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Abstracts



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AN EXPERIMENTAL STUDY AND MODELING OF L-HISTIDINE SOLUBILITY IN CHLORIDE SALTS AQUEOUS SOLUTIONS AT DIFFERENT TEMPERATURES

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Measurements were performed to determine the solubilities of L-histidine in aqueous solutions of various concentrations of chloride salts (NaCl and KCl) by using a thermostatted reactor and gravimetric method from (293.15 to 323.15 K) under atmospheric pressure. The effect of inorganic salts on the solubility of L-histidine was investigated and was found accordingly: sodium chloride > potassium chloride. Results showed that the solubility in pure water and in aqueous chloride solutions increased with increasing temperature. The experimental data were well correlated by the semi-empirical equation. Using the measured solubilities, the standard molar thermodynamic properties of transfer of GA ($\Delta_{tr}G^\circ$, $\Delta_{tr}H^\circ$ and $\Delta_{tr}S^\circ$) from pure water to aqueous solutions of the chloride salts were estimated

Biography

Adel Noubigh has completed his PhD from Tunis El Manar University, Tunisia and Postdoctoral Studies from ENSTA ParisTech. He is serving as an Assistant Professor in the Department of Chemistry, Preparatory Institute for Engineering Studies of Gafsa, Gafsa University, Tunisia and in the Faculty of Science, Northern Borders University, Kingdom of Saudi Arabia. He has published more than 26 papers in reputed journals.

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PHASE TRANSITION INDUCED BAND STRUCTURE ENGINEERING OF BIVO₄ FOR SOLAR FUEL PRODUCTION

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Cost-effective solar water splitting requires earth abundant photocatalytic materials converting photons to working electrons in a highly efficient manner. To develop such suitable photocatalysts, their atomic structure control is of primary importance since their intrinsic attributes (e.g., electronic band structure, electric properties, catalytic activity, etc.) are governed by their atomic configuration. In this regard, BiVO₄'s atomic structure has been engineered via P5+ doping and In³⁺/Mo⁶⁺ dual doping. The significantly enhanced photo-responsive characteristics of the doping-treated BiVO₄ have been systematically studied within experimental and theoretical domains. Specifically, VO₄ and PO₄ oxoanion exchange in monoclinic BiVO₄ significantly reduces its charge-transfer resistance by increasing charge-carrier density, and thus enhances solar-to-hydrogen efficiency up to 29.3 times, as Fig. 1 shows. Notably, this brand-new oxoanion exchange technique can be applied to other various VO₄-based semiconductors to improve their electronic, catalytic and photochemical properties. To upgrade the photocatalytic performance of BiVO₄ further, its electronic band structure was engineered by simultaneously substituting In³⁺ for Bi³⁺ and Mo⁶⁺ for V⁵⁺, which induced partial phase transformation from pure monoclinic BiVO₄ to a mixture of monoclinic and tetragonal BiVO₄. This In³⁺/Mo⁶⁺ doped BiVO₄ has a slightly larger band-gap energy (E_g ~2.5 eV) than usual 'yellow' monoclinic BiVO₄ (E_g ~2.4 eV) and higher (more negative) conduction band edge (-0.1 VRHE at pH 7) than H⁺/H₂ potential (0 VRHE at pH 7). Consequently, as Fig. 2 displays, the In³⁺/Mo⁶⁺ doped BiVO₄ is able to split water into H₂ and O₂ under visible-light irradiation without using any sacrificial reagents (e.g. CH₃OH or AgNO₃). This outcome is the first example of a pure water-splitting photocatalyst responding to visible light without any noble-metal co-catalyst.

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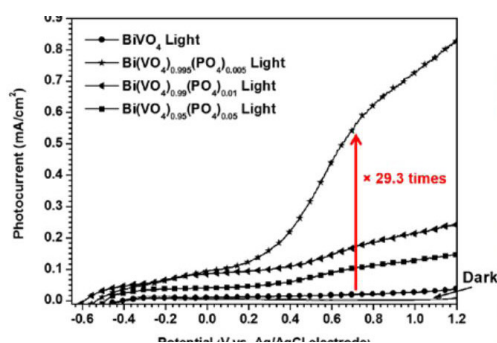


Fig 1: Enhanced photocurrent by PO₄ doping into BiVO₄

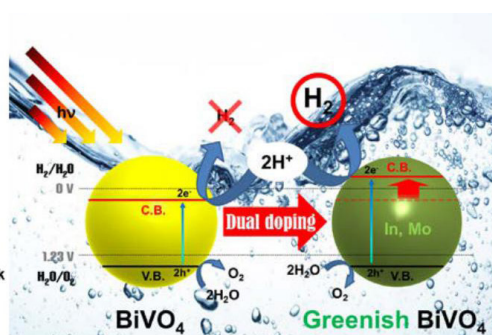


Fig 2: Overall water splitting reaction by In³⁺/Mo⁶⁺ doped BiVO₄

KINETICS AND THERMODYNAMICS OF CORROSION INHIBITION OF CARBON STEEL, MILD STEEL AND SABIC IRON BY SYNTHESIZED N-DODECYL ARGININE SURFACTANT IN ACIDIC ENVIRONMENT: A COMPARATIVE STUDY

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The kinetics and thermodynamic studies of the corrosion inhibition of carbon steel, mild steel and SABIC iron in hydrochloric acid medium by synthesized N-dodecyl arginine surfactant (DAS) as environmentally friendly corrosion inhibitor were carried out using both chemical and electrochemical techniques. It was found that the synthesized surfactant acts as a good corrosion inhibitor for the three investigated steel samples in the tested medium. The inhibition efficiency increased as the concentration of surfactant is increased in the medium but it was found to decrease with increasing concentration of the corrosive medium (HCl) and temperature. The high inhibitive action of the surfactant is discussed in view of adsorption of its molecules on the steel surfaces and forming protective films. Thermodynamic and kinetic parameters have been evaluated and discussed which support the mechanism of physical adsorption of the surfactant. The synthesized surfactant was found to act as a mixed inhibitor. The morphology of the surfaces of the investigated steel samples was shown by scanning electron microscopy (SEM) which supported the presence of good protective films onto the steel surfaces.

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CONSTRUCTION OF AN OXIDIZED POLYPYRROLE MODIFIED ELECTRODE AND ITS APPLICATION FOR DETERMINATION OF COPPER (II) IN ENVIRONMENTAL SAMPLES

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In this study, an electrochemical method for the determination of copper ion has been developed using over oxidized polypyrrole (OPPy) electrode doped with sulfosalicylic acid (SSA). The SSA acts both as a chelating agent and a counter anion within the polypyrrole matrix. In a typical assay, Cu (II) is accumulated on a solid electrode via the formation of a copper-SSA complex. The electrode containing the Cu²⁺ SSA is then transferred to a 0.2M potassium nitrate where it is subjected to differential pulse anodic stripping voltammetry. The resulting stripping peak current was linearly related to the concentration of copper. The method has been optimized with respect to pH (pH=5.0), concentration of chelating agent (0.1M), accumulation time (200s) and reduction potential (0.5V). The detection limit was found to be 4×10⁻⁹ M with a linear range of 1×10⁻⁹-1×10⁻³M. The method has been validated for the determination of copper in environmental samples.

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THE USE OF THE MATRIX-ASSISTED LASER DESORPTION/ IONIZATION TIME-OF-FLIGHT MASS SPECTROMETRY (MALDI-TOF MS) TECHNIQUE FOR THE DEVELOPMENT OF ANTIFUNGAL STRATEGIES

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In the last decades, several epidemiological studies have confirmed the increase in the frequency of invasive fungal infections (IFIs) worldwide, which are currently considered important public health problem. Clinical and experimental evidence has shown that IFIs can be caused by organized communities in the form of biofilms. These structures are characterized by intense metabolic cooperation and great resistance to physical and chemical agents and are defined as dynamic communities of microorganisms strongly adhered to a biotic/abiotic substrate and protected by a matrix rich in exopolymers, especially proteins. The extracellular matrix of the biofilm plays a crucial role in the protection of fungal cells against the immune response of the host besides being considered one of the main mechanisms of resistance to antifungals. Understanding the mechanisms involved in the synthesis of the biofilm matrix is the key point for the development of antifungal strategies. There are several techniques for identifying the components of the biofilm matrix, one of them is the matrix assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS), which allows analyzing the biofilm matrix constituents. Thus, this communication aims to emphasize the use of the MALDI-TOF MS technique as a tool for the development of antifungal strategies.

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BIOPOLYETHER FROM MEDICINAL PLANTS: AS ANTICANCER AGENT

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Within the field of pharmacologically active biopolymers the area of stable polyethers seems rather new and attractive. A new series of linear and regular caffeic acid derived polyether, namely poly[oxy-1-carboxy-2-(3,4-dihydroxyphenyl)ethylene] or poly[3-(3,4-dihydroxyphenyl)glyceric acid] (PDPGA) was isolated and identified in the water-soluble, high molecular weight fractions obtained from *Symphytum asperum*, *S. caucasicum*, *S. officinale*, *S. grandiflorum* and *Anchusa italica* (Boraginaceae). According to data of ^{13}C , ^1H NMR, 2D $^1\text{H}/^{13}\text{C}$ HSQC experiments, the polyoxyethylene chain is the backbone of the polymer molecule. 3, 4-Dihydroxyphenyl and carboxyl groups are regular substituents at two carbon atoms in the chain. The repeating unit of this regular polymer is 3-(3, 4-dihydroxyphenyl) glyceric acid residue. Most of the carboxylic groups of PDPGA from *A. italica* and *S. grandiflorum* unlike the polymer of *S. asperum*, *S. caucasicum* and *S. officinale* are methylated. The 2D DOSY experiment gave the similar diffusion coefficient for the methylated and non-methylated signals of *A. italica* PDPGA. Both sets of signals fell in the same horizontal. This would imply a similar molecular weight for methylated and non-methylated polymers. PDPGA is endowed with intriguing pharmacological properties as anticomplementary, antioxidant, anti-inflammatory, burn and wound healing effect. The synthesis of racemic monomer of PDPGA, 2,3-dihydroxy-3-(3,4-dihydroxyphenyl)propionic acid (DDPPA) and its enantiomers (+)-(2R,3S)-DDPPA and (-)-(2S,3R)-DDPPA was carried out via sharpless asymmetric dihydroxylation of *trans*-caffeic acid derivatives using a potassium osmate catalyst and cinchona alkaloid derivatives (DHQ)2-PHAL and (DHQD)2-PHAL as chiral auxiliaries. PDPGA and DDPPA exerted anti-cancer efficacy *in vitro* and *in vivo* against human prostate cancer (PCA) cells via targeting androgen receptor, cell cycle arrest and apoptosis without any toxicity, together with a strong decrease in prostate specific antigen level in plasma. However, our results showed that anticancer efficacy of PDPGA is more effective compared to its synthetic monomer. Overall, this study identifies PDPGA as a potent agent against PCA without any toxicity, and supports its clinical application.

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IRRADIATION OF WASTEWATER WITH ELECTRON BEAM IS A KEY TO SUSTAINABLE SMART/GREEN CITIES

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The application of electron beam technology for the treatment of sewage water was carried out in this research work. The study was conducted to evaluate the disinfection potential of electron beam radiation (EBR) on sewage water. Results obtained at dose rate of 3 kGy per $\approx 50\mu\text{s}$ were shown to be more efficient for the disinfection of sewage water. At high dose rate of 6 kGy per $\approx 50\mu\text{s}$, the removal percentage of organic load in sewage increased up to 60% of its initial load and also showed a substantial improvement in waste water quality with an efficient decrease in organic load that lead to a better remediation process. On irradiation, the organic matter in sewage water will be degraded via transforming from complex to simpler molecular forms that are easily metabolized by native soil microflora during irrigation. The statistical correlation co-efficient analysis of the data has resulted in the significant r-values of the entire data i.e. $r>68$ which concludes the results to be positively significant and shows strong correlation coefficient. Therefore, this study emphasizes that the feasibility of electron beam radiation (EBR) for sewage water remediation. Further, our study defends that the ionizing radiation can be applied in two ways for treatment of sewage water: remediation at lower dose rate as well as substitution of chlorination at tertiary treatment process and reduction of sewage water's organic load at higher dose rate. Based on the results, it can be concluded that pollution mitigation using ionizing radiation (electron beam accelerators) is an eco-friendly alternative technology, without using chemical disinfectants ensuring robust life to mankind. Irradiated sewage water is fit for irrigation as well as use in industries which will be a promising solution to existing water demand and also a gateway to sustainable management of fragile fresh water resources for developing countries.

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FLEXIBLE, STRETCHABLE AND HEALABLE ELECTRONICS

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Organic electronics based on semiconducting and conducting polymers have been extensively investigated in the past two decades and have found commercial applications in lighting panels, smartphone and TV screens using OLEDs (organic light emitting diodes) technology. Many other applications are foreseen to reach the commercial maturity in future in areas such as transistors, sensors and photovoltaics. Organic electronic devices, apart from consumer applications are paving the path for key applications at the interface between electronics and biology such as in polymer electrodes for recording and stimulating neural activity in neurological diseases. In such applications, organic polymers are very attractive candidates due to their distinct property of mixed conduction: the ability to transport both electron/holes and ionic species. Additionally, conducting polymers offer the possibility to tune their surface properties (e.g., wettability or chemical reactivity) by changing their oxidation state, thus promoting or hindering the adhesion of biomolecules. This feature can be particularly useful for enhancing the biocompatibility of implantable electrodes. My talk will deal with processing and characterization of conducting polymer films and devices for flexible, stretchable and healable electronics. I will particularly focus on micro-patterning of conducting polymer films for flexible and stretchable devices and on healing of conducting polymer films.

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DEMONSTRATION OF IMPROVED PEAK CAPACITY IN OPEN TUBULAR CAPILLARY COLUMN FOR THE SEPARATION OF PEPTIDES AND PROTEINS

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A copolymer layer was attached inside a preconditioned 64 cm long silica capillary column with effective length of 56 cm where internal diameter was 10 μm , after the attachment of 4-chloromethylphenyl isocyanate and dithiocarbamate initiator system. Dibutyl tin dichloride catalyst was used for the effective attachment of ligand to silanol group present on inner capillary. The copolymer immobilized open tubular capillary column resulted in the separation of about 22 peaks (peptides) out of tryptic digest of cytochrome C sample in capillary electrochromatography with high separation efficiency close to 600,000 plates/column (990,000 plates/meter) with peak capacity of 220. The use of a mobile phase of high water content was facilitated by the open tubular nature of the capillary column which make sure the elution of all peptide peaks resulting in relatively short analysis time.

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NEW PATHWAYS FOR ULTRA-ROBUST MOLECULAR ELECTRONICS AND FOR LIGHT SENSITIVE MOLECULAR SWITCHES

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A number of technological challenges need to be overcome to move organic-based thin-film devices from the research stage to the application level. In this talk, avenues toward the realization of organic electronics on the basis of ultrathin functional organic layers are outlined, specifically by leveraging on the self-assembly process at interfaces. As an attempt to, large area molecular junctions of outstanding robustness are presented and we show that they can be realized using densely packed molecular metal-terpyridine complex oligomers, which might enable a versatile platform for functional optoelectronic layers. By electron and optical spectroscopy, the electronic structure of the materials is elucidated and the robustness determined by nanotribological studies. Finally, as an example for biomolecular photoconductors, Sn-cyt C protein layers are shown to act as reversible photo-electrochemical switches upon integration into large area solid state junctions. The electrical properties of this protein system is investigated using a novel Hg-drop setup, allowing to detect the electrical response of the most fragile adsorbate layers.

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THE CONVERGENCE OF TECHNOLOGIES GENERATES CONVERGENCE IN THE REGULATIONS

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The convergence of nanotechnologies generates synergies among different technologies to say, nanotechnologies, neurotechnology, computers and biotechnology. These technologies must converge (7) their regulations, the application of medical devices in nanotechnologies should lead us to a link between the technical committee TC 210 and ISO technical committee 229 link that does not exist in our work in this moment. In this do, an analysis of the management of risk from an optical NC-ISO 14971 (1). Studying the global trend in this respect as imported for manufacturers medical devices worldwide. The convergences of technologies are a consequence of atomic precision, where the boundary between the biotic and abiotic mute blur the interaction. The interaction between nanotechnologies, biotechnology and informatics and communications (NBIC) generates a synergy of unusual consequences of all is known that the industry of semiconductor(5)s is the one of greater precision that is atomic, the new medical devices that will be applied in the teranocis will dose physical principles that will be governed under the laws of quantum mechanics(4), but there are two problems that have not been solved even though, they are, one the non-existence of quantum biology and the transition from quantum to classical mechanics. On the other hand, the redefinition of the international system of units based on the universal constants that will be implemented by 2018 has a deficiency that is the second that redefirms implies redefinition of the meter, the chain of traceability proposed for nanometrology presents a serious difficulty when putting the microcopy of atomic force wing of effect tunnel situation that is changing the verification of the Wiedemann-Franz law (8) at atomic level yields a result where the phononic component is taken into account, a result that launches STM to the cusp of the chain of traceability above inclusive of interferometry.

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INTERFACE ENGINEERING AND FORCE TUNING ELECTRICAL TRANSPORT BEHAVIOUR OF NANO-DEVICES BASED ON ATOMIC LAYERED MoS_2

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High-performance piezoelectricity in monolayer semiconducting transition metal dichalcogenides is highly desirable for the development of nanosensors, piezotronics and photopiezotransistors. Here, we report the experimental study of the theoretically predicted piezoelectric effect in triangle monolayer MoS_2 devices under isotropic mechanical deformation. The experimental observation indicates that the conductivity of MoS_2 devices can be actively modulated by the piezoelectric charge polarization-induced built-in electric field under strain variation. These polarization charges alter the Schottky barrier height on both contacts resulting in a barrier height increase with increasing compressive strain and decrease with increasing tensile strain. The underlying mechanism of strain-induced in-plane charge polarization is proposed and discussed using energy band diagrams. In addition, a new type of MoS_2 strain/force sensor built using a monolayer MoS_2 triangle is also demonstrated. Our results provide evidence for strain-gating monolayer MoS_2 piezotronics, a promising avenue for achieving augmented functionalities in next-generation electronic and mechanical-electronic nanodevices. Developing nanoelectronics that utilize the vertical sub-nanometer thickness of two-dimensional materials is desirable for achieving miniaturization of circuit elements. However, only a few researches have been studied in the vertical transport of atomic layered materials so far. Here, the vertical electrical transport behaviour of bilayer MoS_2 under coupling of photons and force is explored by the use of conductive atomic force microscopy. We found that the current-voltage behaviour across the tip- MoS_2 -Pt junction is a tunnelling current which can be well fitted by a Simmons approximation. Among which, direct tunneling is dominated at low bias voltages whereas Fowler-Nordheim tunneling is happened at high bias voltages. The bias voltages in transition point between direct and Fowler-Nordheim tunneling are matched with the tunnelling barrier height of energy band shape difference. Furthermore, the source-drain current dropping surprisingly appears when we continually increase force in which the dropping point is altered by light provided. The potential mechanism is responsible for the tuning in tunnelling barrier height and width by force and photons. These results provide a new way to design devices that takes advantage of ultrathin two-dimensional materials. Such ultra-short channel length electronic components that possess tunnelling current are important for establishing high-efficiency electronic and optoelectronic systems.

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PHYSICAL ASPECTS AND NANOSCALE CHARACTERIZATION OF PHASE TRANSFORMATIONS IN SHAPE MEMORY ALLOYS

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Shape memory effect is a peculiar property exhibited by series alloy systems in the β -phase fields. Successive martensitic transformations, thermal induced and stress induced martensitic transformations govern shape memory effect in shape memory alloys. Shape memory effect is performed thermally in a temperature interval on heating and cooling after deformation in low temperature phase condition. Thermal and stressing processes govern shape memory effect in physical basis; twinning and detwinning processes govern in crystallographic basis. Thermal induced martensitic transformation occurs as Martensite variants with lattice twinning in crystallographic scale. Twinned Martensite structures turn into detwinned Martensite structure by means of stress induced transformation Martensite variants occur with the cooperative movement of atoms by means of shear-like mechanism. Copper based alloys exhibit this property in metastable β -phase region, which has bcc-based structures at high temperature parent phase field and these structures martensitically turn into the complex stacking ordered structures with lattice twinning reaction on cooling. Lattice invariant shears are not uniform in copper based shape memory alloys and the ordered parent phase structures martensitically undergo the non-conventional complex layered structures on cooling. The long-period layered structures can be described by different unit cells as 3R, 9R or 18R depending on the stacking sequences on the close-packed planes of the ordered lattice. The close-packed planes, basal planes, exhibit high symmetry and short range order as parent phase. The unit cell and periodicity is completed through 18 layers in direction z, in case of 18R Martensite, and unit cells are not periodic in short range in direction z. In the present contribution, X-ray diffraction and transmission electron microscope studies were carried out on two copper based CuZnAl and CuAlMn alloys. These alloy samples have been heat treated for homogenization in the β -phase fields. X-ray diffraction profiles and electron diffraction patterns reveal that both alloys exhibit super lattice reflections inherited from parent phase due to the displacive character of martensitic transformation. X-ray diffractograms taken in a long time interval show that diffraction angles and intensities of diffraction peaks change with the aging time at room temperature. In particular, some of the successive peak pairs providing a special relation between Miller indices come close each other and this result leads to the rearrangement of atoms in diffusive manner.

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QUANTUM MECHANICS MUST BE REVISED DUE TO ITS DIFFICULTIES AND CONTRADICTIONS

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The difficulties and contradictions of quantum mechanics are exhibited and elucidated in detail by virtue of the comparisons between the experimental facts and theoretical results obtained from the solutions of Schrödinger equations with different potentials, which can only give the wave features of microscopic particles, but cannot always exhibit their corpuscle features. These difficulties and contradictions are intrinsic and inevitable for quantum mechanics and cannot be eliminated and overcome in its framework, no matter how of the quantum mechanics or external potentials. The difficulties and contradictions of quantum mechanics indicated clearly that quantum mechanics is only a linear and approximate theory and cannot be used to describe correctly and completely the duality of wave and corpuscle features of microscopic particles. Detailed investigations showed that the difficulties and contradictions are induced by the dispersed effect of microscopic particle arising from the kinetic energy in Hamiltonian of the systems and Schrödinger equations. This implies that the quantum mechanics must be remoulded, its direction or method remoulding are just to add a nonlinear interaction which can stop and restrain the dispersed effect, then the microscopic particles can be localized and have a wave-corpuscle duality in this case once the nonlinear interaction can balance the dispersed effect of the kinetic energy in Hamiltonian and dynamic equations in the systems, thus the difficulties and contradictions of quantum mechanics could be completely eliminated and overcome. The correctness of the conclusion was perfectly verified and confirmed by our investigations. Then the correct direction and way eliminating the difficulties and contradictions of quantum mechanics are found and affirmed, i.e., it is to establish the nonlinear quantum mechanics. In order to demonstrate that it can describe and represent really and exact the properties of microscopic particles, we found further the real mechanisms of the form of nonlinear interaction which is the self-interaction, self-trapping, self-focusing and self-localized in variously physical systems and gave further their concrete representations, which can be always represented by $b|\psi|^2\psi$ in non-relative case. Thus a correct theory of nonlinear quantum mechanics can be established, in which the duality of wave and corpuscle feature of microscopic particles can appear perfectly and naturally.

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QUANTUM RATE COEFFICIENTS FOR THE O + O₂ EXCHANGE REACTION

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Molecular oxygen O₂ is the most important molecule on earth's atmosphere and stratospheric ozone O₃ protects us from the UV radiation. The abundance of ¹⁶O being 99.8%, O₂ and O₃ exclusively formed from it are dominant, thereby giving a reference for any process involving oxygen. A strong enrichment of O₃ (~10%) in both ¹⁸O and ¹⁷O (mass-independent fractionation-MIF) has been observed decades ago and was reproduced in laboratory experiments. Although this phenomenon remains globally unexplained, the three-body recombination O + O₂ + M → O₃ + M is believed to be the main process leading to this enrichment. At sufficiently low pressures, it can be partitioned into two steps: the formation of O₃ in a highly excited rovibrational state, from reaction O + O₂ → O₃^{*} (step 1), and its subsequent stabilization by collision with an energy absorbing partner M (say N₂), O₃^{*} + M → O₃ + M (step 2). Thus, the efficiency of the exchange reaction O + O₂ → O₃^{*} → O₂ + O, involving O₃^{*} as an intermediate, is one of the key parameters to understand ozone formation. We have shown that this reaction, initiated by step 1, is very fast with three identical ¹⁶O atoms involved due to a quantum permutation symmetry effect. Consequently, it competes ferociously with step 2 described above, the latter becoming in this way much less effective. We have reproduced experimentally observed negative temperature dependence for this reaction rate constant when ¹⁸O is involved, along with other groups. We will sum up results of a computationally intensive full-quantum investigation of the dynamics of the ¹⁶O + ³²O₂, ¹⁸O + ³²O₂ and ¹⁷O + ³²O₂ processes supported by an accurate global potential energy surface for the O₃ ground state. Our study based on a time independent quantum mechanical approach demonstrates that all approximate theoretical simulation techniques and calculations previously reported for this process result in considerable inaccuracies, especially because of the neglect of the quantum symmetries such as the nuclear spin symmetry due to the three (or two) identical atoms, ¹⁶O or ¹⁸O.

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INVESTIGATION OF CONVERSION OF CARBON MONOXIDE TO CARBON DIOXIDE ON THE SURFACE OF MIXED NANOCATALYST IN INITIAL TRIMMED OF MODIFICATION OF RADIATION

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The experiments presented in this paper have been performed in the fixed laboratory-built for experiments where the mixed nano-catalyst on the gas stream reactor was refined initially in the γ -radiation. The kinetics of conversion of CO to CO₂ was researched in predefined surface temperature and in partial pressure of carbon-monooxide. Simultaneously, we determined the catalytic activity by analysis of the gas flow leaving the reactor using a quadruple mass spectrometer. During the survey, the surface temperature of catalyst increased steadily, while the conversion speed was risen accordingly. Thus, the share of conversion increases from 43% to 60% in various concentrations of carbon monoxide in the temperature range of T=80-250 oC when compared with the results of non modifiacted radiation experiments on the same catalyst. It is determined that the conversion speed is stable at the interval of partial pressure $\Delta P_{CO}=1\div 14$ mmHg of carbon monoxide in 1 bar pressure of gas mixture on nano-catalyst surface. By carefully comparing the partial pressure during 15 oxidation reduction cycles, we came to the conclusion that at fixed O₂ pressure, the oxidation take place when the CO partial pressure is low than the O₂ partial pressure. In this article, the processes of adsorption and desorption on the surface of the nanocatalyst have been researched. The anion and cation centers greating on the surface of nano-catalyst was studied. Surface effects were studied by EPR and HR spectroscopy. The research has shown that the mixed nano-particles of catalyst could implement on the car catalyst system and other industrial areas for decreasing the pollution level. The selectivity and affectivity of this catalysts are high and could use for a long time and economically is acceptable.

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MULTIADDRESSABLE PHOTOPHYSICAL PROPERTIES OF PHOTOCROMIC DI AND TETRAHYDROINDOLIZES WITH POTENTIAL APPLICATIONS

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Nowadays, numerous branches of photochemistry have been discovered and the study of the phenomenon of color change of organic compounds known as photochromism phenomenon become one of the most important branches of photochemistry. This is due to their potential importance in lenses industry, thin-film, security inks, high density information storage, dye-sensitized solar cell (DSSC), computer chips, imaging optics as well as in medicine such as dental filling technology. Their important applications motivated us to continue our investigation in this field. In this research project, we aimed to synthesize and study the photochromic behavior of di- and tetrahydroindolizes photochromes. Many chemical and photochemical pathways will be followed in order to get over the synthesis problems. Various physical properties such as kinetics, solvent effect, gelations, photodegradation, fluorescence, and many other multiaddressable properties are discovered. We expect that the synthesized compounds will show a wide range of absorption in the UV region, as well as visible light and also have a wide range in the half-life, allowing these series of compounds to have numerous applications in many industrial fields. Irradiation of the photochromic dihydroindolizine (DHIs) with polychromatic light led to ring opening colored betaines which undergo thermal 1, 5-electrocyclization. The kinetic of the thermal 1, 5-electrocyclization was studied by using multichannel FT/UV-VIS spectrophotometer. In addition, some studies on the influence of the substituents on both the DHI and THI regions which are fluorene (A), ester (B) and the heterocyclic base (C) on the photochromic properties which have a significant penetrate in the kinetic properties. From these standpoints and from our experience in this area, we expect that, this work opens a new era in the field of chemistry and photochemistry as well.

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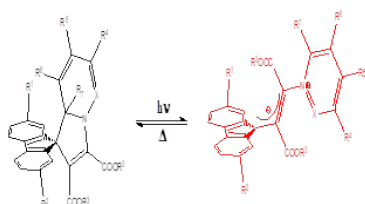


Figure 1: Photo-induced ring opening of the photochromic THI (closed form) to colored betaine (open form) based 1, 5-electrocyclization

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HYDRATED ELECTRON: CAVITY, NONCAVITY OR SOMETHING IN BETWEEN?

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Despite intense investigation, it is still unclear whether the structure of an excess electron in liquid water is best thought of as a quasi-halide ion, where most of the electron resides in a solvent cavity as a non-cavity object with many water molecules packed within the electron's wave function, or something in between. To address this question, we performed a series of mixed quantum/classical simulations with the goal of connecting the structure of simulated hydrated electrons with experiment. We find that traditional cavity models are unable to predict the temperature dependence of the hydrated electron's excited-state lifetime whereas a non-cavity model provides good qualitative agreement with experiment. Cavity models also fail to reproduce features of both static and time-resolved photoelectron spectroscopy (TRPES) experiments including the fact that hydrated electrons are not found near the air/water interface, that solvation dynamics lowers the excited-state energy prior to internal conversion and that solvation of the ground-state is significantly slower than the excited-state lifetime, features that are all well captured with a non-cavity model. We are able to rationalize these observations by comparing free energies of cavity and non-cavity model hydrated electrons. We find that cavity hydrated electrons behave effectively as hard spheres, with large free energy penalties for any incursion of water into the electron's interior. In contrast, there is only a small free energy penalty to remove water molecules from the interior of non-cavity electrons, so that non-cavity electrons have a highly fluxional structure that is non-cavity on average but vary continuously between cavity and non-cavity. The driving force for placing water molecules into the non-cavity electron's interior is entirely entropy-driven, so that non-cavity electrons become more cavity-like on average as the temperature decreases, explaining the experimentally-observed temperature dependence of the hydrated electron's transient absorption spectroscopy and various features of the TRPES experiments.

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NEW APPROACH TO NATURALLY FORM DESIGN NANOSTRUCTURED SEMICONDUCTOR BULK PN HOMOJUNCTIONS FOR OPTO-ELECTRONIC DEVICES

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Planar semiconductor pn junctions constitute an integral part of most optoelectronic devices; they generally require high quality expensive crystals. Bulk heterojunction (BHJ) configuration can circumvent cost, complexity, flexibility and scale-up challenges of conventional pn junctions. Current BHJ structures physically mix organic or inorganic colloidal materials, which invariably create interface mismatch and low doping issues. This paper introduces a radically different thermodynamically-driven, single-step electrodeposition approach; it naturally creates self-stabilized bulk homojunctions, exemplified here by two copper-indium-selenide (CISE) compounds. The resulting film comprises interconnected 3D network of highly-ordered, sharp, abrupt truly-nanoscale pn BHJs; these exhibit unusual electro-optical properties, long lifetime and quantum confinement effects. Unlike colloidal nanocrystals, the CISE nanocrystals are highly doped. Their ordered nanoscale morphology facilitates interpenetration for fast, efficient carrier separation and transport; minimizes recombination and essentially performs the same functions as the high-end, crystalline planar pn junctions. This totality manifests as a significant advance in electrochemical processing of semiconductors, it discloses a generally accessible, very low-cost platform method to create high quality nanocrystalline pn BHJ absorbers with various chalcogenides. These inorganic BHJs can be directly used in devices. With addition of finely band-aligned contact electrodes, these BHJs can transition into high performance devices for LED or solar photovoltaic devices or serve as photoelectrodes for fuel generation. Furthermore, they can be roll-to-roll processed in simple flexible thin-film form factor for easy scale-up.

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HOW TO DESIGN A BI-FUNCTIONAL MOLECULAR CATALYST FOR HYDROGEN PRODUCTION FROM METHANOL?

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We have studied the mechanism of hydrogen production from methanol by two different and well known ruthenium based molecular catalysts: Ru(trop)2dad complex and pincer supported Ru-PNP complex using density functional theory (DFT) in conjunction with *ab initio* molecular dynamics studies (AIMD) with explicit solvation. The results show that while methanol dehydrogenation occurs via a Noyori type (Ru-N) bi-functional mechanism by the Ru(trop)2dad catalyst, the RuPNP complex does not feature the commonly assumed (Ru-N) bifunctional mechanism under the applied reaction conditions. Ru(trop)2dad catalyst does not require any additive (base/Lewis acid) for activity while the RuPNP complex requires 8M KOH for optimal activity. Several other well-known molecular catalysts also require an additive (base/Lewis acid) for hydrogen production from methanol. Therefore, the mechanistic studies on Ru(trop)2dad and RuPNP systems, and the sharp contrast in their respective mechanistic pathways provide guidelines for rational design of additive free and highly active bi-functional catalysts for hydrogen production from methanol. Moreover, these case studies show the importance of an explicit consideration of solvent molecules for realistic computational modelling of minimum energy reaction pathway.

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BIOCOMPOSITE AND INNOVATIVE GREEN CHEMISTRY

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There is a variety of not exploited vegetable fibers in important quantities: palm tree, alfa, rafia, kenaf, etc. Actually, the use of these fibers is limited to the domestic use and paper-maker industry. The FIVBIOP project is an eco-design project which aims to develop a biopolymer composed of an organic thermoplastic matrix and alfa vegetable fibers. Our work is focused on the optimisation of the manufacturing process and the fibers treatment. Our objective is to reduce chemical treatment and use more physical one in order to improve mechanical characteristics. This project allowed the production of a new material with high properties. It associates innovation and sustainability; less waste; biodegradable; less resources depletion; cost reduction; social employment; partnership from Europe and North Africa; a good aspect; new markets: packaging, home and offices decoration; a patented solution; environmentally friendly. We will detail the development of this material and different steps of the project.

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THE POTENTIAL OF GARCINIA ATROVIRIDIS AS THERAPEUTIC AGENTS

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G*arcinia atroviridis* locally known as *asam gelugor* in Malaysia can be found wild in the forest of peninsular Malaysia. Traditionally, *G. atroviridis* has been used as a postpartum medication agent to treat earache, throat irritation, cough, dandruff and stomach ache. The essential oils from different plant parts of *G. atroviridis*, viz., fruit, stem bark and leaf were obtained by hydrodistillation. Analysis by gas chromatography and gas chromatography-mass spectrometry revealed the presence of sesquiterpenoids in the fruit and leaf oils while fatty acids was predominated in the stem bark oil. *In vitro* MTT assay on human breast cancer cells showed that the leaf oil induced anti-proliferative effects in a dose- and time-dependent manner. In a combination treatment with tamoxifen, the leaf oil induced more cell death than the treatment using the drug alone. Thus, there is a need to further explore *G. atroviridis* essential oils as this may lead to the discovery of potential chemotherapeutic agents.

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A COMPOSITE OF MnO_2 COATED WITH GRAPHENE BY GALVANOSTATIC ELECTRODEPOSITION AND ITS HIGHLY ACTIVE AND STABLE CATALYSIS FOR OXYGEN REDUCTION REACTION

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The development of efficient, low-cost and stable electrocatalysts as the alternative to platinum for the oxygen reduction reaction (ORR) plays key roles in several important energy storage and conversion technologies such as fuel cells, metal-air batteries. Manganese oxides (MnO_x) have been widely investigated as a promising non-precious catalyst for ORR because of its abundance, low cost, environmental friendliness. Nevertheless, the practical applications of these materials are greatly impeded by its lower energetic efficiencies which is primarily ascribed to their poor conductivity and relatively lower amount of catalytically active sites. Moreover, MnO_x catalysts are prone to aggregate in recycling use which may further decrease the ORR catalytic activity and stability. Herein, a composite consisting of spherical MnO_2 coated with reduced graphene oxide ($MnO_2@RGO$) has been prepared by step galvanostatic electrodeposition (Figure 1). Firstly, MnO_2 is deposited on the electrode surface by anodic galvanostatic method by the following process $Mn^{2+} + 2H_2O \rightarrow MnOOH + e^- + 3H^+ \rightarrow MnO_2 + 4H^+ + 2e^-$. And then a three-dimensional composite of reduced graphene oxide (RGO) coating MnO_2 is obtained through cathodic galvanostatic reduction of GO to RGO. The formed core-shell structure not only prevent graphene sheets from damage caused by pressure of MnO_x on the surface of graphene which may thereby maximizing the catalyst conductivity extremely, but also reduce the agglomeration of MnO_x particles. In addition, owing to the larger specific surface area of graphene on the outer layer and its stronger electron-donating ability than MnO_2 , the asprepared composite is easier to adsorb and activate O_2 . To the best of our knowledge, few research reports have been involved on the galvanostatic preparation of MnO_2 -graphene core-shell composite and its application for ORR hitherto.

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