ZnTAzP-IVP)] (5c) have been tested as receptors for Cl- and Br- anion sensing. UV-visible titrations reveal that both 5b-c host systems exhibit strong anion binding affinities [1].

Keywords : Click chemistry ; Cyclic voltammetry ; sensation

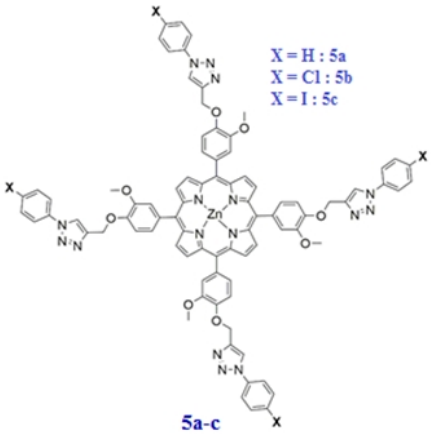

Figure 1 : Structure of [ZnTAzP-RVP)] complexes. 5a: X = H, 5b: X = Cl and 5c: X = I.

[1] L. C. Gilday, N. G. White, P.D. Beer, Dalton Trans, **41**, 7092–7097 (2012).

Synthesis, antidiabetic activity and molecular docking study of rhodanine-substitued spirooxindole pyrrolidine derivatives as novel α-amylase inhibitors

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Abstract :
In this contribution, we describe an elegant one-pot reaction to synthesize a new family of rhodanine-fused spiro[pyrrolidine-2,3'-oxindole] derivatives in good to high yields along with high regio and diastereoselectivity. The protocol involves a three-component 1,3-dipolar cycloaddition, combining (Z)-5-arylidine-2-thioxothiazolidin-4-ones, glycine methyl ester and isatins. Its general applicability has verified by thorough variation of the starting material substrates featuring a wide scope of different sterically and electronic parameters. The resulting spiroheterocycles were evaluated for their in vitro α-amylase inhibitory activities, showing a good α-amylase inhibition with respect to the control drug Acarbose. To understand the mode of binding interactions of synthetic molecules with active sites of α-amylase enzyme, molecular docking studies were performed. The most potent compounds were further screened in vivo for their antidiabetic activity in alloxan-induced diabetic rats and caused a considerable reduction in blood glucose level.

Keywords : Spirooxindole pyrrolidine, Antidiabetic, α-Amylase, 1,3-Dipolar cycloaddition, Molecular docking.

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Journées des Doctorants, 20 & 21 Décembre 2021
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JDD 2020 – PSRSN14

QUANTIFICATION ET INSERTION DU 2-X-3,5-DINITROTHIOPHENE DANS L'ECHELLE UNIVERSELLE DE MAYR

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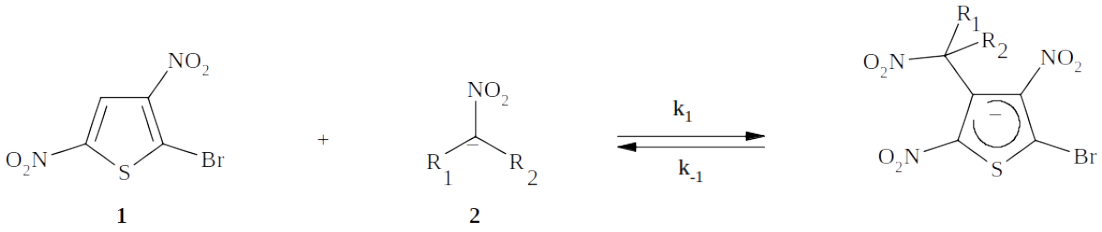
Abstract :
Nous rapportons dans la présente communication l'étude cinétique approfondie de la réaction de couplage du 2-bromo-3,5-dintrothiophène 1a et 1b avec une série d'anions nitroalcanes 2a-c dans l'eau à 20 °C.



1

1a: X = Br
1b: X = NH_2

2

2a : R_1 = H, R_2 = H
2b : R_1 = H, R_2 = CH_3
2c : R_1 = CH_3, R_2 = CH_3

$$\log k\ (20\ °C) = s_N\ (E + N) \qquad (1)$$

Les diverses corrélations structure-réactivité obtenues ont permis d'une part, de quantifier les paramètres d'électrophilie E du 2-X-3,5-dintrothiophène 1a et 1b selon l'approche de Mayr (Eq (1)), et d'autre part de discuter l'effet de la basicité des anions nitroalcanes 2a-c sur la constante de vitesse bimoléculaire.

Mots-Clés : Equation de Mayr, Carbanions, Corrélation Structure-Réactivité.

[1] S. Soussi, W. Gabsi, T. Boubaker. Int. J. Chem. Kinet., 2018, 46, 582-590.
[2] H. Mayr, M. Patz. Angew. Chem. Int. Ed. Engl., 1994, 33, 938.
[3] H. Ayachi, H. Raissi, F. Mahdhaoui, T. Boubaker. Int. J. Chem. Kinet., 2020, soumis.

École doctorale Matériaux, Dispositifs et Microsystèmes
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JDD 2020 – PSRSN15

Anti scaling magnetic processes in natural waters.

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Abstract:
Calcium carbonate scaling is often a major problem in different aspects of industrial processes and domestic installations. The influence of magnetic treatment on the precipitation of calcium carbonate has always attracted the attention of researchers. The techniques adopted to examine the effect of this anti-scaling process are generally based on chemical and electrochemical scaling tests. Permanent magnets were placed in the designed treatment devices that consisted in synthetic water samples whose composition is similar to that of underground Tunisian water (hardness 25°F). Magnetic strength was varied between 0.33 T to 0.5 T to investigate its effect on scale reduction. Indeed, we tried to deposit calcium carbonate by electrochemical reduction of oxygen at negative potential (-1V/SCE) and we studied on metal electrode by chronoamperometry. It was showed that, at the rotation speed of 1200 turn/min the scaling time increased after magnetization with 0.33T from 50 minutes to 185 minutes. In addition, in function of time and at 0.5T, the result proved that 18 hours was the optimal time to obtain the maximum increase until 233 minutes. So the effect of magnetization can persist even after treatment (memory effect). The Scanning lectron Microscopy (SEM) was with EDS analysis to identify the morphology of the scale deposit.

Mots-clés : scaling, magnetic treatment, anti-scale, chronoamperometry.

Electrochemical study of modified glassy carbon electrode by nickel nanoparticle and poly-2-nitroaniline for dopamine detection

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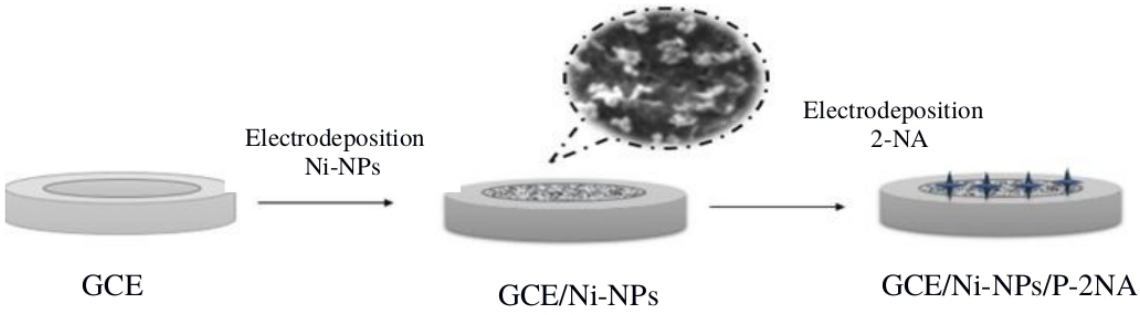
Abstract :
In this study, nickel nanoparticle was first deposited and followed by the electropolymerization of 2-nitroaniline monomer at the surface of glassy carbon electrode for the determination of dopamine (DA) which represents an important neurotransmitter and plays a significant role in the function of the central nervous, renal and hormonal system. The performance of modified surfaces based on the nanocomposite matrix was investigated using cyclic voltammetry and differential pulse voltammetry.
This sensor was characterized by a wide linear range from 5.10 -7 mol.L -1 to 2.10 -4 mol.L -1 , a low limit of detection of 5.10 -7 mol.L -1 and an adequate sensitivity of 0,078 µA/mol.L -1 .



Schematic illustration of the sensor fabrication based on GCE/Ni-NPs/P-2NA obtained by electrodeposition method.

Keywords: Nickel nanoparticle, Dopamine, Biosensor.

PREPARATION, SPECTROSCOPIC CHARACTERIZATION AND MOLECULAR STRUCTURE OF A MANGANESE (III) PORPHYRIN COMPLEX

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Abstract:
Synthetic iron and manganese porphyrins resemble the active centers of heme-containing biological systems. Manganese porphyrins are also widely used in the biomimetic studies of cytochrome P-450 [1], catalases [2] and other enzymes [3]. We have prepared a new coordination compound ; the manganese (III) porphyrin complex $[Mn^{III}(TMPP)(C_7H_{10}N_2)_2].SO_3CF_3$. This species was characterized by UV-Visible, IR, mass spectrum, cyclic voltammetry and X ray crystallography techniques.

Keywords : Manganese, Porphyrin complex,

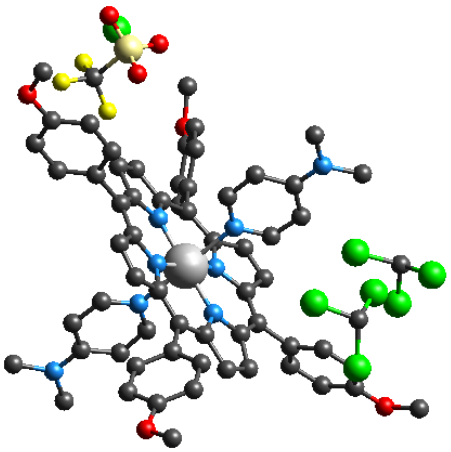

Figure 1 : The manganese (III) porphyrin complex $[Mn^{III}(TMPP)(C_7H_{10}N_2)_2].SO_3CF_3$

[1] : D. Mansuy, Coord. Chem. Rev. **125**, 129-141. (1993).
[2] H. Srour, P. Le Maux, S. Chevance, G. Simonneaux, Coord. Chem. Rev, **257**, 3030-3050. (2013).
[3] I. Batinic-Haberle, Z. Rajic, A. Tovmasyan, J.S. Reboucas, X.D. Ye, K.W. Leong, M. W. Dewhirst, Z. Vujaskovic, L. Benov, I. Spasojevic, Free Radicals Biol. Med,. **51**, 1035-1053 (2011).

Degradability of novel biobased (co)polyesters under different environmental conditions

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Abstract :
Over the past few decades, the search for sustainable chemicals, polymers and materials has intensified. Most recently, interest has focused on isosorbide and furan monomers and their polymers because of their potential to replace equivalent fossil-based products [1]. In this regard, a series of fully biobased poly(isosorbide 2,5-furandicarboxylate-co-dodecanedioate) (co)polyesters (PIsFDDs) were successfully synthesized for the first time from Isosorbide (Is), 2,5-furandicarboxylic acid (FDCA), and 1,12-dodecandioic acid (DDA) using the melt polycondensation method.
A comprehensive evaluation of degradation in phosphate buffer solution (PBS), sea salts, and enzymatic environment indicated that the insertion of DDA monomer into the PIsFDD chain promotes noticeable degradation, resulting in weight loss up to 13 and 15% for the PIsFDD (co)polyesters with 40 and 90 mol% DDA, respectively, after only 63 days. Based on the results obtained in this work, PIsFDDs were found to be promising biobased polymers suitable for applications in sustainable and environmentally friendly plastic packaging.

Keywords : biobased (co)polyesters, hydrolytic degradation, enzymatic degradation, in sea salts degradation.

[1] Vilela, C.; Sousa, A.F.; Fonseca, A.C.; Serra, A.C.; Coelho, J.F.J.; Freire, C.S.R.; Silvestre, A.J.D. The quest for sustainable polyesters-insights into the future. Polym. Chem, 5, 3119–3141 (2014). doi:10.1039/c3py01213a.

Matériaux Organiques et Environnement «MOE»

Numerical modeling of dye transport in unsaturated layered soil

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Abstract :
With the fast development in industrial scale, the problem of water and soil pollution has become more serious. In fact, the use of organic dye in many industrial products may threaten the water systems. To minimize this contaminant migration in the soil, the use of capillary barriers is proposed as an efficient solution. Therefore, a numerical model was developed and validated in this study based on Richard's equation and advection-dispersion equation coupled with adsorption model. The effect of number of layers have been undertaken. The results shows that the soil heterogeneity has a significant effect on methylene blue (MB) adsorption through layered media.

Key words: soil pollution, adsorption, methylene blue, layered soil.

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JDD 2020 – PMOE02

Synthesis, spectroscopic and structural characterization of a new Cadmium(II) porphyrin complex

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Abstract :
The aim of this work is first the synthesis of a new cadmium(II) Metalloporphyrin with formula [K(222)(H2O)][CdII(TMPP)(NCO)].2(CH2Cl 2) (I) where TMPP is the meso-tetra(para-methoxyphenyl)porphyrinato and 222 is the cryptand-222. Compound (I) was prepared by the reaction of the [Cd(TMPP)] staring material with an excess of potassium cyanate salt and an excess of the cryptand-222 in dichloromethane. This complex was characterized by UV–visible, IR and proton NMR spectroscopy. We also characterized this species by single crystal X-ray Molecular structure. The data collection was made at low temperature (150 K) and complex (I) crystalizes in the triclinic crystal system with the P-1 space group. The cell parameters are: a = 12,7952(12) Å, b = 14,1757(10) Å, c = 21,1761(19) Å → = 94,466(3)▼, ↑ = 106,439(3)° and ✚ =97,601(3)°. V = 3624,6(5) Å3, Z = 2, R1 = 0,0397 and wR2 = 0,1094. The Cd (II) cation is chelated by the four pyrrole N atoms of the porphyrinate anion and additionally coordinated by an N-cyanato ligand in an apical site. The K+ ion is chelated by the six oxygen atoms and two nitrogen atoms of the cryptand-222 mol-ecule and is further coordinated by a water molecule.

Keywords: Cadmium (II) porphyrin coordination compound; X-ray crystal structure; UV– visible spectra; IR spectra.

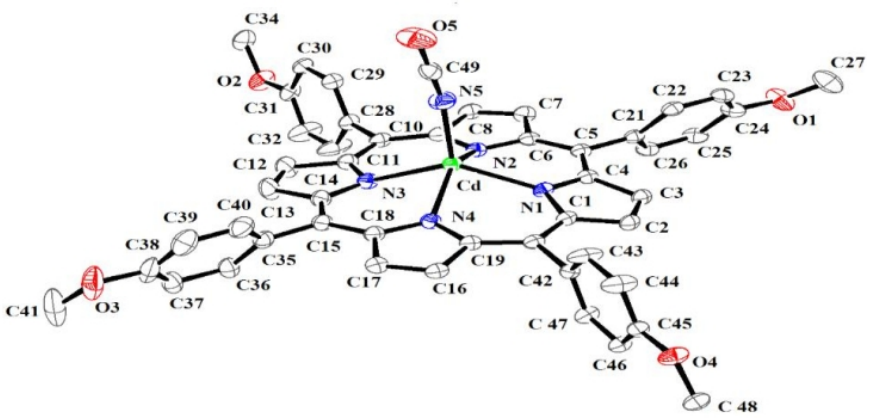

Figure 1: Molecular structure of [CdII(TMPP)(NCO)]- ion complex

New organic materials with a conjugated p-electron

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Abstract:

New organic materials with a conjugated p-electron system providing intramolecular charge-transfer properties have been elucidated. In a particular embodiment, the studied organic materials denoted as M1, is based on a two bromo-distyrylbenzene motives, with N-ethylcarbazole group as central core, has been synthesized and characterized. Then, four benzocarbazole were designed as symmetrical D(-p-A)2 type materials were N-ethylbenzocarbazole as the electron donor, stylben as π-bridge and cyanoacrylic acid (CbzA1), rhodanine-3-acetic acid (CbzA2), indenedione (CbzA3), cyanobenzthiazolevinylene (CbzA4) as the electron acceptor were elucidated.

The relation between the electronic structure and the optical properties of these kinds of π-conjugated materials and their photovoltaic performances was investigated. Herein, All calculations were performed using the Density Functional Theory (DFT) and the Time-Dependent DFT (TD-DFT) in both gas and solution phases, showing a good correlation with the corresponding experimental measurements. The lowest-lying absorption spectra can be mainly attributed to intramolecular charge transfer (ICT), and the fluorescence spectra can be mainly described as originating from an excited state with intramolecular charge transfer (ICT) character. We calculated the charge transfer parameters, and some Reactivity Descriptors. Also we investigated the effects N-atom substitution on the photophysical properties of these push–pull organic materials.

Keywords: Carbazole; DFT calculations; Intramolecular Charge transfer (ICT), DSSC device.

Electro-optical properties enhancement in MEH-PPV by incorporation of DABMN small organic molecules

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Abstract :
The solution-processable organic semiconductors are viable cost-effective candidate for several active components in organic optoelectronic and photonic devices and offer high flexibility and large area uniformity. The present work reports a novel solution-processable organic composite formation of p-N,N-dimethyl-amino-benzylidene-malononitrile (DABMN) and poly [2-methoxy-5-(2-ethylhexyloxy)-1, 4-phenylenevinylene] (MEH-PPV). The microstructure and the electro-optical performance of the MEH-PPV: DABMN composite films were investigated. The morphological and optical investigations of the composite reveal interaction between DABMN and MEH-PPV. The photoluminescence spectra of the composite showed an apparent quenching suggesting the transfer of charge between the two composite materials. The current-voltage characteristic of the composite device exhibits a Schottky diode type behavior with a low threshold voltage. From conductance measurements, the interface state density and trap states time constant of MEH-PPV and MEH-PPV: DABMN were calculated as [2.02 ×1014 eV-1 m-2, 0.42 10-6 s] and [1.27 ×1014 eV-1 m-2, 0.21 10-6 s], respectively. This result was compared to the literature and showed that the DABMN enhances the composite performance.

Key words: solution-processable organic semiconductors, DABMN, composite films, Interface state density, organic optoelectronic.

Electronique et Microélectronique «EME»

Conception et implémentation d'un système d'apprentissage profond pour la détection des anomalies dans les images médicales.

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Abstract :

L'énorme progrès des appareils d'acquisition des images médicales a offert dans nos jours la disponibilité des données volumineuses qui rend l'analyse de l'image très intéressante mais difficile. Cette croissance rapide des modalités des images médicales exige des efforts considérables et fastidieux de la part des experts médicaux qui peuvent présenter des grandes variations dans les résultats des analyses d'un expert à un autre. La solution alternative est d'utiliser des techniques à machine d'apprentissage pour automatiser le processus de diagnostic, cependant, les méthodes traditionnelles d'apprentissage ne sont pas suffisantes pour traiter des problèmes complexes. En associant le traitement des images médicales avec la machine d'apprentissage cela permet de traiter des grandes images médicales avec un diagnostic précis et efficace. Des techniques permettent non seulement de sélectionner et d'extraire des caractéristiques, mais aussi de mesurer la cible prédictive et de fournir des modèles de prédiction exploitables pour aider les chercheurs, les physiciens et les médecins de manière efficace.

On se propose dans ce sujet de réaliser des applications de détection des anomalies pour les images médicales par des techniques d'apprentissage profond et accumuler les résultats de traitement et les classer dans un serveur firebase. Selon le type d'application on évalue les plateformes utilisées qui seront capables d'assurer le traitement en temps réel. Des optimisations algorithmiques permettent d'accélérer le traitement seront proposées. On peut envisager des divers types de traitement hardware/software en particulier les plateformes d'analyse et les outils de BigData.

Miniaturized Antenna design for UHF Small Satellite Communication

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Abstract :
The (Ultra High Frequency) UHF radio amateur band is a very popular radio band for CubeSat Communications. The longer wavelength accompanied with the UHF band results in antennas that are relatively big compared to the size of a CubeSat. To communicate in this band, CubeSats are therefore equipped with linear wire antennas in dipole or turnstile configuration. Compared to patch antennas which are used to communicate in the S-band, these linear wire antennas have the downside that they need a deployment mechanism. This deployment mechanism increases the risk of failure during the mission, and subsequently asks more attention during design, integration and testing of the CubeSat. Furthermore, this system adds extra mass to the CubeSat and it takes up space that could be used by other subsystems.
In this work, we elaborate the design and simulation of a planar low profile antenna solution for a CubeSat operating around 920 MHz. The main feature of the proposed antenna is its miniaturized size. The miniaturization procedure is given in detail, and the electrical performance of this small antenna is documented. Two main miniaturization techniques have been applied, i.e. dielectric loading and distortion of the current path by adding a meander line and ground in the same side. The size reduction of λ/5 compared to the conventional reference antenna is achieved in this study. The proposed antenna has a simple structure and small size of 50*80*1.635 mm3 or about 0.153λ0 * 0.245 λ0. It has an S11 of -31.11dB obtained by simulation and a measured S11 of -19 dB. Simulation results show that the meander line antenna produces an omnidirectional radiation pattern with a maximum gain of 1.8dB and a measured gain of 1.5dB. A good agreement between the simulation and the measured results of the return loss was also obtained, which shows the potential of this approach.

Keywords : meander line antenna, UHF communication, FR-4, CubeSat.

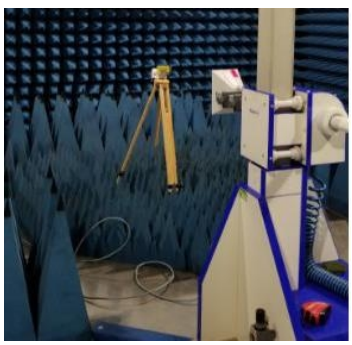

Figure 1: Measurement setup of the antenna radiation pattern in the anechoic chamber.

A Virtual Sensor Network Architecture Based on Cloud Computing for Wireless Sensor Network

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Abstract:
The paper proposes a novel approach to support the usability and sharing of WSNs by multiple applications using the Cloud computing as an emerging technology that offers many processing and storing capabilities at different levels. Virtualization is the key technology that may potentially enable this sharing. A novel Architecture of Virtual Sensor Network is discussed for routing sensed data between virtual sensors. Finally, the evaluation of the proposed architecture confirms its suitability to be adopted as a potential concurrent for the integration of WSNs in the Cloud Computing.

Key words: Wireless Sensor Network, Cloud Computing, Virtual Sensor Network.

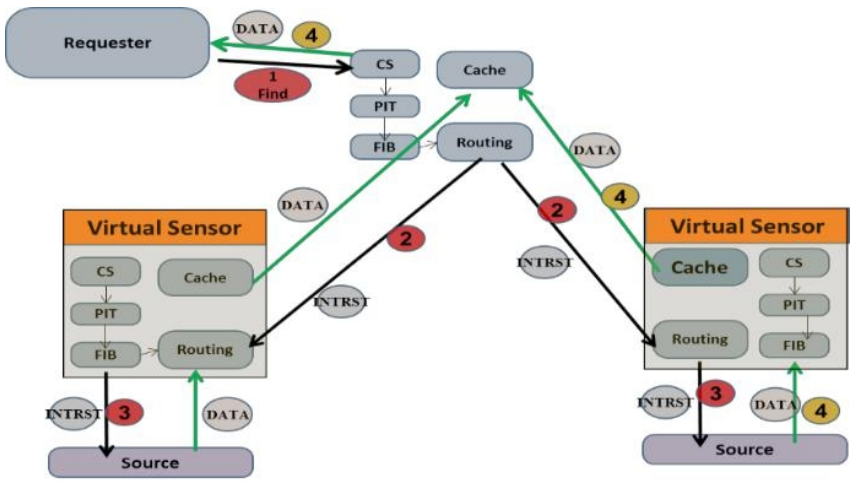

Figure: Adopted routing scheme

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Contribution aux applications de traitement des images hyper spectrales spatiales

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Abstract :
Les images hyper spectrales sont des images multidimensionnelles repérées dans un hyper-cube. Le traitement des images hyper spectrales nécessite un système hardware très puissant et offrant un parallélisme suffisant pour le traitement. Ce type d'équipement nécessite de l'énergie électrique excessive. En associant le traitement hyper spectral avec de l'intelligence artificielle tel que les CNN et le Deep Learning, les plateformes matérielles ne sont pas capables de faire du traitement en temps réel ou bien dans un délai faible avant d'afficher les résultats. On se propose dans ce sujet de réaliser des applications d'observation de la terre par des images hyper spectrales spatiales, filmée par des satellites, dotée avec de l'intelligence artificielle, pour détecter et reconnaitre des objets et des effets. Par exemple, détecter les feux dans les forêts, détecter des intrusions frontalières, chercher les nappes et courants d'eau avec étude de la qualité de l'eau, ...
Des optimisations algorithmiques permettent d'accélérer le traitement par adéquation algorithme/architecture. De même une étude d'adéquation architecture/algorithme permet d'optimiser la plateforme matérielle comme noyau exécutif. On peut envisager tout type de hardware, en particulier les cloud-plateformes. Une évaluation des performances de l'application et une évaluation des performances des plateformes permet de classer les systèmes hardware en fonction du type d'application.

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Crosstalk analysis in homogeneous Raised-cosine multi-core 6-mode fiber

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Abstract :
We designed a Raised-cosine (RC) 6-LP mode homogeneous multicore fiber (MCF) for high density optical interconnect application. The proposed fiber supports long-distance multimode transmission around 1.550 µm band. The core-to-core crosstalk impact has been studied numerically with respect to bending radius, core pitch, transmission distance, wavelength, and core diameter for all 6-LP modes. In anticipation of further reduction in crosstalk levels, the trench-assisted cores have been presented for all respective designs. We have also shown the different lattice structures of 7-core and 12-core RC- 6-LP mode homogeneous MCF.

Key words: crosstalk, multicore fiber, multimode fiber, bending radius

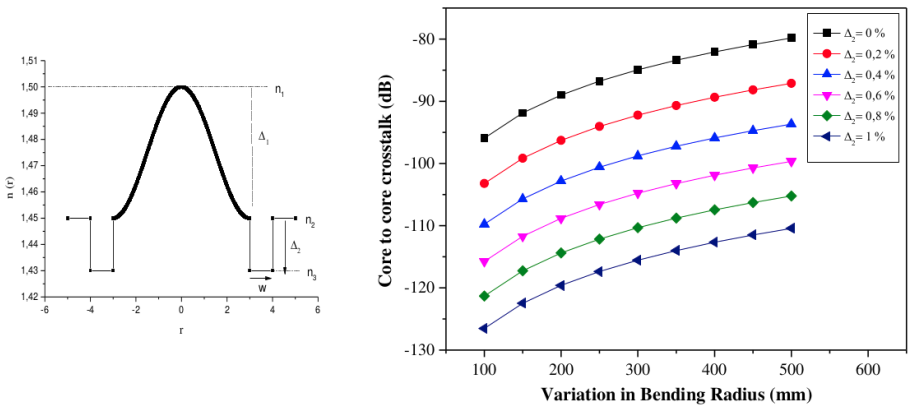

Figure 1: Relation between bending radius and crosstalk for LP 01 mode at w=2µm

Contribution à la recon naissance de forme d'images par les mé thodes à noyaux

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Abstract :
Le cancer est un problème d'une extrême importance ayant des implicatio ns sociales et financières pour la santé publiqu e. Différents types de cancers ont déjà été rapportés dans la littérature et peuvent être classés selon le type de cellules initialement affectées. Le cancer du sein est le principal problème de santé des femmes. La détection précoce du cancer du sein peut être obtenue par des techniques de mammographie qui permettent de visualiser la structure tissulaire du sein. Le d iagnostic assisté par ordinateur (CAD) des mammographies tente d'aider les radiologues à fournir une procédure automatique pour détecter d'éventuels cancers dans les mammographie s.
Le travail présenté vise à développer un modèle CAD qui peut classer les mammographies cancéreuses (anormales) ou no n cancéreuses (normales) suivies de bénignes ou malignes. Dans le présent modèle, une égalisation d'histogramme adaptatif à contraste lim ité (CLAHE) est utilisée pour prétraitement d 'image, Transformation discrète de Tchebichef (DTT) pour l'extraction de caractéristiques et KPCA pour la réduction de dimension. Ensuite, une machine d'apprentissage extrême basée s ur le noyau utilisant trois types de noyau différents (Rbf-KELM, Wav-KELM et Poly-KELM) est utilise pour classer les mammographies comme normales ou anormales, et en outre, bénignes ou malignes.
Le présent modèle atteint la plus haute précision de 100% pour la base de données MIAS [1].

Mots-clés : imagerie médicale, classification, machine d'apprentissage, cancer de sein

[1] Suckling J, The MiniMIAS database, Mammographic Image Analysis Society—MIAS, www.wiau.man.ac.uk/services / MIAS/MIAScom.html.

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Traffic signs recognition for advanced driving assisting system using deep learning

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Abstract :
Advanced Driving Assistance System (ADAS) are widely used in to-day cars. It has been a revolutionary approach to make roads safer by assisting the driver indifficult situations like collusion, or the assistance in respecting road rules.
Intelligent ADAS are used to assist drivers in difficult driving situations. Indeed, the ADAS can assist them in the continuous control of the vehicle. In addition, the ADAS system can access the vehicle functionalities like engine and brakes, and apply numerous actions to avoid dangerous situation like collusions with other vehicle or with pedestrians. Generally, an ADAS system is composed of a number of sensors (camera included). In the research presented here, the visual information provided by the cam-eras will be used to help the ADAS system to recognize and interpret correctly the road signs.
In this work, we introduce a road signs recognition application for an ADAS system to recognize and understand traffic signs. This application is based on a deep learning technique; in particular, it uses Convolutional Neural Networks (CNN). The proposed CNN achieves high performance in road sign classification with the correct recognition rate of 99.75%.

Keywords: intelligent advanced driving assistance system, deep learning, convolutional neural networks, traffic signs classification.

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Area Efficient Implementation for LED Lightweight Block Cipher on FPGA

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Abstract :
The LED (Light Encryption Device) is one of the lightweight block algorithms used to provide security for small private data on resource-limited devices. In this work, we have proposed serial hardware architectures for LED lightweight block cipher algorithm with key length 128-bit. This architecture of LED is implemented in FPGA device Xilinx Spartan-3. Then, it is compared with existing implementations for the LED.

Keywords : LED Block Cipher, Lightweight Block Ciphers, Hardware architectures, area optimization.

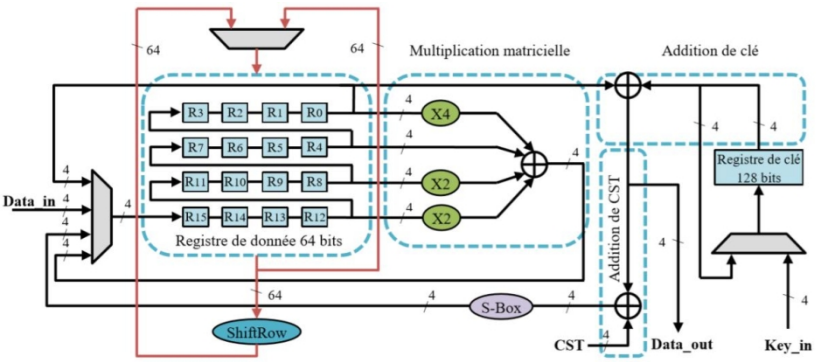

Figure 1 : Merci Proposed serial architecture of Piccolo.

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[2] C. Marchand, L. Bossuet, and K. Gaj, Area-oriented comparison of lightweight block ciphers implemented in hardware for the activation mechanism in the anti-counterfeiting schemes, INTERNATIONAL JOURNAL OF CIRCUIT THEORY AND APPLICATIONS, (2016).

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Object classification model for autonomous vehicles using Machine Learning and Deep Learning

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Abstract :
This paper aims to make a comparison between machine learning and deep learning techniques used in the field of object detection. We chose to work on the road signs shape classification to make this comparison and see the results. For the machine learning technique, we chose to extract the characteristics of the road sign using the Sobel filters and the oriented gradient histogram (HOG) and for the classification, we used the Support Vector Machines (SVM). For the deep learning technique, we chose to work with a Convolutional Neural Network (CNN) model. To improve the quality of the results to be obtained we tried to work with the same database.

Keywords : Machine Learning, Deep Learning, Comparison, Classification, Road signs.

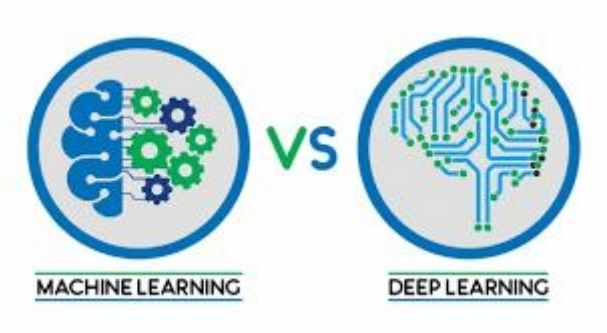

Figure 1 : Machine Learning Vs Deep learning (Performance comparison).

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A Convolutional Neural Network Approach for Reducing HEVC Complexity

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Abstract:
With the development of video coding technology, the High Efficiency Video Coding (HEVC) provides better coding efficiency compared to its predecessors H.264/AVC. HEVC improves Rate Distortion (RD) performance significantly with increased encoding complexity. Due to the adoption of a large variety of Coding Unit (CU) sizes, at RD optimization level, the quadtree partition of the CU consumes a large proportion of the encoding complexity. Hence, the computational complexity cost remains a critical issue that must be properly considered in the optimization task. In this paper, a deep learning-based fast CU partition method for inter-mode HEVC is proposed, in order to optimize the complexity allocation at CU level. Firstly, we construct a large-scale training database including substantial CU partition data. Secondly, a deep Convolutional Neural Network (CNN) is proposed to predict the CU partition at inter-mode. Experimental results demonstrate that the proposed deep CNN can reduce the encoding time by 53.99% with 0.195% BitRate degradation compared to the original HEVC. Consequently, the HEVC encoding complexity can be drastically reduced by replacing the brute-force RDO search with deep CNN to decide the CU partition at inter-mode.

Keywords: HEVC, CU partition, Deep Learning, CNN, Complexity reduction.

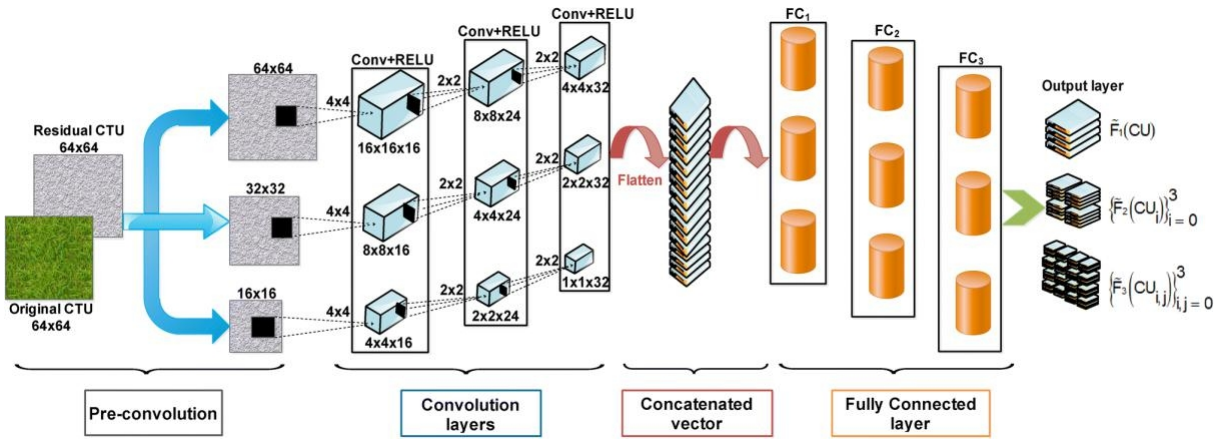

Figure 1: *Deep CNN architecture*

1. S. Bouaafia, R. Khemiri, F.E. Sayadi, M. Atri, Fast CU Partition Based Machine Learning Approach for Reducing HEVC Complexity, J. Real-Time Image Processing, pp. 1–12, 2019.