



# ملخص الأبحاث العلمية

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# Summary of Scientific Research

اليوم العلمي السادس  
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Scientific Day  
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# قسم الرياضيات والاحصاء

**Mathematics and Statistic Department**

## Extension Of S-Plurisubharmonic Currents Across Zero Sets of Psh Functions

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Complex Variables and Elliptic Equations, Published online: 28 Nov 2018

### Abstract

In this paper, we study the extension of  $S$ -plurisubharmonic currents of bi-dimension  $(p; p)$  across zero sets of plurisubharmonic functions. More precisely, we show that the extension of the current  $g^\alpha T, \alpha > 1$  exists for every non-negative plurisubharmonic function  $g$  and negative  $S$ -plurisubharmonic current  $T$  defined outside  $A = \{z \in \Omega; g(z) = 0\}$  as soon as the  $(2p - 1)$ -Hausdorff measure of  $A$  vanishes. By some examples we show the astonishing fact that in some sense this result is sharp.

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## On the integrability of 2D Hamiltonian systems with variable Gaussian curvature

A. Elmandouh

Nonlinear Dynamics 93: 933–943 (2018)

Mathematics and Statistics Department, College of Science, King Faisal University.

### Abstract:

In this work, we consider the integrability of a general 2D motion of a particle on a surface with variable Gaussian curvature under the influence of conservative potential forces. Although this system has a kinetic energy relying on the coordinates, it remains homogeneous. The homogeneity of the system generally enables us to find a particular solution that can be utilized to derive the necessary conditions for the integrability by studying the properties of the differential Galois group of the normal variational equations along this particular solution. We present a new theory that can be applied to determine the necessary conditions for the integrability of Hamiltonian systems having a variable Gaussian curvature.

### References

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## **Controllability of Fractional Evolution Inclusions with Noninstantaneous Impulses**

JinRong Wang , AG Ibrahim , D O'Regan

International Journal of Nonlinear Sciences and Numerical Simulation 19,3-4,(2018),1-14

### **Abstract**

This paper, is concerned with the controllability issue fractional semilinear differential inclusions with non-instantaneous impulses. Using weak sequentially closed operators , we establish sufficient conditions to guarantee the controllability result. We don't assume that the semi-group is compact or a compactness type condition on the multivalued function Finally two examples are given to illustrate our theory.

### **References**

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- R, A. Debbouche, N.I. Mahmudov, Approximate controllability of fractional stochastic differential inclusions with nonlocal conditions, Appl. Anal. 95(2016), 2361–2382.

## Rivulet Flow Of Generalized Newtonian Fluids

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Physical Review Fluids, 3, 083302 (2018) 1–24

### Abstract

Steady unidirectional gravity-driven flow of a uniform thin rivulet (i.e., a rivulet with small transverse aspect ratio) of a generalized Newtonian fluid down a vertical planar substrate is considered. The parametric solution for any generalized Newtonian fluid whose viscosity can be expressed as a function of the shear rate and the explicit solution for any generalized Newtonian fluid whose viscosity can be expressed as a function of the extra stress are obtained.

### References

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## **Magneto-electro-thermal bending of FG-graphene reinforced polymer doubly-curved shallow shells with piezoelectromagnetic faces**

Mohammed Sobhy

Composite Structures 203 (2018) 844–860.

### **Abstract**

In this paper, an analytical treatment is developed for the magneto-electro-thermal bending of composite doubly-curved shallow shells reinforced by functionally graded graphene platelets (FGGPLs) surrounded by two piezoelectromagnetic (PEM) face sheets with various boundary conditions. According to new piece-wise mixture rules, four kinds of FGGPLs reinforced doubly-curved shells are considered. These shells are assumed to be exposed to thermal load, external electric voltage and magnetic potential. The material properties of FGGPLs multi-layered doubly-curved shallow shells are assumed to be varied in the shell thickness direction according to the suggested piece-wise distribution. Each layer of the composite shell is composed of polymer matrix reinforced with uniformly distributed graphene platelets. A four-variable shell theory is considered to describe the displacement field. In accordance with this theory, four equilibrium equations are derived from the virtual work principle. The governing equations are analytically solved to obtain the displacements, electric displacements, magnetic induction and stresses in the composite shells. A parametric study is presented to investigate the effects of the shell curvatures, boundary conditions, electric potential, magnetic potential, temperature rise and graphene platelets distribution type on the deflection, electric displacements, magnetic induction and stresses in FGGPLs reinforced laminated doubly-curved shells. It is found that the increment in the GPLs weight fraction and decrement in temperature increase the strength of the present structure.

### **References**

- Kiani Y, Akbarzadeh AH, Chen ZT, Eslami MR. Static and dynamic analysis of an FGM doubly curved panel resting on the Pasternak-type elastic foundation. *Composite Structures* 2012;94(8):2474-2484.

## **Extensions of proper efficiency in complex space**

Mamdouh Elbrolosy & Ebraheem Youness

Mathematical Methods in the Applied Science, Volume 41, 2018, 5792-5800

### **Abstract**

In this paper we extend proper efficiency concepts for a vector optimization problem in complex space. The relationships among the concepts due to Benson, Borwein, Kuhn-Tucker and Geoffrion are discussed under some convexity and constraints qualification conditions. The necessary and sufficient conditions for a feasible point to be a properly efficient solution are established. The results are generalizations of the concepts of proper efficiency and their related theorems from real to complex space and complete the existing ones.

### **References**

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## A question about saturated chains of primes in Serre conjecture rings

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Ricerche di Matematica, (2018) 67; 447-456

### Abstract

We propose to give a positive answer to the following question: is  $R\langle X, Y \rangle$  strong  $S$  when  $R\langle X \rangle$  is strong  $S$ ? in case  $R$  is obtained by a  $(T, I, D)$  construction, where  $I$  is an intersection of finitely many maximal ideals of  $T$ .

### References

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## Lelong numbers of $m$ -subharmonic functions

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J. Math. Anal. Appl. 466 (2018) 1373–1392

### Abstract

In this paper we study the existence of Lelong numbers of  $m$ -subharmonic currents of bidimension  $(p, p)$  on an open subset of  $\mathbb{C}^n$ , when  $m + p \geq n$ . In the special case of  $m$ -subharmonic function  $u$ , we give a relationship between the Lelong numbers of  $ddc u$  and the mean values of  $u$  on spheres and balls. As an application we study the integrability exponent of  $u$ . We express the integrability exponent of  $u$  in terms of volume of sub-level sets of  $u$  and we give a link between this exponent and its Lelong number.

### References

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## Differential equation and inequalities of the generalized $k$ -Bessel functions

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### Abstract

We introduce and study a generalization of the  $k$ -Bessel functions of order  $\nu > -k$ , where  $k$  is any nonnegative integer. We indicate some representation formulae for the introduced functions. We show that the generalized  $k$ -Bessel function is a solution of a second-order differential equation. By some judicious choice of parameters in the definition of the function, we investigate about its monotonicity and log-convexity. Several inequalities, including well-known Turán type inequality, are established. We propose an open problem regarding the pattern of the zeroes of the function.

### References

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## **Free vibration characteristic of laminated conical shells based on higher-order shear deformation theory**

Saira Javed

Composite Structures, vol. 204, 15 Nov. 2018, Pages 80-87

### **Abstract**

The purpose of this research is to analyse the free vibration of composite laminated conical shells based on higher order shear deformation theory. The vibrational behavior of multi-layered conical shells are analyzed for simply supported end condition. The coupled differential equations in terms displacement and rotational functions are obtained. These displacement and rotational functions are invariantly approximated using cubic and quintic spline. A generalized eigenvalue problem is obtained and solved numerically for an eigenfrequency parameter and an associated eigenvector of spline coefficients. The different materials are used to show the parametric effects of shell's length ratio, cone angle, stacking sequence and number of lamina on the frequency of the conical shells. The numerical results obtained using spline approximation are validated through existing literature.

### **References**

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## Differential Inclusions of Fractional Order In Infinite Dimensional Banach Spaces

Ebtisam Saud Abdulrahman Alasmari  
Supervisor :Prof. Ahmed Gamal Ibrahim

### Abstract

In this work we establish new existence theorems of solutions for impulsive differential inclusions of fractional order  $\alpha \in (1,2)$ , in infinite dimensional Banach spaces. Moreover, we give the conditions that guarantee the compactness of the set of solutions. Our technique depends on applying an appropriate fixed point theorem and on using the properties of the measure of noncompactness.

### References

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## Wedge Product of Positive Currents

Noura Alssaiid and Hassine El Mir

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### Abstract

In this paper, we study some properties of plurisubharmonic currents. More precisely, we study the existence of the current  $T \wedge dd^c u$  where  $T$  is a currents of order zero of bi-dimension  $(p,p)$ , and  $u$  is a locally bounded plurisubharmonic function.

### References

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## **Controllability of Nonlocal Fractional Non-instantaneous Impulsive Semilinear Differential Inclusions**

By Mariam Ibrahim Alsultan

Supervisor: Prof. Ahmed Gamal Ibrahim

### **Abstract**

This work is concerned to seek out suitable conditions that insure the existence of mild solution for nonlocal fractional non-instantaneous impulsive semilinear differential inclusions, where the linear part is the infinitesimal generator of a  $C_0$ -semigroup in infinite dimensional Banach space with confirmation not to assume any regularity conditions expressed in terms of measures of non-compactness.

### **References**

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## Slicing And Extension Of Currents

Mona Mohammed Almuhanha and H. El Mir

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### Abstract

In this thesis, we study The existence of the slices of positive closed current  $T$  that is defined on  $\Omega$  such that the  $2(n-k)$ -Hausdorff measure of the singular support of  $T$  is zero. Also, by our new example we show the condition on  $B$  for every  $z \in B$  the slice of  $T$  at  $z$  can be extended to positive closed current on  $\{z\} \times \Delta^{(n-k)}$  in Ben Messaoud and El Mir result is sharp to extend the current on  $\Omega$

### References

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## **A novel shear and normal deformation theory for hygrothermal bending response of FGM sandwich plates on Pasternak elastic foundation**

M. A. Abazid, Muneerah S. Alotebi and M. Sobhy

Structural Engineering and Mechanics (ISI/Q2), 67(3), (2018), 219-232

### **Abstract**

This paper deals with the static bending of various types of FGM sandwich plates resting on two-parameter elastic foundations in hygrothermal environment. The elastic foundation is modeled as Pasternak's type, which can be either isotropic or orthotropic and as a special case, it converges to Winkler's foundation if the shear layer is neglected. The present FGM sandwich plate is assumed to be made of a fully ceramic core layer sandwiched by metal/ceramic FGM coats. The governing equations are derived from principle of virtual displacements based on a shear and normal deformations plate theory. The present theory takes into account both shear and normal strains effects, thus it predicts results more accurate than the shear deformation plate theories. The results obtained by the shear and normal deformation theory are compared with those available in the literature and also with those obtained by other shear deformation theories. It is concluded that the present results are slightly deviated from other results because the normal deformation effect is taken into account. Numerical results are presented to show the effects of the different parameters, such as side-to-thickness ratio, foundation parameters, aspect ratio, temperature, moisture, power law index and core thickness on the stresses and displacements of the FG sandwich plates.

### **References**

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# قسم علوم الحياة

**Biological Sciences Department**

## **Polyphasic characterization of *Delftia acidovorans*, a facultative methylotrophic bacterium isolated from rhizosphere of *Eruca sativa***

Ashraf Khalifa and M. Almalki

Biological Sciences Department, College of Science, King Faisal University.

### **Abstract**

In this study, one bacterial strain, ESM-1, was isolated from rhizosphere of *Eruca sativa*, growing in Al Hofouf, Saudia Arabia, after enrichment with methanol as a sole carbon and energy source in a batch culture. ESM-1 was characterized by a polyphasic approach. The strain was identified as *Delftia acidovorans* at similarity level of 99.9% of the 16S rRNA gene sequences. Results of the Biolog Gen III MicroPlate test system showed that strain ESM-1 reacted positively to 47 (50%) including the one-carbon compound formic acid, and partially positive to 6 (~6.4%) out of the 94 different the traits examined. The total cellular fatty acids composition of the strain ESM-1 was (C16:1 $\omega$ 7c/C16:1 $\omega$ 6c) and C16:0) and matched that of *Delftia acidovorans* at a similarity index of 0.9, providing a robustness to the ESM-1 identification. Furthermore, ESM-1 displayed a complex polar lipid profile consisting of phosphatidylethanolamine, phosphatidylglycerol, glycolipid, aminolipid, in addition to uncharacterized lipids. The DNA G+C content of the strain was 66.6 mol%. Phylogenetic analyses based on 16S rRNA gene sequences showed that the strain ESM1-1 was clearly clustered within the *Delftia* clade and constructed a monophyletic subcluster with *Delftia acidovorans* NBRC14950. The results addressed that ESM-1 is a facultative methylotrophic bacterium indigenous to Al Hofouf region and opens the door for potential biotechnological applications (e.g., bioremediation) of this strain, in future. Additionally, these findings assure that the total cellular fatty acid analysis and 16S rRNA gene are reliable tool for bacterial characterization and identification.

### **References**

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**Diatomite improves productivity and quality of *Moringa oleifera* grown in greenhouse**

Fadia El-Sherif, Doha El Zain, Yun-Kiam Yap,

Department of Biological Sciences, College of science, King Faisal University.

Full paper: El-Sherif et. al., Electronic Journal of Biology, 2018, Vol. 14(1): 1-6

**Abstract**

*Moringa oleifera* Lam. is a tropical perennial, soft-wooded tree. Different parts of the tree have been used as traditional medicine, food, plant growth enhancer, animal feed, water coagulant, cosmetic ingredient, and biodiesel raw materials. In this study, we have investigated the effects of diatomite, a rich source of silicate on the growth and active compounds content in *Moringa oleifera*. We have irrigated our plants with 3 different concentrations (2.5, 5.0 and 10.0 g/L), of diatomite solution. Our results indicated that plants irrigated with 2.5g/L of diatomite shown highest rate of improvement in growth parameters such as plant height, number of branch, leaves, and roots, as well as fresh and dried weight of stem, leaves, and roots as compared to the control (irrigated with water only) and plants irrigated with 5 or 10 g/L diatomite. The enhancement in growth parameters is supported by the increased in photosynthetic pigments. The amount of total phenolic and flavonoid as well as tocopherol and apigenin in the leaves and roots samples shown slight increment in all the diatomite treatment groups as compared to the control. Taken together, our results suggest that 2.5g/L diatomite irrigation improve the growth of *Moringa oleifera* by increasing the photosynthetic capacity of the plants.

**References**

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## First isolation and characterization of pathogenic *Aeromonas veronii* bv. *veronii* associated with Ulcerative Syndrome in the indigenous *Pelophylax ridibundus* of Al-Ahsaa, Saudi Arabia

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Journal: Microbial pathogenesis 117 :361-368

### Abstract

Virulent microbial pathogen infections are the main cause for amphibian decline worldwide. In the present study, a bacterial strain named RDL-2, which was isolated from the skin of infected *Pelophylax ridibundus* larvae, was cultured and then phenotypically and biochemically characterized using scanning electron microscopic observations and the API20E strip and Biolog Gen III MicroPlate system. The 16S rRNA gene sequence of this strain was also obtained and used in strain identification and phylogenetic analysis. Healthy *P. ridibundus* larvae were also challenged with RDL-2 and monitored to determine clinical signs consistent with the disease. RDL-2 was identified as *Aeromonas* 16S rRNA gene sequence displayed the highest homology to that of *A. veronii* bv. *veronii* (99.9%). Koch's postulates were fulfilled confirming that *A. veronii* is the causal agent of Ulcerative Syndrome, and this study is, therefore, the first report of *A. veronii* as a pathogen for the marsh frog indigenous to the Al-Ahsaa region. The aetiology of *A. veronii* as a potential poikilothermic pathogen shown here will expedite the development of diagnostic tests and methods for eradicating this emerging disease.

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## Cyanobacteria as Nanogold Factories: Chemical and Anti-Myocardial Infarction Properties of Gold Nanoparticles Synthesized by *Lyngbya majuscula*

Esam M. Bakir, Nancy S. Younis, Maged E. Mohamed and Nermin A. El Semary

### Abstract

*Lyngbya majuscula* was isolated from the Al Oqair area, Al-Ahsa Government, Eastern Province, Kingdom of Saudi Arabia. The cyanobacterium was initially incubated with 1500 mg/mL of HAuCl<sub>4</sub> for two days. The blue-green strain turned purple, which indicated the intracellular formation of gold nanoparticles. Prolonged incubation for over two months triggered the extracellular production of nanogold particles. UV-visible spectroscopy measurements indicated the presence of a resonance plasmon band at ~535 nm, whereas electron microscopy scanning indicated the presence of gold nanoparticles with an average diameter of 41.7 ± 0.2 nm. The antioxidant and anti-myocardial infarction activities of the cyanobacterial extract, the gold nanoparticle solution, and a combination of both were investigated in animal models. Isoproterenol (100 mg/kg, SC (sub cutaneous)) was injected into experimental rats for three days to induce a state of myocardial infarction; then the animals were given cyanobacterial extract (200 mg/kg/day, IP (intra peritoneal)), gold nanoparticles (200 mg/kg/day, IP), or a mixture of both for 14 days. Cardiac biomarkers, electrocardiogram (ECG), blood pressure, and antioxidant enzymes were determined as indicators of myocardial infarction. The results showed that isoproterenol elevates ST and QT segments and increases heart rate and serum activities of creatine phosphokinase (CPK), creatine kinase-myocardial bound (CP-MB), and cardiac troponin T (cTnT). It also reduces heart tissue content of glutathione peroxidase (GRx) and superoxide dismutase (SOD), and the arterial pressure indices of systolic arterial pressure (SAP), diastolic arterial pressure (DAP), and mean arterial pressure (MAP). Gold nanoparticles alone or in combination with cyanobacterial extract produced an inhibitory effect on isoproterenol-induced changes in serum cardiac injury markers, ECG, arterial pressure indices, and antioxidant capabilities of the heart.

### References

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## Anticancer potential of NFκB targeting apoptotic molecule “Flavipin” isolated from endophytic *Chaetomium globosum*

SenthilKumar V, Kumaresan S, Tamizh M.M, HairulIslam M.I, Thirugnanasambantham K.  
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### Abstract

**Background:** Anticancer compounds from natural sources have drawn attention due to their structural diversity and relatively lesser side effects. Endophytic fungi are one such natural resource from, which plethoras of anticancerous compounds have been isolated.

**Purpose:** The objective of the study was to isolate and characterize the bioactive metabolite from *Chaetomium globosum* that exhibits astonishing antiproliferative activity against cancerous cell lines.

**Methods:** Flavipin was isolated by bioassay-guided fractionation and identified using FT-IR, EI-MS and NMR studies. MTT assay was used to determine cytotoxicity. Real time PCR and Western blotting were used to analyze the expression of apoptosis related genes and its proteins, respectively.

**Results:** Flavipin inhibited proliferation of A549, HT-29 and MCF-7 cancer cells in dose dependent manner with an IC<sub>50</sub> concentration of 9.89 μg/mL, 18 μg/mL and 54 μg/mL, respectively, At IC<sub>50</sub> concentration cancerous cells exhibited cell shrinkage and fragmentation of DNA, which indicated that flavipin induced apoptotic cell death. Furthermore, western blotting results also showed down-regulation of NFκB.

**Conclusion:** This is the first report on the antiproliferative activity of flavipin isolated from endophytic *C. globosum*. Flavipin induced apoptosis at low concentrations in cancer cell lines (A549, HT-29) and exhibited itself as a potential anticancer agent.

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<https://doi.org/10.1016/j.homp.2014.10.001>

## Traditionally practiced medicinal plant extracts inhibit the ergosterol biosynthesis of clinically isolated dermatophytic pathogens

Chellappandian M, Saravanan M, Pandikumar P, Harikrishnan P, Thirugnanasambantham K, Subramanian S, Hairul-Islam M.I, Ignacimuthu S

Department of biological sciences, School of science, King Faisal University.

### Abstract

Objective: Control drug resistant microbes is urgently needed. This study evaluates the antidermatophytic potential of 18 selected ctive. —Development of new plant drugs to medicinal plants used by traditional healers in Theni and Virudhunagar Districts of Tamil Nadu, India.

Materials and methods. — Selected plant parts were collected, shade dried and powdered. Plant powders were extracted with ethanol and their antifungal potency was investigated against and clinical dermatophytes.

Results and discussion. — The ethanol extract of *Phyllanthus reticulatus* leaves showed good antifungal activity compared to other plant extracts. The MIC and MFC for *Phyllanthus reticulatus* were 62.5 and 250 mg/mL against *M. pachydermatitis* and *T. rubrum* respectively. The ethanol extract of *Phyllanthus reticulatus* leaves was more biocompatible to host cells than other active extracts.

Conclusion. — Our study indicated that the ethanol extract of *Phyllanthus reticulatus* leaves showed promising activity against dermatophytes. It could be a potential material for future development of antidermatophytic agents.

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**Pinocembrin, a novel histidine decarboxylase inhibitor with anti-allergic potential in vitro**

Hamza H, HairulIslam M.I, Saravanan S, Chellappandian M, Ragul K, Durga A, Venugopal K, Senthilkumar V, Senthilkumar P, Thirugnanasambantham K. Biological Sciences Department, College of Science, King Faisal University.

**Abstract**

Pinocembrin (5, 7- dihydroxy flavanone) is the most abundant chiral flavonoid found in propolis, exhibiting antioxidant, antimicrobial and anti-inflammatory properties. Thus, current study aimed at investigating the effects of Pinocembrin on IgE-mediated allergic response in vitro. A special emphasis was directed toward histidine decarboxylase (HDC) and other proallergic and pro-inflammatory mediators. Preliminary studies, using a microbiological model of *Klebsiella pneumoniae*, provided first evidences that suggest Pinocembrin as a potential thermal stable inhibitor for HDC. Applying docking analysis revealed possible interaction between Pinocembrin and mammalian HDC. In vitro studies validated the predicted interaction and showed that Pinocembrin inhibits HDC activity and histamine in IgE-sensitized RBL-2H3 in response to dinitrophenol (DNP)-bovine serum albumin (BSA) stimulation. In addition, Pinocembrin mitigated the damage in the mitochondrial membrane, formation of cytoplasmic granules and degranulation as indicated by lower  $\beta$ -hexoseaminidase level. Interestingly, it reduced range of pro-inflammatory mediators in the IgE-mediated allergic response including tumor necrosis factor (TNF)- $\alpha$ , interleukin (IL)-6, nitric oxide (NO), inducible NO synthase (iNOS), phosphorylation of inhibitory kappa B ( $\text{I}\kappa\text{B}$ )- $\alpha$ , prostaglandin (PGE)-2 and cyclooxygenase (COX)-2. In conclusion, current study suggests Pinocembrin as a potential HDC inhibitor, and provides the first evidences it is in vitro anti-allergic properties, suggesting Pinocembrin as anew candidate for natural anti-allergic drugs.

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## **Metabolic Diversity of The Diesel-Oil-Degrading Bacterium, *Achromobacter Pulmonis* Hdk3, Obtained from Eastern Region Of Saudi Arabia**

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Botany and Microbiology Department, Faculty of Science, University of Beni-Suef, Beni-Suef, Egypt

### **Abstract**

Herein, a diesel oil-degrading bacterial strain designated HDK3 was obtained from a soil sample collected from Al Mizan Gas station, Eastern region of Saudi Arabia using the enrichment culture method. The strain was characterized morphologically, phenotypically and genotypically. Besides, the capability of HDK3 to biodegrade diesel oil was estimated using GC-MS analysis. The strain formed a white, convex and an entire colony. The results obtained from the 16s rRNA gene sequencing analysis highlighted that the strain could be identified as *Achromobacter pulmonis* at an identity level of 98.89%. Observations derived from the Biolog system highlighted that the strain could consume a wide range of carbon and energy sources and grew in presences of many stressors such as NaCl, antibiotics and dyes. Additionally, HDK3 showed an ability to degrade the C14-C19 compounds in diesel as revealed by the Gas chromatography-mass spectrometry (GC-MS). In conclusion, the strain HDK3 exhibited a metabolic diversity along with its capability to metabolize diesel oil, in that way provides an ecofriendly approach for its exploitation in hydrocarbon bioremediation.

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## **A simple and reliable protocol for long-term culture of murine bone marrow stem cells that retained their in vitro and in vivo stemness**

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Department of Biological Sciences, College of science, King Faisal University.

### **Abstract**

**Background:** Bone marrow derived stromal stem cells (BMSCs) are a clonogenic cell population that is characterized by self-renewal capacity and differentiation potential into osteoblasts, and other mesenchymal cell types. Mouse BMSCs (mBMSCs) are difficult to be cultured and propagated in vitro due to their replicative senescent phenotype, heterogeneity and high contamination with plastic adherent hematopoietic progenitors (HPCs).

In this study, we described long-term culture of homogenous population of mBMSCs using simple and highly reproducible approach based on frequent subculturing (FS) at fixed split ratio in the presence of basic fibroblast growth factor (bFGF).

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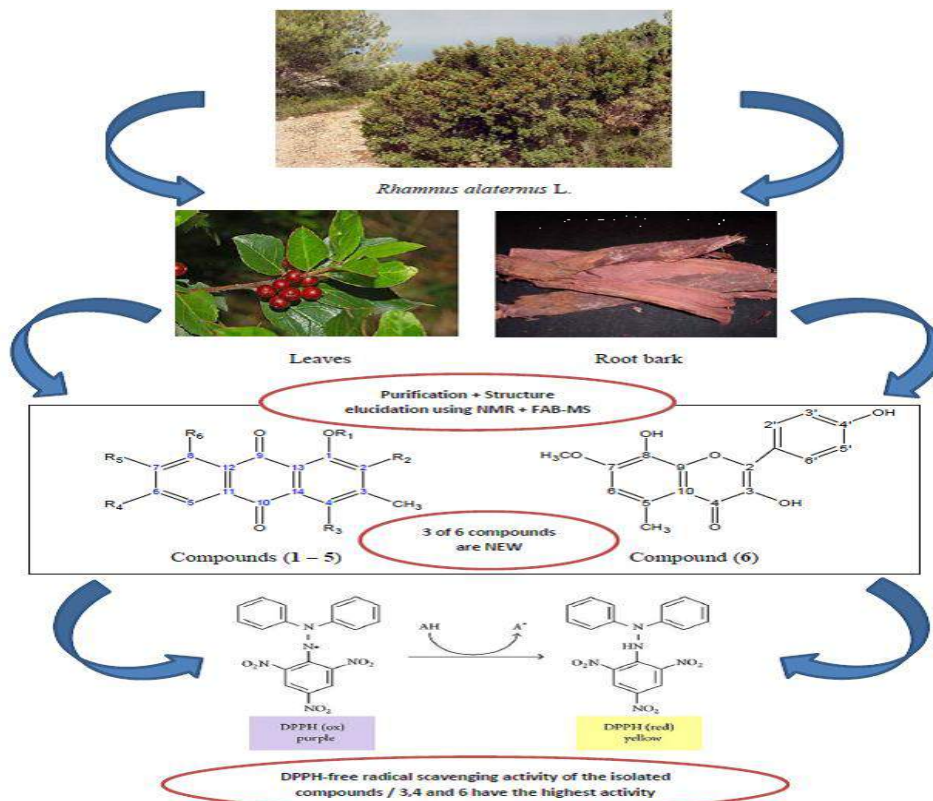
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## Isolation and identification of new anthraquinones from *Rhamnus alaternus* L and evaluation of their free radical scavenging activity

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\*Department of Biological Sciences, College of Sciences, King Faisal University.

### Abstract



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## **Advantages of bioconjugated silica-coated nanoparticles as an innovative diagnosis for human toxoplasmosis**

Ibrahim Aly, Eman E. Taher, Gehan EL naina, Hoda EL Sayed, Faten A. Mohammed, Rabab S. Hamad, Elsayed M. Bayoumy

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Acta Tropica 177 (2018) 19–24

### **Abstract**

This work aimed to evaluate the advantage of bioconjugation of SiO<sub>2</sub>NP with PAb against Toxoplasma lyzate antigen (TLA) as an innovative diagnostic method for human toxoplasmosis. This cross-sectional study included 120 individuals, divided into Group I: 70 patients suspected for Toxoplasma gondii based on the presence of clinical manifestation. Group II: 30 patients harboring other parasites than T. gondii Group III: 20 apparently healthy individuals free from toxoplasmosis and other parasitic infections served as negative control. Detection of circulating Toxoplasma antigen was performed by Sandwich ELISA and Nano-sandwich ELISA on sera and pooled urine of human samples. Using Sandwich ELISA, 10 out of 70 suspected Toxoplasma-infected human serum samples showed false negative and 8 out of 30 of other parasites groups were false positive giving 85.7% sensitivity and 84.0% specificity, while the sensitivity and specificity were 78.6% and 70% respectively in urine samples. Using Nano-Sandwich ELISA, 7 out of 70 suspected Toxoplasma-infected human samples showed false negative results and the sensitivity of the assay was 90.0%, while 4 out of 30 of other parasites groups were false positive giving 92.0% specificity, while the sensitivity and specificity were 82.6% and 80% respectively in urine samples. In conclusion, our data demonstrated that loading SiO<sub>2</sub> nanoparticles with pAb increased the sensitivity and specificity of Nano-sandwich ELISA for detection of T.gondii antigens in serum and urine samples, thus active (early) and light infections could be easily detected.

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**DNA vaccination using recombinant *Schistosoma mansoni* fatty acid binding protein (smFABP) gene**

Ibrahim Aly, Gehan EL naina, Rabab S. Hamad, Mona Kilany, Hamed A. Ghramh, Aly Alshehri, Saad M.

Dajem, Essam H. Ibrahim

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Experimental Parasitology 194 (2018) 53–59

**Abstract**

This work was carried out to investigate the possible effect of DNA vaccination against *Schistosoma mansoni* infection using recombinant *S. mansoni* fatty acid binding protein (rsmFABP). The smFABP gene was cloned into the eukaryotic expression vector pcDNA1/Amp in order to obtain an smFABP-pcDNA1 recombinant plasmid (DNA vaccine) and was used for the intramuscular DNA vaccination of out-bred Swiss albino mice prior to infection with *S. mansoni* cercariae. Infected groups, either DNA vaccinated or unvaccinated, were treated with PZQ at week 6 post-infection. After 8 weeks post-infection, all mouse groups were sacrificed and parasitological, immunological and histopathological parameters were studied. DNA vaccinated mice showed a high titer of anti-smFABP-IgG antibodies and acquired significant protection (74.2%,  $p < 0.01$ ) against *S. mansoni* infection, with a reduction in ova and granuloma counts. DNA vaccinated and PZQ treated animals had higher titers of anti-smFABP-IgG antibodies and decreased (87%,  $P < 0.001$ ) parenchymal granulomas compared to the DNA vaccinated PZQ untreated group. Infected mice, either non DNA vaccinated or vaccinated, had very high collagen content and fibrous granulomas (74%) compared to the PZQ treated group (10.3% fibrous granuloma) and PZQ treated + DNA vaccinated group (0% fibrous granuloma). In conclusion, DNA vaccination had protective and anti-pathological effects in naive mice and greatly improved the pathological status in PZQ-treated animals, suggesting an immunological and pathological modulating effect of PZQ treatment.

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## **Bacterial contamination and health risks of drinking water from the municipal non-government managed water treatment plants**

Salama A. Ouf & Ramy S. Yehia & Ahmed S. Ouf & Rania F. Abdul-Rahim

### **Abstract**

The average total count of bacteria detected after four stages of treatments in the investigated plants was 32 CFU/1 mL compared to 2330 cfu/mL for raw water, with a reduction percentage of 98.6. Although there is a relatively high removal percent of bacterial contamination from the water sources, however, several bacterial pathogens were identified in the produced water prepared for drinking including *Enterococcus faecalis*, *Escherichia coli*, *Pseudomonas aeruginosa*, and *Shigella* spp. After 3 days of water incubation at 30 °C, the amount of bacterial endotoxins ranged from 77 to 137 ng/mL in the water produced from the municipal plants compared to 621–1260 ng/mL for untreated water. The main diseases reported from patients attending different clinics and hospitals during summer 2014 at the surveyed locations and assuredly due to drinking water from these plants indicated that diarrheas and gastroenteritis due to *E. coli* and *Campylobacter jejuni* constituted 65.7% of the total patients followed by bacillary dysentery or shigellosis due to *Shigella* spp. (7.9%) and cholera due to *Vibrio cholera* (7.2%). There was an increase in serum aspartate aminotransferase (AST), alanine aminotransferase (ALT), and alkaline phosphatase (ALP) as well as urea and creatinine values of guinea pigs consuming water produced from the non-governmental plants for 6 months indicating remarkable liver and kidney damages. Histological sections of liver and kidney from the tested animal revealed liver having ballooning degeneration of hepatocytes and distortion and fragmentation of the nuclei, while the section of the kidney showed irregularly distributed wrinkled cells, degenerated Bowman's capsule, congested blood vessels, and inflammatory cells.

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### **Monitoring metal levels in water and multiple biomarkers in the grouper**

**(*Epinephelus tauvina*) to assess environmental stressors on the Arabian Gulf coast of Saudi Arabia**

Ashraf M Abdel-Moneim, Mohamed A Al-Kahtani, Omar M Elmenshawy, Hany Elsaywy, Aly M Hafez and  
Marwa A Genena

Toxicology and Industrial Health, 2018, Vol. 34(5) 301–314

#### **Abstract**

In this field study, the levels of heavy metals (Pb, Fe, Co, Cu, and Zn) in water and a suite of biochemical and histological biomarkers in the grouper (*Epinephelus tauvina*) were assessed at four sites in the Arabian Gulf. Samples were taken from a relatively non-urban reference site, called Salwa (S1), and three effluent-dominated sites, namely Al-aziziyah in southern Dammam city (S2), the Al-Jubail coast (S3), and Manifa (S4). Toxic metals, namely Pb and Co (at all sites) and Fe (at S3), were elevated in water samples relative to the internationally permissible limits. In fish, induced levels of heat shock protein 70 (HSP70) in the liver at S3 and S4 were higher than those of the reference fish at S1. Additionally, the level of the lipid peroxidation (LPO) product (malondialdehyde (MDA)) was significantly increased in gills (at S3) and liver (at S2 and S3). There was an inhibition of catalase activities in the gills of fish from S2 to S4 and significantly higher activity levels of superoxide dismutase in the gills of fish from S4. Histopathological features such as aneurysms in gill vessels, deformed gill lamellae, increases in liver melano-macrophage centers, and hepatocellular necrosis were most abundant at sites where significant pollution problems exist (i.e. S2–S4). The results reveal that the eastern coast of Saudi Arabia, in the Arabian Gulf, is still contaminated, as indicated by elevated HSP70, LPO content and numbers of histological lesions, and that monitoring of contaminants and their effects should be continued in this region.

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**In-vitro selection of salt tolerant Jojoba (*Simmondsia chinensis*)**

Nouf Ali Alyousif

Supervisors

Prof. Dr. Salah Khattab and Dr. Yap Yun Kiam

Department of Biological Sciences, College of science, King Faisal University.

**Abstract**

Jojoba (*Simmondsia chinensis*) is a dioecious, long-lived perennial shrub widely grown in semi-arid regions. Its waxy seed oil has been widely used in cosmetic and pharmaceutical products. Propagation of jojoba by seeds is not suitable for commercial scale cultivation due to high male bias ratio, long flowering and seed set as well as high heterogeneity in seed raised plants. Therefore, selection of high salt tolerance clone and micro-propagation of these clones in-vitro to establish supply of high salt tolerance clone for commercial scale cultivation of jojoba in Saudi Arabia is desired.

Seeds from selected cultivar of jojoba will be aseptically germinated in media containing different concentration of salt to impose salt stress in the growth media. Plants germinated in media containing high salt concentration will be micro-propagated in multiplication media to generate multiple shoots. Shoots will be rooted, and the rooted plantlets will be transplanted to green house.

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## **Isolation and characterization of bacterial biofertilizers from Al-Ahsa region**

Heba Adel AlAli.

Supervisors

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Department of Biological Sciences, College of science, King Faisal University.

### **Abstract**

The main idea is to isolate species of bacteria from different areas of Al-Ahsa that can be used as biofertilizers to increase the fertility of the soils and enhance the growth of some plants in the eastern region of Saudi Arabia. Application of biofertilizers decreases the usage of synthetic fertilizers that have deleterious environmental effects. However, there is not a lot of information available about the bacterial species that can be employed in the process of biofertilization in the eastern province of Saudi Arabia specially in Al-Ahsa are limited. Characterization of bacterial strains by phenotype and biochemical properties. Bacterial strains with high production of plant stimulanting agents will be identified using the 16S rRNA gene sequencing. Phylogenetic tree will be constructed. The ability of the selected strains will be tested for improving the growth of some plants such as *Abelmoschus esculentus* and *Pisum sativum* which have economic importance.

The expected outcome of this study is to obtain effective and ecofriendly bacterial biofertilizers.

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قسم الكيمياء

**Chemistry Department**

## Polyhydrazide incorporated with thiadiazole moiety as novel and effective corrosion inhibitor for C-steel in pickling solutions of HCl and H<sub>2</sub>SO<sub>4</sub>

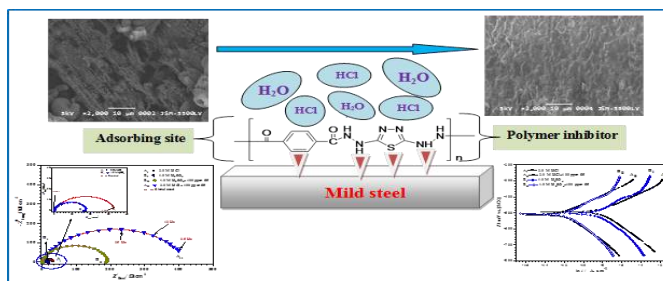
Abdelwahed R. Sayed, Hany M. Abd El-Lateef

Chemistry Department, College of Science, King Faisal University.

Macromolecular Research 26 (10) (2018) 882–891.

### Abstract

Polyhydrazide incorporated with thiadiazole moiety (S5) was prepared and its chemical configuration was confirmed by different spectroscopic methods. The inhibitive action of S5 polymer and its monomer 2,5-dihydrazinyl-1,3,4-thiadiazole (M1) on the C-steel corrosion in pickling acids solution was investigated by weight loss, potentiodynamic polarization (PDP) and electrochemical impedance spectroscopy (EIS) measurements. PDP method exhibited that the investigated polymer is mixed-type corrosion inhibitor in both acids (HCl and H<sub>2</sub>SO<sub>4</sub>). The data revealed that S5 compound is a good inhibitor for C-steel in studied acids, and protection efficiency (P%) follows this sequence: H<sub>2</sub>SO<sub>4</sub><HCl. Also, it was found that, the P% of the S5 polymer is higher than that obtained for its monomer (M1). Adsorption of the titled polymer obeyed the isotherm of Langmuir and involves both chemical and physical adsorptions. Scanning electron microscopy (SEM) investigations established the protective layer formation from the studied polymer on the metal substrate and shield it from direct Cl<sup>-</sup> and/or SO<sub>4</sub><sup>2-</sup> attack.



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## **Spectrofluorimetric method for atenolol determination based on gold nanoparticles**

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<sup>3</sup> Textile Research Division National Research Center, Dokki Cairo, Egypt

### **Abstract**

A simple and sensitive spectrofluorimetric method for determination of atenolol (ATE) using gold nanoparticles (AuNPs) was developed. The method is based on the quenching effect of atenolol on photoluminescence of AuNPs at  $\lambda_{em} = 705$  nm. Variables affecting luminescence of gold nanoparticles such as the solvent, pH value and surfactant were studied and optimized. The method was preliminarily validated according to ICH guidelines. A linear correlation was recorded within the range of 1.0–10 mgmL<sup>-1</sup> ATE with the coefficient of determination R<sup>2</sup> of 0.999. The limit of detection and limit of quantitation for atenolol were found to be 0.87 and 2.64 mg mL<sup>-1</sup>, resp. Good recoveries in the range of 98.7–100.0 % were obtained for spiked samples. The proposed method was applied successfully to assaying atenolol in pharmaceutical formulations.

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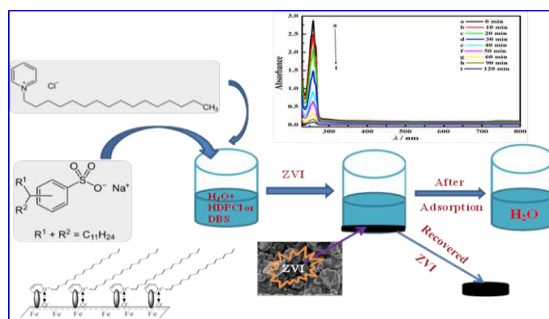
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## Adsorption and Removal of Cationic and Anionic Surfactants From Wastewater Using Zero-Valent Iron Nanoparticle

Mai M. Khalaf Ali, Hany M. Abd El-Lateef, Mahmoud M. Saleh  
Chemistry Department, College of Science, King Faisal University.  
Journal of Molecular Liquids 268 (2018) 497–505.

### Abstract

It is known that, surfactants have mimicked the influence of human estrogen, which can be a serious threat to human health. Therefore, reduction of the surfactants amount present in such water is critical from both economic and an environmental perspective. This study is dedicated for adsorption of surfactants on Zero-Valent Iron (nZVI). As a nano-adsorbent, nZVI is synthesized by simple and economic method then characterized using various surface and structural techniques. Nano-ZVI is tested as potential adsorbent for the removal of a cationic surfactant, and anionic surfactant from dilute solutions. The effects of different experimental parameters such as the amount of nZVI, the initial surfactant concentration, pH, shaking speed, and temperature on the system performance have been studied. The obtained thermodynamic parameters demonstrate the easiness and spontaneity of the adsorption process with favorable adsorption extent to the HDPCl compared to the DBS. This was attributed to the difference in the molecular structures. Reusing of spent nZVI is possible with adequate removal efficiencies of the surfactant molecules through multiple regeneration cycles.



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## Fine-template synthetic process of mesoporous TiO<sub>2</sub> using ionic/nonionic surfactants as potential remediation of Pb(II) from contaminated soil

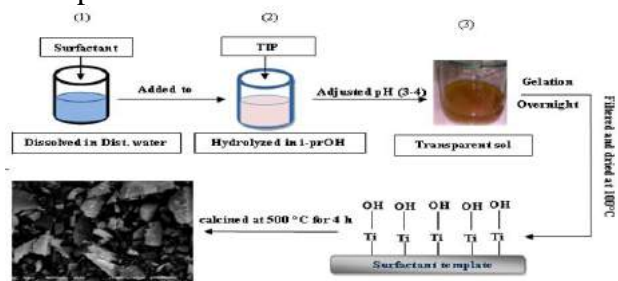
Mai M. Khalaf Ali, Hany M. Abd El-Lateef

Chemistry Department, College of Science, King Faisal University.

International Journal of Environmental Science and Technology (2018)

### Abstract

Urban and agricultural soils have been turned out polluted via heavy metals and metalloids assemblages due to mining and manufacturing; the earth enforcement of wastewater irrigation, pesticides, animal manures, sewage sludge, and fertilizers; and the accidental accumulation of coal combustion residues, petrochemical spills, and other atmospheric depositions. Excess heavy metal accumulation in soils cannot be controlled, resulting in long-term residuals that are toxic to humans, animals and ecosystems. Hence, it is important to develop an efficient remediation method for agricultural soil polluted by heavy metals. This trend of research deals with preparation of mesoporous TiO<sub>2</sub> by a simple approach using sol gel method by various surfactant templates. These obtained nano adsorbents are examined as functional adsorbents for lead ions up taking from contaminated soil specimens. The optimum conditions of 25 °C, 5, and 0.1 g were obtained for temperature, pH and amount of adsorbents, respectively. The obtained results revealed that about 97.6, 99.1, and 95.3 % of total adsorptive capacity were obtained for Ti C, Ti S, and Ti P, respectively at 100 mg/L of Pb (II) ions in soil solutions during 120 min. These findings recommended these nano adsorbent TiO<sub>2</sub> as adequate adsorbents in remediation process of Pb enriched soil.



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## Nickel Phosphate/Carbon Fibers Composite for High-performance Supercapacitors

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### Abstract

This article reports the use of crystalline nickel phosphate/carbon fibre (NiPh/CFs) nanocomposites as an electrode material for pseudocapacitor applications. The NiPh particles are synthesised by a cost-effective one-pot method, which is based on refluxing nickel and phosphate precursors at 90 °C. The crystallinity and structural morphologies of the synthesised particles are characterized by X-ray diffraction (XRD) and field-emission scanning electron microscopy (FE-SEM). Also, the N<sub>2</sub> adsorption/desorption isotherms are recorded. The Brunauer–Emmett–Teller (BET) method is used to calculate the specific surface area. The electrochemical performance of pristine NiPh and NiPh/CFs composite electrodes are investigated in an alkaline solution of 0.5 M of KOH. The specific capacitances were calculated using cyclic voltammograms at a potential scan rate of 100 mV s<sup>-1</sup>. For the pristine electrode the calculated specific capacitance was 4.3 F g<sup>-1</sup> and for the composite NiPh/CFs electrode it was 699.2 F g<sup>-1</sup>. The significant improvement in the performance is attributed to the high surface area and enhanced electronic conductivity of the NiPh/CFs composite electrode. Also, the composite electrode shows outstanding stability and delivers 1000 cycles with excellent capacitance retention.

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## **A facile Synthetic Route to novel Polyamides-Based on Thieno[2,3-b]thiophene and Their Application for Corrosion Inhibition Behavior**

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Chinese J. Polym. Sci. 36 (7) (2018) 835–847.

### **Abstract**

Polyamides containing thieno[2,3-b]thiophene moiety have been prepared via a simple polycondensation reaction of the diaminothieno[2,3-b]thiophene monomer 1a with different kinds of diacid chlorides (including, oxaloyl, adipoyl, sebacoyl, isophthaloyl, terephthaloyl, 4,4'-azodibenzoyl, 3,3'-azodibenzoyl, p-phenylene diacryloyl) in the presence of LiCl anhydrous as a catalyst and NMP as solvent through low-temperature solution polycondensation technique. The chemical structures of model compound and synthesized polyamides have been confirmed by FT-IR, nuclear magnetic resonance spectroscopy (including, <sup>1</sup>H-NMR and <sup>13</sup>C-NMR) and elemental analysis. In addition, the thermal stability, crystallinity structure and surface morphology of synthesized polyamides were characterized via Thermogravimetric analysis (TGA), Wide-angle X-ray diffraction analysis (WXRd) and scanning electron microscope (SEM). Also, the corrosion inhibition behavior of selected examples of polyamides was studied; the inhibitive effect of the investigated polymers for carbon steel in 1.0 M HCl was studied using potentiodynamic polarization (PDP) and electrochemical impedance spectroscopy (EIS) methods. PDP results displayed that the polyamides containing thieno[2,3-b]thiophene moiety can be act as mixed-type inhibitors. The inhibition efficiency (P %) was found to be in the range 67.13-96.01%. There is an increase in P% by the synthesized polymers in comparison to the starting monomer. The adsorption of these polymers was found to obey Langmuir adsorption isotherm.

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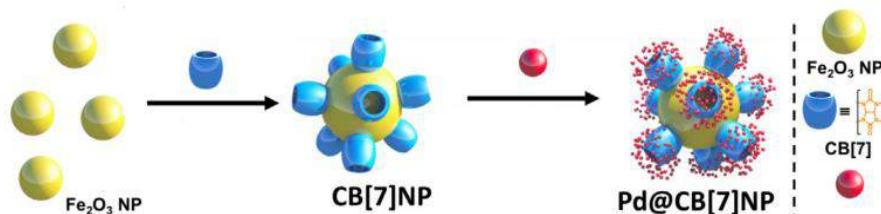
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## Palladium Functionalized Iron Oxide Nanoparticles for catalytical activity: An XPS Study

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Chem. Eur. J. 2018, 24, 2349 – 2353 (IF = 5.16)

### Abstract

Iron oxide nanoparticles were coated with Cucurbit[7]uril (CB[7]) macrocyle and then loaded with palladium (II) to form nano-catalysts (Pd@CB[7]NPs). These nanoparticles catalysed with high efficiency Suzuki–Miyaura and Sonogashira cross-coupling reactions.



Scheme 1: Schematic representation of coating of iron oxide nanoparticles with Pd(II)

Conversions and yields were uniformly high and the nano-catalysts could be recovered with a magnet and reused several times (6 times for Suzuki–Miyaura reaction) without loss of activity. Beside the catalytic activities, we present in this work an X-Ray Photoelectron Study (XPS) to figure out the strong interactions with CB[7] and palladium on the surface of these nanoparticles.<sup>1</sup>

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## **Speciation of Trace Metals in Sediment: Modified Tessier Sequential extraction Scheme versus BCR Scheme**

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### **Abstract**

Modified Tessier sequential chemical extraction scheme connected with ICP-MS was compared with the European Community Bureau of Reference (BCR) procedure for extraction of As, Cd, Co, Cr, Cu, Fe, Mn, Ni, Pb, Se, V and Zn for sediment samples collected from the coast of Sabah and Sarawak, Malaysia. Reliability of the obtained data was achieved by calculating the recovery of the fractions results for the two sequential extraction methods. The distribution of the concentration of the elements through the chemical fractions showed that no significant differences between the two procedures for all elements under study with an exception of Zn element. According to the recovery calculation, both techniques are an equally competitive procedure for extraction of As, Cu, V, Se, Co and Pb. BCR is a superior technique for Mn and Fe over the modified Tessier procedure, while for Cr, Ni and Zn element the later one is the preferable method.

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## Green Synthesis of Iron Nanoparticles by *Acacia nilotica* Pods Extract and its Catalytic, Adsorption, and Antibacterial Activities

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### Abstract

Iron nanoparticles (FeNP) were synthesized using *Acacia nilotica* seedless pods extract. The synthesized FeNP were characterised by Fourier transform infrared (FTIR), UV/Vis spectroscopy, dynamic light scattering (DLS), electron microscopy (TEM), scanning electron microscopy (SEM), transmission and energy dispersive X-ray EDX. EDX spectroscopy showed the presence of elemental iron and oxygen indicating that the nanoparticles are essentially present in oxide form. UV absorption in the range of 450-550 nm confirmed the formation of FeNP. DLS indicated an average FeNP particle size of 229 nm. The synthesized FeNP was tested for adsorption and oxidation degradation of methyl orange (MO) under different conditions and found to be effective in both degradation and adsorption processes. Furthermore, the synthesized FeNP has the potential to terminate the pathogenicity of several human opportunistic pathogens; belongs to gram negative and gram-positive bacteria and one species of candida as well.

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## Tuning Optical Properties Of Chalcone Derivatives: Computational Study

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Bayach, A. D'Aléo, and P. Trouillas, *J. Phys. Chem. A*, 2019, 123, 1, 194-201

### Abstract

The conformational feature of non-covalent complexes of two borondifluoride chalcone derivatives was assessed using DFT-D2. The corresponding optical properties were analyzed based on TD-DFT calculations. As already described in such complexes, the  $\pi$ -stacking interaction existing between both fragments allowed formation of a new absorption band corresponding to the  $S_0 \rightarrow S_1$  transition. However, this band appears very close to the most intense band corresponding the  $S_0 \rightarrow S_2$  transition.

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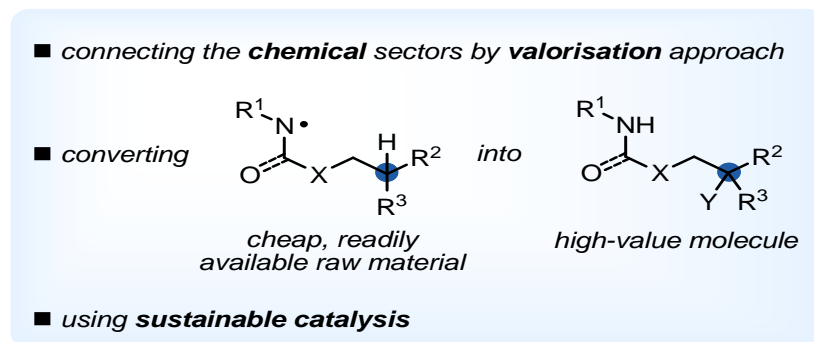
## Valorisation of Organic Molecules

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### Abstract

Valorisation is a phenomenal process of utilizing scientific knowledge in practice. In a nutshell, it is directly linked with “innovation” and “transfer of scientific knowledge”. In collaboration with the University of Manchester (QS ranking: 29<sup>th</sup> in the world, 6<sup>th</sup> in the UK), we have applied this approach to fabricate cheap and readily available raw materials into high-value organic molecules (Figure 1), with applications spanning from pharmaceutical ingredients to agrochemicals. The research team of King Faisal University performs in-depth computational calculations to gain mechanistic insight while the research team at the University of Manchester carries out chemical synthesis



**Figure 1:** Research design towards valorisation of organic molecules

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## Carbon Cobalt Nanostructures as an Efficient Adsorbent of Malachite Green

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### Abstract

Carbon-cobalt nanostructures CCoNS 1 and 2 were prepared by pyrolysis of the cis-dichlorobis(1,10-phenanthroline-N,N')-cobalt(II) complex 3 in the absence or presence of anthracene respectively. DFT calculation was used to estimate ligand dissociation energy of cobalt complex, the energy cost for the formation of cobalt particles which catalyze the formation of carbon nanostructures.

Nanostructures 1 and 2 were tested as adsorbents to uptake malachite green dye (MG) from aqueous solution. The optimum conditions for adsorption such as time, pH were determined. Adsorption isotherms of MG by adsorbents 1 and 2 were fitted in terms of Langmuir, Freundlich, Temkin, and D-R models, and the capacities were calculated.

Adsorption thermodynamic and activated thermodynamic parameters were evaluated. The kinetics of adsorption process were also studied.

Column kinetic adsorption of malachite Green of CCoNS (2) was fitted by Thomas, Yoon Nelson, and Yan et al model.

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## Synthesis of polar unique 3d metal-imine complexes of salicylidene anthranilate sodium salt.

### Homogeneous catalytic and corrosion inhibition performance

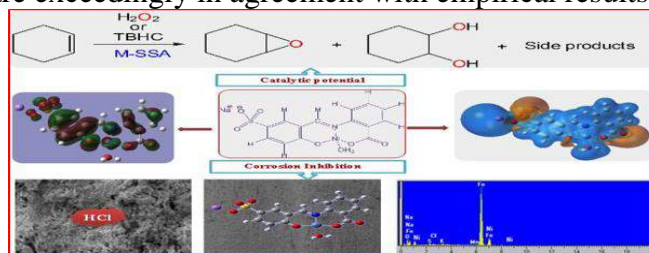
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Journal of the Taiwan Institute of Chemical Engineers 88 (2018) 286–304.

#### Abstract

Three polar Ni(II)-, Cu(II)- and Zn(II)-complexes (M-SSA) of salicylidene anthranilate sodium salt ligand were synthesized. The ligand (H<sub>2</sub>SSA) and its corresponding metal-complexes are characterized by alternative physico-chemical tools in which H<sub>2</sub>SSA acts as tridentate bi-basic chelating agent. Catalytic potential of M-SSA was investigated in the homogenous oxidation of 1,2-cyclohexene at 80 °C in acetonitrile, water or under solvent-free condition. M-complexes exhibit high catalytic reactivity with high chemoselectivity in acetonitrile. Cu-SSA shows the highest catalytic potential for the oxidation of 1,2-cyclohexene than Ni-SSA or Zn-SSA. The lowest yield of the epoxy-product was obtained in water due to the hydrolysis ring opening reaction affording 1,2-cyclohexanediol. The inhibition performance of H<sub>2</sub>SSA and M-SSA on the carbon steel corrosion (CS) in HCl was studied using electrochemical techniques. The inhibition capability was increased with increasing inhibitor dose. The adsorption of inhibitors on the surface of CS obeyed the Langmuir isotherm paradigm. Surface characterizations (SEM/EDX) revealed that the investigated compounds adsorbed on CS surface and form protective layer that shield the surface from direct corrosion attack. The experimental data have been completed by density functional theory treatment. The obtained theoretical results are exceedingly in agreement with empirical results catalytically and inhibitory.



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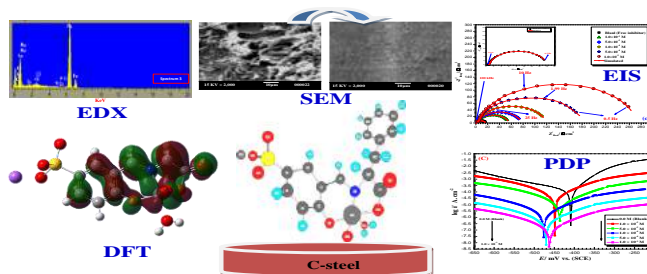
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## Anionicoxide-vanadium Schiff base amino acid complexes as potent inhibitors and as effective catalysts for sulfides oxidation: Experimental studies complemented with quantum chemical calculations

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Journal of Molecular Liquids 250 (2018) 307–322.

### Abstract

Three anionic oxide-vanadium Schiff base N-salicylideneamino acid complexes are derived from the reaction of sodium salicylaldehyde-5-sulfonate with phenylalanine (VO-1), alanine (VO-2) or glycine (VO-3), followed by mixing with vanadyl sulfate monohydrate. Inhibition effect of VO-1, VO-2 and VO-3 is investigated for the corrosion of carbon steel in chloride acid solution. From the electrochemical measurements, VO-complexes protect carbon steel from corrosion, yielding maximum inhibition efficiency up to 94.7% in the presence of 1.0 mM VO-1 inhibitor. All VO-complexes act as mixed-type inhibitors. The SEM and EDX investigations provided the appearance of an inhibitor layer encasement the steel surface. Catalytic efficiency of VO-complexes is measured in the symmetric and asymmetric oxidation of sulfides by using an aqueous  $H_2O_2$ . All complexes show high catalytic potentials towards sulfides oxidation. VO-1, VO-2 and VO-3 are optimized at B3LYP/GEN and B3LYP/LANL2DZ levels of theory in gas and aqueous phases. Theoretical results agree with the experimental reactivity of the VO-complexes, as corrosion inhibitors and catalysts for sulfides oxidation.



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## **Porous Cobalt Carbon Nanocomposites for Electrode Materials and Water Treatment Crystal Structure of Cobalt Precursor in Pyrolytic Synthesis**

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### **Abstract**

Carbon nanostructures are of great importance due to their unique properties and interesting applications. A simple method is conducted for the synthesis of cobalt-carbon nanocomposites by solid-state pyrolysis starting from cobalt complexes of N- and O- donor ligands. Highly porous carbon nanostructures embedding cobalt nanoparticles were obtained of size ranging from 10 nm to 200 nm according to SEM and TEM analysis. The presence of cobalt and cobalt oxides nanoparticles is evidenced by XRD, EDX and XPS. A good graphitization degree is revealed by Raman scattering. The electrochemical behavior of glassy carbon electrode modified by the newly nanocomposites show good electrochemical response using cyclic voltammetry and potassium ferrocyanide as a redox couple. In addition, the adsorption efficiency of pyrolytic product of a mixed-ligand complex of 2,2- bipyridine and terephthalate dianion (Pyro 92) toward Crystal Violet dye is tested using both batch and column methods. Pyro 92 shows adsorption capacity of 214 mg/g at 25 Co. Freundlich isotherm model matched the experimental data very well and adsorption kinetic obeyed pseudo-second-order. The adsorption capacity of a fixed-bed column is 36.29 mg/g. Cobalt phenanthroline aqua complex, “a catalyst precursor for solid-state pyrolysis of nanocarbon” was synthesized and characterized using Single-crystal X-ray Diffraction.

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## **Synthesis and crystal structures of new Ni(II) complexes with bipyridine, 1,10-phenanthroline and terphthalic acid: Ligand-based coordination competition**

Safiah A. Alramadhan, Prof Hassan Hammud

Chemistry Department, Faculty of Science, King Faisal University.

### **Abstract**

In this work, we have designed and synthesized new nickel complexes with bipyridine, 1,10-phenanthroline and terphthalic acid using the three layer-based diffusion method into adequate sizes for single crystal X-ray diffraction analysis (SCXRD). The detailed crystallographic data including selected geometric parameters and hydrogen bond were also investigated. Complexes (A-E) were produced with good single crystals that were used for further crystal structure analysis.

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## Nicel Complexes Pyrolysis for Production of Graphitic Carbon Nanocomposite for Electrodes, Gas storage & Water Treatment

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### Abstract

New graphitic carbon nickel nanocomposites GCNiN were prepared by solid state pyrolysis of 2,2'-bipyridine, 1,10-phenanthroline and terephthalate nickel complexes. The pressure of inert gas, temperature and time of heating stages, amount of aromatic additional carbon source, and silica matrix has been optimized in order to obtain the highest graphitic GCNiN with finest nanoparticles and greatest porosity and surface area. This has been proved by characterization of GCNiN with modern physical techniques. The structures were characterized using Scanning Electron Microscope (SEM) and Transmission Electron Microscope (TEM) indicating the presence of nanoparticles made up of graphitic shell and nickel cores and some carbon nanotubes. The elemental analysis and chemical environment were studied using EDX, XPS and XRD. High graphitization degree is indicated by Raman scattering analysis. Surface area and pores sizes and gas adsorption were determined by BETT analysis.

The structures of four nickel complexes with potential catalytic pyrolysis precursors were determined by X-Ray single crystal characterization.

The electrochemistry of glassy carbon electrode modified by GCNiN and GCNiN-Si were studied using cyclic voltammetry and potassium ferrocyanide redox couple.

The adsorption of crystal violet by GCNiN-Si was fitted to different isotherm models and kinetics. Column adsorption data was fitted to Thomas, Yoon-Nelson, and Yan et al.

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## Prevalence and characterization of *Escherichia coli* resistant to broad-spectrum cephalosporin from patients visiting King Fahed Hospital

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<sup>4</sup> Charles Nicolle Hospital, Laboratory of Microbiology, 1006 Tunis, Tunisia.

### Abstract

The present study investigated *E. coli* from patients visiting King Fahed Hospital. It was conducted to evaluate the prevalence of *E. coli* resistant to 3rd generation cephalosporins (3rd GC) and to characterize them. The prevalence of *E. coli* resistant to 3rd GC was 22.7% (27/119). ESBL and cephalosporinase phenotypes were detected in 25 and 2 isolates, respectively and the majority of the isolates were multidrug resistant. Genes encoding resistance to 3rd GC detected were blaCTX-M-15 (n=21), blaCTX-M-27 (n=5) and blaCTX-M-9 (n=1); blaCMY-42 (n=2, one of them co-harbored blaCTX-M-15). qnrS1 gene was detected in 12 strains, among them six concomitantly harbored the aac(6')Ib-cr. There is a serious need of additional epidemiologic surveillance and strict control measure implementation in order to limit their diffusion.

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## Protective Effect of Silymarin against Acrylamide Induced Testicular Toxicity in Rats

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### Abstract

Infertility is one of the major health problems in life and approximately about 30% of this problem is due to male factors. Acrylamide (AA) has multiple chemicals and industrial applications. It is produced during cooking of carbohydrate-rich foods at very high temperature (> 120°C). Animals were randomly divided into four groups of six animals each. Our data showed that administration of AA caused a significant reduction in serum testosterone and an increase in follicle stimulating hormone and luteinizing hormone levels in intoxicated rats. Furthermore, AA induced lipid peroxidation, decrease the activities of the studied antioxidant enzymes and sperm quality. In addition, it caused histological and DNA damages in the testis. However, the co-administration of silymarin mitigated the toxicity of AA by partially normalization of these biochemical parameters, improvement of the sperm quality and the histopathological changes. On the other hand, silymarin did not able to counteract the damaged DNA.

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## **Synthesized Porphyrins for Catalysis of Water Splitting Oxygen Evolution Reaction**

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### **Abstract**

Free-base porphyrin, and its cobalt and copper complexes were synthesized in good and quantitative yields respectively. The chemical structure of the synthesized porphyrins was confirmed by spectroscopic techniques (FT-IR, NMR, MS, and UV-Vis). Subsequently, the porphyrins were used as electrocatalysts for the oxygen evolution reaction (OER) in 1 M KOH. The cobalt-porphyrin complex showed the best performance in term of a low band gap value and a high catalytic activity with good stability towards the OER.

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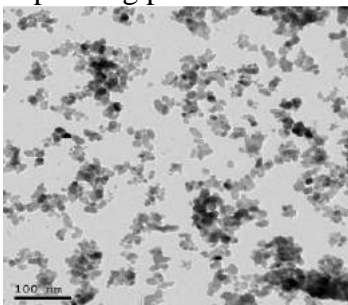
## Nickel Ferrite Nanoparticles: Synthesis, Characterization and its Electrocatalytic Application

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### Abstract

Ferrite  $MFe_2O_4$  Nanoparticles is an important material since it is involved in many applications including catalytic oxidation reactions and photo catalytic reactions. When it is prepared in nanoscale, its magnetic, surface and catalytic properties are enhanced dramatically. It is the aim of this work to fabricate  $NiFe_2O_4$  (NFO) in nanoscale with cost effective methods e.g. sol-gel technique at different experimental conditions. The effects of different parameters such as calcination temperature on the synthesis process and the properties of produced particles was studied. The synthesized NFO was characterized using different surface and structural characterization techniques including BET surface area determination, X-ray diffraction spectroscopy, XRD, scanning electron microscopy, SEM, transmission electron micrograph, TEM. Also, electrochemical techniques such as cyclic voltammetry (CV) were used for its characterization. Probe reaction such as oxygen evolution reaction (OER) and /or glucose oxidation were used as a probe reaction to assess the electro-catalytic performance of the synthesized NFO at different experimental conditions. The surface and structural properties of the NFO are correlated with the performance towards the electro-catalytic reaction. The effects of different operating parameters on the process performance was studied.



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**قسم الفيزياء**  
**Physics Department**

### **Purity temperature dependency for coupled harmonic oscillator**

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#### **Abstract**

We consider the thermal aspect of a system composed of two coupled harmonic oscillators and study the corresponding purity. We initially consider a situation where the system is brought to a canonical thermal equilibrium with a heat-bath at temperature  $T$ . We adopt the path integral approach and introduce the evolution operator to calculate the density matrix and subsequently the reduced matrix density. It is used to explicitly determine the purity in terms of different physical quantities and therefore study some limiting cases related to temperature as well as other parameters. Different numerical results are reported and discussed in terms of the involved parameters of our system.

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## Nitrogen-doped porous carbon and interlinked urchin-like NiCo<sub>2</sub>O<sub>4</sub>@3DNF framework as an asymmetric supercapacitor

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### Abstract

An aqueous potassium ion-based asymmetric supercapacitor has been successfully developed using nitrogen-doped porous carbon (NPC) derived from waste orange peel and sea urchin-like intercrossed and interconnected NiCo<sub>2</sub>O<sub>4</sub> array on Ni foam for negative and positive electrodes, respectively. A negative electrode was designed using NPC developed via hydrothermal method. Subsequent KOH activation of waste orange peel resulted in NPC. NPC yielded a typical electrical double layer capacitor with a high capacitance of 268 F/g, and robust cyclic stability (100%) with up to 4000 cycles and good working potential (0 to -1V) in an aqueous electrolyte. Hydrothermally synthesized urchin-like intercrossed and interlinked NiCo<sub>2</sub>O<sub>4</sub>@NF was used as a negative electrode with a high capacitance of 1300 F/g at a current density of 1 A/g and excellent rate as well as enhanced cyclic performance up to 2000 cycles. NiCo<sub>2</sub>O<sub>4</sub>//NPC-assembled asymmetric supercapacitor exhibited excellent life cycle with 100% capacitance retention up to 8000 cycles.

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## Mechanical and electronic properties of 1D Single-layer MoS<sub>2</sub> under elastic strain

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### Abstract

In this study we implement first principles calculations (DFT calculations) on a model of MoS<sub>2</sub>\_NR (NanoRibbons). Our calculations revealed that, depending on the MoS<sub>2</sub>\_NR edge structure, the MoS<sub>2</sub>\_NR is either magnetic or nonmagnetic. Applying strain on MoS<sub>2</sub>\_NRs zigzag terminal structures aiming for investigating the dependence of their energy bands, density of states, and magnetic properties on the NR width and terminal type. Due to the decreasing of orbital overlap, the bonding–antibonding splitting of these states is reduced. As a result, Upon  $\epsilon=0.0$ , the single-layer MoS<sub>2</sub> shows a behavior of semiconductor with direct gap, while it transits into indirect semiconductor within region  $\epsilon \geq 0.10$ . Then it behaves as metal in region  $0.06 \leq \epsilon \leq 0.1$ , further, the valance band maximum VBM moves upward, the conduction band minimum CBM moves downward, and the band gap decreases. Band gap does not vanish until the (VBM) and (CBM) cross the Fermi level, and the semiconductor-to-metal transition emerges.

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### **Numerical simulation of entropy generation due to unsteady natural convection in a semi-annular enclosure filled with nanofluid**

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#### **Abstract**

A numerical study has been carried out to investigate the natural convection and entropy generation for different nanofluids within an inclined half-annulus heated from above. The conservation equations in cylindrical coordinates are solved using an in-house FORTRAN code based on the finite volume method coupled with multigrid acceleration. Water-based nanofluid containing various types of nanoparticles (Au, Ag, Cu and CuO) are used to examine the fluid flow and potential heat transfer enhancement in the annulus. The effective thermal conductivity and viscosity of nanofluids are calculated using the Maxwell–Garnetts (MG) and Brinkman models, respectively. The results demonstrate clearly that the average entropy generation due to heat transfer ( $\langle \text{STG} \rangle$ ) is strengthened by increasing  $\Phi$  and Ra. Furthermore, for small inclination angles  $\gamma=0^\circ$  and  $45^\circ$  ( $\langle \text{SVG} \rangle$ ) and ( $\langle \text{STG} \rangle$ ) values are reduced as RR is augmented, whereas, their values were observed to strengthen when RR increases for large tilt angles  $\gamma=90^\circ$ ,  $135^\circ$  and  $180^\circ$ . So, several important issues are highlighted that deserve greater attention.

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## Feasibility of using hollow double walled Mn<sub>2</sub>O<sub>3</sub> nanocubes for hybrid Na-air battery

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### Abstract

Synthesis of the strongly anisotropic materials, such as highly porous hollow double walled cubes are considered excellent approach to maximize the diffusion of electrolytes. Herein, hollow doubled walled (HDW) Mn<sub>2</sub>O<sub>3</sub> nanocubes (NCs) were synthesized by facile hydrothermal method followed by calcination method. The growth of nanocubes were studied by performing hydrothermal reaction at different times ranging from 3 to 9 h. Thereafter, the feasibility of prepared HDW NCs as air cathode in hybrid Na-air battery was systematically investigated. Among all, the sample prepared by 9 h hydrothermal treatment showed superior performance than 3 and 6 h samples. The fabricated hybrid Na-air cell using HDW Mn<sub>2</sub>O<sub>3</sub> NCs displayed 330 mV overpotential gap and 90% electrical energy efficiency at 5 mA g<sup>-1</sup> current density, maximum of 0.2 W g<sup>-1</sup> power density and good cyclic stability up to 75 cycles which is attributed to the highly porous nature of material that allows efficient diffusion of electrolyte ions and oxygen from air. Thus, present investigation suggests that HDW Mn<sub>2</sub>O<sub>3</sub> NCs can be a potential air cathode and can be utilized in other metal-air battery systems.

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## Theoretical Investigation of the X-ray photoabsorption spectra of Argon Near the KL-edge

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### Abstract

The X-ray photoabsorption spectrum of Argon near the KL-edge have been investigated by calculating the transition probabilities of double electron excitations from the ground state. The final excited states included the double electron excitations  $[1s2p]5p2, [1s2p]6p2, [1s2p]4p5p, [1s2p]4p6p, [1s2p]4s5s, [1s4p]4s6s$ . The method of the calculations was done using relativistic multi-configurational Dirac-Hartree Fock method, Breit Interactions and Quantum electrodynamics effects was also included in the calculations. Comparison of the calculations with previous measurements of the X-ray photoabsorption spectrum of Argon showed reasonable agreement.

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## Investigation of the X-ray Photoabsorption Spectrum of Potassium near K, KN and KL edges; Transition probabilities for single and double electron excitations

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Journal of Electron spectroscopy, January, 2018,

### Abstract

We present new calculations for the transition probabilities and transition energies for single electron K shell excitations and double electron KN and KL shell excitations in atomic Potassium in the energy range 3610-3650 eV. The calculations were carried out to investigate the X-ray photoabsorption spectrum of atomic Potassium using Multi-configurational Dirac-Hartee Fock method. The transition probabilities were convoluted in Lorentzian line shapes, a rough estimate of the effect of photoionization was also taken into account, comparison of the calculations with previous measurements of the X-ray photoabsorption spectrum of atomic Potassium near K, KN and KL edges showed relatively good agreement.

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## Effects of deposition parameters on photo catalytic activity of Ti(W)Ox thin films

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### Abstract

One of the most pervasive problems related to today's world is inadequate access to clean water and sanitation. New suitable technologies must be developed to permit the use of solar energy to help solving both the energy and water problems. The goal of our research in this project is to develop a solar photo catalysis based on Tungsten doped Titanium Dioxide Ti(W)Ox film for water purification and self cleaning purposes. It is predicted that the incorporation of W atoms on TiOx will result in charge separation by avoiding electron and holes to recombine and increased recombination life times. Synergistic enhancements in photo-catalysis and surface super-hydrophilic characters are also expected by W-doping. We have deposited Ti(W)Ox films using the magnetron sputtering technique on float glass substrates. Such films can be directly deployed to find effect of solar energy induced photocatalysis on the contaminant degradation from waste water. In the thesis, we have modified the sputtering parameters such as the chamber pressure, duration of deposition and RF power of sputtering gun to optimize Ti(W)Ox growth process. Chemical states present in the Ti(W)Ox films are determined using X-ray photoelectron spectroscopy and extent of W incorporation in the TiOx is estimated. Quantitatively, the photo-catalytic activity Ti(W)Ox is evaluated from the process the photo-degradation indicated using the color (650 nm) change in methylene blue (MB) dye during continuous ultraviolet irradiation. The surface wettability is also determined from contact angle measurements for the self-cleaning surface applications.

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## **Sol-gel synthesized Co-doped anatase TiO<sub>2</sub> nanoparticles: Structural, optical, and magnetic characterization**

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### **Abstract**

A simple sol-gel method was used to synthesize cobalt doped TiO<sub>2</sub> nanoparticles. Co doping concentration within the range 0, 2, 4, 6 and 8 mol. % were prepared. structural, optical, surface morphology and magnetic characterization of samples under the effect of changing the Co concentration. X-ray diffraction (XRD), Fourier transform infrared (FTIR), UV/Vis/NIR Diffuse Reflectance Spectroscopy (DRS), UV-visible absorption, transmission electron microscopy (TEM), and vibrating sample magnetometer (VSM) System techniques were employed. XRD results confirmed the formation of TiO<sub>2</sub> (titania) nanoparticles in anatase phase for all the undoped and Co-doped samples. The microstructure studies of the samples confirmed the incorporation of Co ions into the host titania matrix is occurring via substitution for the Ti sites. All the investigated samples exhibited a room temperature ferromagnetic (RTFM) behavior as observed by VSM measurements. The optical energy gap (E<sub>g</sub>) ~ 3.59 eV. The absorption band shows shift from 510 nm to 720 nm as Co concentration is increased. An extension of the band gap into the visible light region with Co doping as confirmed by DRS study.

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## Dielectric Behavior of Spark Plasma Sintered BaTi<sub>0.7</sub>Zr<sub>0.3</sub>O<sub>3</sub> Relaxor Ferroelectric

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### Abstract

Oxide ferroelectric materials with a high dielectric constant are of great importance in many electrical applications, such as capacitors, actuators, memory storage and microwave devices. Barium titanate zirconate [BaTi<sub>1-x</sub>Zr<sub>x</sub>O<sub>3</sub>] ceramics are interesting materials for these applications. These ceramics have a grain size in micrometer range and the dielectric constant was found to increase with the increase of grain size. In the current study, we are planning to investigate the dielectric properties of fine-grained BaTi<sub>0.7</sub>Zr<sub>0.3</sub>O<sub>3</sub> (BTZ30) ceramics. These ceramics are prepared by combination of mechanical milling, solid state reaction and spark plasma sintering (SPS). The SPS technique will produce dense fine-grained ceramics. The product ceramics are characterized by X-ray diffraction and scanning electron microscopy (SEM). The dielectric and transport properties of the investigated ceramics will be studied by impedance spectroscopy over wide ranges of temperature (-150 – +200 °C) and frequency (1 – 107 Hz). The dielectric data have been analyzed by the original or modified Curie-Weiss law and the relaxation process in the materials has fitted by Vogel-Fulcher model.

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### **Fast degradation of green pollutants through nanonets and nanofibers of the Al-doped zinc oxide**

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Acta Metallurgica Sinica (English Letters) 31, 533–546 (2018)

#### **Abstract**

In this study, series of nanolayered structures of Zn–Al LDHs were prepared by urea hydrolysis. Nanofibers and nanonets of the Al-doped ZnO were formed via the decomposition of the nanolayers under high pressure and temperature. Nanospheres were also prepared for comparison. The different morphologies of the prepared nanomaterials were confirmed by several techniques. An improvement for the optical properties of the doped zinc oxides was observed through narrowing of their band gap energies because of transforming the nanolayers to nanonets and nanofibers. The photocatalytic activities of the prepared nanomaterials were studied through photocatalytic degradation of the pollutants of acid green dyes. Complete decolorization and mineralization of green dyes happened in the presence of the nanolayers and nanospheres within 4–6 h, while the nanonets and the nanofibers achieved the complete decolorization and degradation of the dyes at shorter time 1.3 h. These results could be explained through the kinetic study of the photocatalytic degradation of dyes. It was concluded that the nanonets and the nanofibers were very effective for the photocatalytic degradation of pollutants.

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## Accelerating the Photocatalytic Degradation of Green Dye Pollutants by Using a New Coating Technique for Carbon Nanotubes with Nanolayered Structures and Nanocomposites

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Chemistry Open 7, 833 – 841 (2018)

### Abstract

The present study has two aims, first to accelerate the degradation of pollutants by coating carbon nanotubes (CNTs) with nanoplatelets or nanocomposites of aluminum zinc oxides and second to fabricate an advanced photocatalyst. Accordingly, Zn-Al layered double hydroxides (LDHs) were grown in the presence of functionalized CNTs during urea hydrolysis. The presence of CNTs led to the formation of LDH nanoplatelets, and TEM images showed that the CNTs were coated with nanoplatelets.

The nanoplatelets were thermally treated to form nanocomposite-coated CNTs. Raman spectra demonstrated the successful coating of CNTs with LDHs and nanocomposite. The coated CNTs were very effective in the photocatalytic degradation of industrial pollutants. A kinetics study demonstrated that the rate of photocatalytic degradation of green dye in the presence of CNTs coated with aluminum zinc oxide nanocomposite was five times faster than with the aluminum zinc oxide nanocomposite.

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## Designing Magnetic Layered Double Hydroxides and Two-Dimensional Magnetic Nano-Nets of Cobalt Ferrite through a Novel Approach

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Applied Science 8, 2099 (2018)

### Abstract

The present study has a dual aim of supporting magnetic nanoparticles over the nanolayers of LDHs and designing two-dimensional magnetic nano-nets of cobalt ferrite. In this trend, nanoparticles of  $\text{CoFe}_2\text{O}_4$  were prepared and supported by Co-Fe LDH through urea hydrolysis. The nanolayered structures of Co-Fe LDH were confirmed by X-ray diffraction, energy-dispersive X-ray spectrometry, FT-IR spectra, thermal analyses, and transmission electron microscopy. In addition, they indicated that 13.2%  $\text{CoFe}_2\text{O}_4$  were supported over Co-Fe LDH. Transformation of the nanolayered structures of Co-Fe LDH to nano-nets was achieved by the catalytic effect of the supported  $\text{CoFe}_2\text{O}_4$  nanoparticles through solvent thermal technique. X-ray diffraction patterns and transmission electron microscopy images confirmed the transformation of the supported Co-Fe LDH to nano-nets of cobalt ferrite. In order to indicate the effect of the LDH for designing the nano-nets, nanoparticles of cobalt ferrite were prepared by the same technique without LDH. The magnetic behavior of the nano-nets and the supported Co-Fe LDH were measured and compared with the nanoparticles through vibrating sample magnetometer technique. The magnetic parameters indicated that the prepared nano-nets have ferromagnetic behavior and high coercivity. However, the prepared nanoparticles revealed a superparamagnetic state and low coercivity. The experimental results concluded that the incorporation of nanoparticles with nanowires into nano-net structures has been found to be an efficient way to improve their magnetic properties and prevent their agglomerations. Finally, layered double hydroxides are an important source for constructing magnetic nanolayered structures and nano-nets.

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## Influence of Iron Doping on Structural, Optical and Magnetic Properties of TiO<sub>2</sub> Nanoparticles

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### Abstract

In this study, various concentrations of Fe doped TiO<sub>2</sub> nanoparticles have been successfully synthesized using the sol-gel method. A variety of characterization techniques as ultra-violet visible (UV-Vis) spectroscopy, X-ray diffractometer (XRD), vibrating sample magnetometry (VSM) and field emission scanning electron microscopy (FESEM) were employed to analyze the prepared nanopowders. XRD measurement confirmed the substitution of Fe ion without disturbing the tetragonal crystal system of TiO<sub>2</sub>. The crystallite size was found to decrease and lattice strain increases upon doping estimated by Williamson Hall plot. Furthermore, the average grain size calculated by FESEM found was between 10 and 30 nm for pure and doped TiO<sub>2</sub>. UV-Vis spectroscopy showed an increase in absorption accompanied red shift and increase in band gap energies from 3.36 to 3.62 eV with the addition of Fe. The FTIR spectroscopy was employed to confirm the presence of functional groups in the fabricated nanopowders. Upon mixing the saturation magnetization (M<sub>s</sub>) varying from (2.12 to 1.51)10<sup>-2</sup> emu/g was observed.

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## Uniaxial tension/ compression effects on the electrical properties of carbon nanotube bundles: A first-principles study.

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### Abstract

In this work, we studied the effect of uniaxial tension/compression on the electrical properties of carbon nanotube bundles within the framework of density functional theory. The bundles consist of mono-chirality single-walled carbon nanotubes. The band gap response of the bundles shows different electrical characteristics including band gap opening, closing and non-linear behaviors, where the affected band gap is significantly dependent on the chirality of the constituent tubes. Calculations reveal that the bundles express a systematic down-shift in the Fermi energy as a consequence of the applied tension, and a systematic up-shift in the Fermi energy in response to the applied compression. Furthermore, the simulation results show a nonlinear behavior in Fermi energy for bundles under test. This nonlinear behavior in Fermi energy may be caused by asymmetrical electronic effects in both conduction and valance bands. For all bundles, the weak wall-to-wall interactions have considerable effects on electrical properties compared to single-walled carbon nanotubes. We hope this study does not only provide helpful enlightenment on the effects of uniaxial strain on electrical properties of bundles, but also opens exciting opportunities for potential applications of piezoresistive nano-devices.

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## Micromagnetic Modeling of Barium Hexaferrite Thin Films by RF Magnetron Sputtering

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Results in Physics 8, 587-591 (2018) <https://doi.org/10.1016/j.rinp.2018.01.003>

### Abstract

The synthesis and characterization of thin M-type barium hexaferrite (BaFe<sub>12</sub>O<sub>19</sub> or BaM) films on silicon are reported. Multilayer insitu technique was employed to anneal the films at 850-900°C for 10 minutes. The thickness dependence of the magnetic properties of the BaM films has been investigated using VSM. For the BaM 150 nm thickness film, acicular BaM grains were present having their c-axis randomly oriented. For the BaM films thicker than 150 nm, lattice relaxation favors the c-axis to be aligned in the film plane. The Micromagnetic simulation was used to model the out-of-plane and the in-plane hysteresis loops. We have achieved good matching between the experimental data and the model. Using the micromagnetic model, we have estimated the deflection angle of c-axis from the normal plane  $\theta = 25^\circ$  for the 150 nm thick film.

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## Haeckelite structure, carbon nanotube, optical properties, transverse electric field, and density functional theory

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### Abstract

Optical properties of Haeckelite structure as well as pristine carbon nanotubes were studied. Density functional theory was used to analyze optical absorption, reflectivity, dielectric function, conductivity, refractive index and loss function under transverse electric field. Our calculations illustrate noticeable reducing of spectra peaks in addition to blue/red shift corresponds lower/ higher frequency. We also investigated the effect of transverse electric field on static values of reflectivity, dielectric function and refractive index. Our results show significant variations between pristine.

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## Self-Cleaning Surfaces Based on Pure and Doped TiO<sub>2</sub> Ultra-Thin Films

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### Abstract

Self-cleaning property of TiO<sub>2</sub> film derives from its two intrinsic properties; photocatalysis and superhydrophilicity. In addition, TiO<sub>2</sub> can decompose organic contaminant or kill bacteria adhering to the surface under illumination of (UV) light.

In this work, we developed self-cleaning surfaces based on pure and N-doped TiO<sub>2</sub> ultra-thin films. Amorphous TiO<sub>2</sub> thin films were prepared by DC-magnetron sputtering deposition at room temperature. We investigated the effect of deposition parameters as deposition time, pressure and nitrogen flow rate on the photocatalytic activity and the surface wettability of TiO<sub>2</sub> thin films. The surface wettability was tested by controlled contact angle measurement (CA) and photocatalytic activity. Self-cleaning tested by effective photodegradation in Methylene Blue (MB) dye in respect to UV illumination. X-ray photoelectron spectroscopy (XPS) , scanning electron microscope (SEM) were employed to analyze the chemical structure and the surface topography in order to understand the difference in performance of samples. Finally, we successfully obtained super hydrophilic ultra-thin films with the ability to decompose pollutant.

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## **Entanglement in two coupled harmonic oscillators under the influence of an external constant electromagnetic field**

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### **Abstract**

Recently among the possible approaches that have been used in exploring some basic features of the entangled massive states, we cite the coupled harmonic oscillators' theory. This is why we intend here to study the entanglement in two coupled harmonic oscillator under the influence of an external constant electromagnetic field. To do this, we first make use of suitable unitary transformation that enable us to get the solutions of the energy spectrum. These are used to construct the associated coherent states in the standard way.

In order to evaluate the degree of the entanglement between the states obtained, we calculate the purity function in terms of coherent states as well as in terms of the number states. The interesting emerging property be a dependence of the purity function on the coupling parameter of the system which scales well with need of controlling easily the degrees of entanglement. Analysis in terms of the coupling parameter reveals the condition for which the system is strongly entangled.

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## **Dilute magnetic properties of $\text{Ni}_x\text{Sn}_{1-x}\text{O}_2$ Semiconductor: Optical, Electrical and Magneto-Transport Investigations**

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### **Abstract**

Transition metal (Ni) doped tin-oxide ( $\text{SnO}_2$ ) is a dilute magnetic ternary semiconductor (DMS) alloy, which is a valuable material in variety of spintronics and thermoelectric applications. In the thesis research work,  $\text{Ni}_x\text{Sn}_{1-x}\text{O}_2$  ( $x = 0, 0.001, 0.01, \text{ and } 0.1$ ) powder samples are prepared by using sol-gel method and synthesis parameters are optimized to obtained single-phased pure ternary solid solution. In addition to this, chemical states, optical, morphological, optical, thermo-gravimetric, structural and compositional analyses of the alloy is performed using XRD, TGA, Raman, PL, XPS and SEM techniques. Magneto-electric characterization of the DMS alloy is also performed using Physical property measurement system (PPMS) to evaluate magneto-resistance in the pellets of  $\text{Ni}_x\text{Sn}_{1-x}\text{O}_2$ . The change in magneto-resistance is expected from the Ni doping related changes in oxygen vacancies and chemical states.

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### **Effects of deposition parameters on Photo-catalytic activity of Ti(W)Ox thin films**

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#### **Abstract**

One of the most pervasive problems related to today's world is inadequate access to clean water and sanitation. New suitable technologies must be developed to permit the use of solar energy to help solving both the energy and water problems. The goal of our research in this project is to develop a solar photo catalysis based on Tungsten doped Titanium Dioxide Ti(W)Ox film for water purification and disinfection purposes. It is predicted that the incorporation of W atoms on TiOx will result in charge separation by avoiding electron and holes to recombine and increased recombination life times. Synergistic enhancements in photo-catalysis and surface super-hydrophilic characters are also expected by W-doping. We have deposited Ti(W)Ox films using the magnetron sputtering technique on float glass substrates. Such films can be directly deployed to find effect of solar energy induced photocatalysis on the contaminant degradation from waste water. In the thesis, we have modified the sputtering parameters such as the chamber pressure, duration of deposition and RF power of sputtering gun to optimize Ti(W)Ox growth process. Chemical states present in the Ti(W)Ox films are determined using X-ray photoelectron spectroscopy and extent of W incorporation in the TiOx is estimated. Quantitatively, the photo-catalytic activity Ti(W)Ox is evaluated from the process the photo-degradation indicated using the color (650 nm) change in methylene blue (MB) dye during continuous ultraviolet irradiation. The surface wettability is also determined from contact angle measurements for surface oxidative sterilization applications in presence of radiation.

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## **New Preparation Approach and Physical Properties of Pol(vinyl Alcohol) loaded Graphene**

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### **Abstract**

Previous publications showed that, graphene sheets polymer nanocomposites were prepared by incorporating previously prepared graphene into the polymer matrix through two or more successive steps. In this work, graphene sheets were exfoliated inside the polymer matrix solution for certain period in one step. This approach was easy to perform, low cost, high mass production of graphene and, almost, produces effective results. In this respect, electrolytic solution from poly(vinyl chloride), PVA, and salt dissolved in water in which exfoliation process took place inside for different times and got films of PVA loaded with different concentrations of graphene sheets. The dielectric permittivity, dielectric loss, and AC electrical conductivity had maximum values at 10 min of exfoliation time.

Cool-Cool impedance plots show semicircles behavior with lowest radius for samples prepared at 10 min. The elastic modulus was found to has a maximum value at exfoliation time of 30 min. exfoliation of graphene sheets inside the polymer matrix solution was found to decrease the glass transition temperature.

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## **Electronic and Structural properties of strained double-walled carbon nanotubes: Density functional theory study.**

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### **Abstract**

In this work we utilized Density Functional Theory to investigate theoretically the electrical and structural properties of double walled carbon nanotubes (DWCNTs) upon applying uniaxial strain. We used three different types of zigzag single walled carbon nanotubes (SWCNTs) to build the DWCNT cells. These nanotubes are chosen with different sizes and electrical properties including metallic and semiconductors tubes. For all nanotubes we carried out total energy calculations and smooth curves were observed which is a good indication that the nanotubes are intact no fracture occurred. Furthermore we, found that all understudy DWCNTs have total energies less than their constituents SWCNTs before and after applying uniaxial strain. This can be attributed to the presence of Van der Waals forces between the wall to wall layers, which is considered as a reasonable explanation of the DWCNT more stability compared to SWCNT. Interestingly, band gap response to uniaxial strain of DWCNTs has been investigated and analyzed for the three tube types, Furthermore, we have found the band gap of DWCNTs is less than or close to the least band gap of its constituents SWCNT. This was explained by the charge transfer from the outer-tube to the inner-tube in DWCNTs in addition to the overlap between the orbitals of conduction band of the inner nanotube and the valence band of the outer nanotube. We also investigated the dependence of Fermi level on uniaxial strain for all nanotubes. Fermi level show mixed linear and nonlinear downshifts in Fermi level in response to the applied strain on all nanotubes except (8,0)SW. In (8,0)SW we have noted the opposite due to its smallness diameter.

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## **Influence of doping and processing conditions on the structural, electrical and dielectric properties of $\text{CaCu}_3(\text{Ti}_{4-x}\text{Al}_x)\text{O}_{12}$ ceramics**

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### **Abstract**

A series of samples having the compositions of  $\text{CaCu}_3(\text{Ti}_{4-x}\text{Al}_x)\text{O}_{12}$  ( $x=0:0.2$ ), CCTAO, have been prepared. Conventional sintering (CS) at  $1100\text{ }^\circ\text{C}$  for 12 h were used to obtain the dense ceramics from the synthesized powders. XRD patterns show that all CCTAO ceramics showed a CCTO-like pure phase. The microstructure studies by FE-SEM showed that the grain size increases from 13 to  $175\text{ }\mu\text{m}$  when increasing the concentration Al. All the CS CCTAO ceramics showed giant dielectric constant ( $\epsilon' > 10^4$ ) at room temperature and 9 kHz. With increasing Al content, the resistivity of the ceramics was found to decrease while both the dielectric constant and dielectric loss increases. Interestingly, it was found that  $\text{Al}^{3+}$  ions act as electron donors that result in the decrease of resistivity of the Al-doped CCTO ceramics.

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## كتيب ملخص الأبحاث العلمية - اليوم العلمي السادس 2019

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