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Abstracts

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# ADVANCED NANOTECHNOLOGY

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# GEOEXCHANGER SYSTEM FOR BUILDINGS HEATING AND COOLING

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**Geothermal heat pumps (GSHPs), or direct expansion (DX) ground source heat pumps, are a highly efficient renewable energy technology, which uses the earth, groundwater or surface water as a heat source when operating in heating mode or as a heat sink when operating in a cooling mode. It is receiving increasing interest because of its potential to decrease primary energy consumption and thus reduce emissions of the greenhouse gases (GHGs). The main concept of this technology is that it uses the lower temperature of the ground (approximately <32°C), which remains relatively stable throughout the year, to provide space heating, cooling and domestic hot water inside the building area. The main goal of this study was to stimulate the uptake of the GSHPs. Recent attempts to stimulate alternative energy sources for heating and cooling of buildings have emphasised the utilisation of the ambient energy from ground source and other renewable energy sources. The purpose of this study, however, was to examine the means of reducing of energy consumption in buildings, identifying GSHPs as an environmental friendly technology able to provide efficient utilisation of energy in the buildings sector, promoting the use of GSHPs applications as an optimum means of heating and cooling, and presenting typical applications and recent advances of the DX GSHPs. The study highlighted the potential energy saving that could be achieved through the use of ground energy sources. It also focused on the optimisation and improvement of the operation conditions of the heat cycle and performance of the DX GSHP. It is concluded that the direct expansion of the GSHP, combined with the ground heat exchanger in foundation piles and the seasonal thermal energy storage from solar thermal collectors, is extendable to more comprehensive applications.**

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# OPTOELECTRONIC, MAGNETIC AND STRUCTURAL PROPERTIES OF DOUBLE PEROVSKITE MATERIALS AFFECTING IN NANOTECHNOLOGY FIELD

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**In this paper, we have investigated the structural, electronic, magnetic and optical properties of cubic double perovskite $Sr_2CrZrO_6$ using the full-potential linearized augmented plane wave method (FP-LAPW), based on the density functional theory (DFT) as implemented in the WIEN2K code. The exchange correlation potentials is treated by the generalized gradient approximation (GGA), GGA+U where U is on-site coulomb interaction correction as well as modified Becke-Johnson (mBJ) which have been used to correct the potential. Calculations were performed with the Birch-Murnaghan approach to determine the equilibrium phase, lattice, bulk modulus and its pressure derivative. The results display a half-metallic ferromagnetic ground state for the cubic double perovskite $Sr_2CrZrO_6$ compound due to the strong correlation effect of transition metal Cr(3d-t2g) states with the integer value of the total magnetic moment. Furthermore, we found a direct gap (Γ-Γ) around the Fermi level, making this material $Sr_2CrZrO_6$ a competent candidate for optoelectronic and spintronic applications in the future of Nanotechnology.**

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# THE CONVERGENCE OF TECHNOLOGIES, GENERATES CONVERGENCE IN THE REGULATIONS

**Guillermo Valdes Mesa**
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The convergence of Nanotechnologies generates synergies among different technologies to say, nanotechnologies, neurotechnology, computers and biotechnology, these technologies must converge 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. Studying the global trend in this respect as imported for manufacturers medical devices worldwide. The convergences of technologies is 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 semiconductors 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, 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 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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# INTERFACIAL STRESSES IN EXTERNALLY FGM PLATED RC BEAMS

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**In this paper, an improved theoretical solution for interfacial stress analysis is presented for simply supported concrete beam bonded with a sandwich FGM plate. Interfacial stress analysis is presented for simply supported concrete beam bonded with a sandwich plate. This improved solution is intended for application to beams made of all kinds of materials bonded with a thin plate, while all existing solutions have been developed focusing on the strengthening of reinforced concrete beams, which allowed the omission of certain terms. It is shown that both the normal and shear stresses at the interface are influenced by the material and geometry parameters of the composite beam. A numerical parametric study was performed for different simulated cases to assess the effect of several parameters. Numerical comparisons between the existing solutions and the present new solution enable a clear appreciation of the effects of various parameters. The results of this study indicated that the FGM sandwich panel strengthening systems are effective in enhancing flexural behavior of the strengthened RC beams.**

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# A NONLOCAL TIMOSHENKO BEAM MODEL FOR FREE VIBRATION ANALYSIS OF CHIRAL SINGLE-WALLED CARBON NANOTUBES

**Tahar Hassaine Daouadji, Tayeb Bensattalah and Mohamed Zidour**
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**In this study, nonlocal Timoshenko beam theory has been implemented to investigate the free vibration response of chiral single-walled carbon nanotubes (SWCNTs). According to nonlocal Timoshenko vibration equation for SWCNTs, The analytical solution is derived and two solutions for vibration are obtained. Influence of nonlocal small-scale coefficient, the vibrational mode number, the chirality of carbon nanotube and aspect ratio of the (SWCNTs) on frequency of the SWCNTs are studied and discussed. The results indicate significant dependence of natural frequencies on the chirality of single-walled carbon nanotube with increase in the nonlocal small-scale coefficient, the vibrational mode number and the nanotube aspect ratio of length to diameter.**

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# NUMERICAL MODELLING ON NANO STRUCTURED COATING IN SUSPENSION PLASMA SPRAY

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**Suspension plasma spray is a promising technique for nano-structured coatings and nano-powder synthesis where nano-particles are injected into the plasma jet with the help of liquid precursors. When the particles fly through the plasma flame, their mass, momentum and energy will dramatically change due to the interaction with the flame. A comprehensive model was developed to investigate the suspension spraying in the radio frequency inductively coupled plasma torch. The model is based on hybrid Eulerian/Lagrangian coordinate system to illustrate the suspension behavior, such as suspension droplets collision, heating and evaporation; nano or agglomerate particles heating, melting and evaporation. Special considerations are directed to the suspension droplets collision, non-continuum effects and the influence of evaporation on heat transfer. After validation with experimental data, the comprehensive particle model is used to predict the trajectory, velocity, temperature and size of the in-flight nano- or agglomerate particles. A parametric analysis has been performed to find the way of controlling the operating conditions for desirable final particle status. The parameters that have a significant influence on the spray process are identified. The relationship between the predicted height of droplet complete evaporation and the droplet initial diameter is deduced. Finally, results also calculate the critical size of an ethanol droplet suspended with zirconia particles, which will be completely vaporized under present conditions.**

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# AB-INITIO STUDY OF STRUCTURAL, OPTOELECTRONIC AND MAGNETIC PROPERTIES OF CO2MNSI HEUSLER ALLOYS

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[2]University of Mascara, Algeria

**We performed first-principle calculations to investigate the structural, optoelectronic, and magnetic properties of Co2MnSi Heusler alloys using density functional theory based on full- potential linearized augmented plane wave (FP-LAPW) method. We employed three approaches LSDA, LSDA+U and Hybrid on-site exact exchange, where the Hubbard correction U is calculated by constraint LDA for Co and Mn. Our results showed the half- metallicity character with integral magnetic moment of 5μB, which agrees with the Slater- Pauling rule. Our findings suggest that these materials are potential candidates for manufacturing Spintronic devices and Nanotechnology.**

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# INFLUENCE OF THERMALLY INDUCED POLY TO SINGLE CRYSTALLINE STRUCTURAL PHASE TRANSITION ON PHOTOLUMINESCENCE AND OPTICAL ABSORPTION BEHAVIOR OF ZNO.78CD0.22S QUANTUM DOTS FOR PHOTO ELECTRONIC APPLICATIONS

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In this paper, we conduct a first trial to study the dependence of photoluminescence (PL) emission, and optical absorption edge of $Zn_{0.78}Cd_{0.22}S$ quantum dots on thermally induced - poly to single crystalline structural phase transition and morphological changes, along with excitation wavelength. It is found that, increasing annealing temperature (Ta) results in two structural phase transitions: firstly, from polycrystalline cubic to crystalline hexagonal $Zn_{0.78}Cd_{0.22}S$ structures at Ta 500°C, secondly, from polycrystalline cubic to single crystalline predominant ZnO hexagonal structure at 600°C, accompanied by an increase in XRD peaks intensity, sharpness, the crystallite size, the reduction of the internal local strain and the dislocation density, and consequently red shift of the optical gap. In addition, analysis of HRTEM images and SAED patterns, FTIR and Raman spectra indicates good agreement with XRD results. Moreover, the deconvoluted PL emission spectra at excitation wavelength 325 nm of the as-prepared and annealed nanoparticles up to 500°C demonstrate UV- blue emission bands at 362, 395, 443, and 523 nm, which quenched and red shifted to 402, 469, 509, 540 nm with increasing ex to 370 nm, along with the evolution of new emission bands at 594, 637, and 685 nm. In addition, the as-synthesized $Zn_{0.78}Cd_{0.22}S$ colloidal solution at ex of 325 nm reveals multiple broad emission bands associated with quenching and red shift in the PL intensity with increasing ex to 370 nm. Increasing Ta up to 500 oC at ex of 370 nm results in quenching and red shift of the overall PL spectra, whereas at ex of 325 nm, no change is observed. Moreover, $Zn_{0.78}Cd_{0.22}S$ nanopowder at either 600 or 700 oC at ex 370 nm reveal new and red shifted PL emission bands, along with a drastic increase in PL intensity by one order of magnitude higher than that observed at ex 325 nm. The unusual excitation wavelength dependent enhancement and blue shift of PL in $Zn_{0.78}Cd_{0.22}S$ nanopowder has demonstrated. Trapping and recombination radiative levels have been identified and the corresponding energy band diagrams are suggested.

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# MRI AND FLUORESCENT ACTIVE PLASMONIC NANOMATRYOSHKA

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**Engineering a compact, near-infrared plasmonic nanostructure with integrated image-enhancing agents for combined imaging and therapy is an important nanomedical challenge. To overcome this challenge we designed a nanostructure with NIR plasmonic signatures composed of a 50 nm Au core surrounded a SiO2 inner-shell doped with contrast agents and an outer Au shell. The plasmon resonance of this nanostructure, known as a nanomatryoshka (NM), can be tuned to the desired wavelength by varying the thickness of the layers. The encapsulated contrast agents used in this study are: Fe (III)-DOTA, Gd(III)-DOTA, and fluorescent dyes. The Fe (III)-NM based contrast agents are found to have relaxivities two times greater than the widely used Gd(III)-DOTA, providing a practical alternative for T1 MRI contrast agent that eliminates Gd(III) patient exposure entirely. Additionally, the internalization of fluorescent dyes and MRI contrast imaging agents within the NM substantially reduces the toxicity while maintaining a free nanoparticles surface for further bio-functionalization.**

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# NEW MAGNETIC NANOPARTICLE CATALYST FOR THE SYNTHESIS OF PHARMACEUTICALLY ACTIVE TETRAZOLOPYRIMIDINES

**Oleg M Demchuk[1], A Maleki[2], J Rahimi[2], A Z Wilczewska[3] and R Jasinski[4]**

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**Substituted pyrimidines are very important biologically and pharmaceutically active agents in the medicinal chemistry and drug discovery processes. A multicomponent reaction (MCRs) is ideal synthetic strategy to construct diverse molecular scaffolds of tetrazolopyrimidines starting from a few simple materials or intermediates. In connection with our continuous interest in designing new efficient and green protocols for synthesis of new biologically active compounds, we developed sonochemical approach for the one-pot four-component synthesis of 5-methyl-7-aryl-4,7-dihydrotetrazolo[1,5-a]pyrimidine-6-carboxylic esters, obtained in the reaction of 2-cyano-guanidine, sodium azide, various aromatic aldehydes and methyl or ethyl acetoacetates in the presence of a catalytic amount of new functionalized hybrid organic-inorganic nanoparticle magnetic metal oxide core–shell based [1] catalyst $Fe_2O_3$@$SiO_2$-$(CH_2)_3$NHC(O)$(CH_2)_2$PPh2.This is the first design, preparation, full characterization and application of the present nanomaterial and also the first ultrasound irradiated synthesis of the biologically and pharmaceutically important heterocyclic compounds in water used as a green solvent. The novel protocol offers several advantages such as high yields, short reaction times, mild reaction conditions, environment-friendly reaction media, easy isolation of the products, simple preparation and recoverability of the nanocatalyst by an external magnet and reusing several times without significant loss of activity. The details of our studies, which describe a scope and generality of the one-pot, simple and high atom economy strategy of synthesis of tetrazolopyrimidine derivatives with respect to various starting materials, will be presented.**

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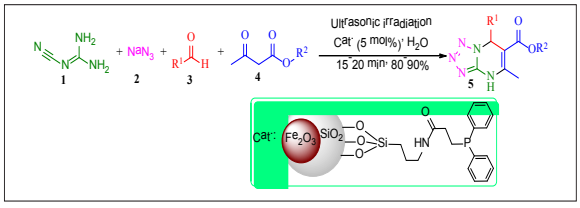


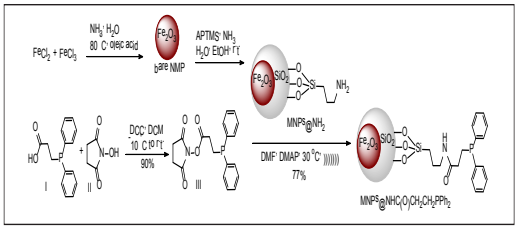

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# CONCENTRATION OF TITANIUM DIOXIDE (TIO2) FROM IRAQI SANDS OF AL-AMAJ REGION

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**TiO2 is one of very important oxides in ceramic industries, glass and glassed ceramic for its chemical, optical, thermal, electrical properties which made it the most common and widely used compound among other titanium compounds. Ores are considered as essential resources of the engineering materials. Generally decreasing of metals percentages in ores by the time has been noted in metallurgical industries. But modern progress of technical means maintains investment ability of the ore which was rather poor for an earlier period. The chemical analysis of Iraqi sand of Al Amaj region declares that it contains low grade of titanium dioxide and within 0.95% percentage. The analysis of volume fraction distribution of the sand indicates that it is fine sand and the larger fraction is with particle size less than 150 µm. TiO2 content distributed unregularly within the different particle volumes, and its larger fraction is concentrated in the fine volume fractions which are less than 150 µm. The concentration process by shaking table increased TiO2 percentage in the ore from 0.95% to 23% with recovery percentage of 72% when the solid fraction percentage is 20% and the feeding rate is 1 L/min. The magnetic separation processes of the concentrate that produced from the shaking table which accomplished by high intensity wet magnet lead to ilmenite with concentration of 57.8% and recovery of 83.8%. The parameters of this process are solid percentage of 20%, feeding rate of 1 L/min and magnetic force of 6.63 kjaws.**

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# NANOSENSORS: AN IMPROVED TOOL FOR EFFICIENT RESERVOIR CHARACTERIZATION AND OIL EXPLORATION

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**Nanosensors have recently attracted the oil and gas industries for acquiring a panoramic insight of the oil reservoirs. Such nanodevices are found to be advantageous as compared to the conventional mechanical, electrical and optical sensors used in reservoir characterisation and oil exploration. The indispensable need for developing sensing devices that work efficiently under high-pressure/high-temperature conditions of the reservoir has paved way for nanosensors. This new class of nanomaterials have overpowered the conventional sensing techniques. Conventional sensing techniques are incapable of acquiring data at a large distance from the injection point. Recent developments have shown that carbon and silicon based nanosensors can be used in reservoir characterization and hydrocarbon detection. Moreover nanosensors in combination with certain conventional monitoring systems are anticipated to substantially improve the imaging outcomes thereby assisting the oil and gas industries in tuning the oil recovery methods for profitable outputs. Nanosensors provide accurate 3D reservoir characterization and even slight improvement in the sensing capability of hydrocarbon detection and insitu chemical compostion will produce exponential benefits. This paper provides an overview of how nanosensors prove to be more efficient than the conventional sensing systems used for reservoir characterization and hydrocarbon detection by the oil and gas industries till now.**

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# DETERMINATION OF VERAPAMIL HCL IN PHARMACEUTICAL PREPARATIONS BY A FLUORESCENT NANO PROBE BASED ON CDTE/CDS/ZNS QUANTUM DOTS

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**Introduction:** This research was aimed to design a method to determine verapamil HCl in dosage forms by using CdTe/CdS/ZnS core-shell QDs as a fluorescent probe.

**Methods:** CdTe/CdS/ZnS quantum dots were prepared by one pot method and analyzed. An analytical technique based on fluorescence quenching of QDs was developed to quantify verapamil in commercially available preparations. Various reaction parameters were optimized and the method developed was validated. One way ANOVA and Post Hoc tests at 5% significance level, were performed to justify the significance of variation in observations.

**Results:** Linear range of the verapamil concentration was 0.25-5 µg/mL while limit of detection was 0.05µg/mL. Recovery and relative standard deviations were NMT±10% of the actual amount and <5.9%, respectively. Foreign materials, common metal ions and pharmaceutical excipients of dosage forms, had little interference. Verapamil content in the tablets and injections was NMT±10% of the stated amount and it conformed to the specifications of both the British Pharmacopoeia and the United States Pharmacopoeia. In case of statistical analysis, p-value was <0.05 in almost all levels of all parameters until the optimized level of system.

**Conclusions:** It can be concluded from the results that the method designed is simple, reliable, cost effective, selective, rapid and sensitive enough to be used for quantitative measurement of the verapamil HCl in dosage forms for quality control purposes.

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# NANOSCALED POLYSACCHARIDES IN SOLUTION: SCALING LAWS OF HYALURONAN

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Ionic polysaccharides (e.g. hyaluronan (HA)) are currently used in a range of sizes, or molar masses, in an increasing number of nanomaterials for biocompatible applications. The aim of this work is to predict the scaling law of HA, in aqueous salt solution, by applying simple and low-cost methods of green degradation and molar mass determination. In this respect, moderately concentrated solutions of native and different ultraviolet (UV) -degraded HA in NaCl aqueous solution were prepared. The corresponding molar masses were obtained via one-point method of viscosity measurements. It has been observed that the progress of molar mass production, via HA degradation, was UV-dose dependent. The graphical interpretation method of kinetic analysis confirmed the first order degradation rate, which is an indication of a random session on the glycosidic bonds. The viscosity data were treated via Flory-Fox's theory to get molecular parameters such as: the hydrodynamic radius (RH, η), radius of gyration (RG, η), coil density (Pcoin, η), critical concentration (C η*) and second virial coefficient (A2,η). It has been found that: RH, η and RG, η represents UV-dose decreases; while, Pcoin, η, C η* and A2,η represents UV-dose increases. The results were explained according to the influence of size and excluded-volume.

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# MORPHOLOGY/PERFORMANCE RELATIONSHIP OF POLYMER BASED NANOCOMPOSITE PIECES OBTAINED BY INJECTION MOLDING

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**Polymer nanocomposites are materials that have great potential in a variety of applications. By incorporating nanoscale particles of a filler material, the performance and properties of the bulk material can be drastically altered. Indeed, quite exceptional improvements can be achieved with small amounts of filler. To make nanocomposites economically viable, i.e. use them in massive applications, their production must use common processing equipment, and additional processing steps should be avoided. Many thermoplastic-composites are processed by an injection moulding process. It is generally accepted that the performance of polymer nanocomposites is intimately related to the degree of dispersion of the nanofiller: good dispersion and exfoliation may lead to the expected improvement in properties. This dispersion depends on factors such as the affinity and compatibility of the filler with the matrix, the matrix viscosity and the applied thermo-mechanical level, which depends on the processing conditions. The understanding of the fracture, microdeformation and mechanics of failure of nanocomposites is crucial for engineers. In this work the relationship between processing and performance is reviewed for different injected thermoplastic pieces. The combined effects of the moulding technique and the nano filler on the properties of the polymer composites are reported. Also, the effect of the occurrence of in-homogeneities, such as weld lines or flow lines in microstructure and therefore in performance are summarized.**

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