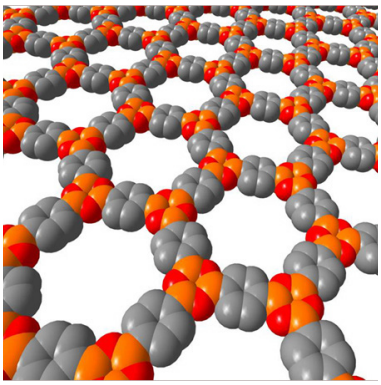
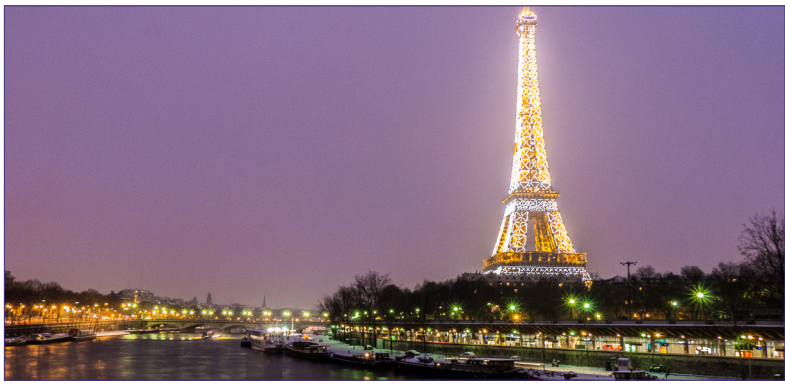
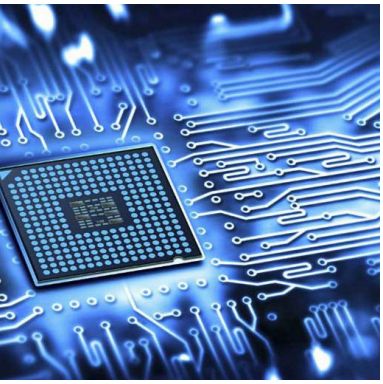
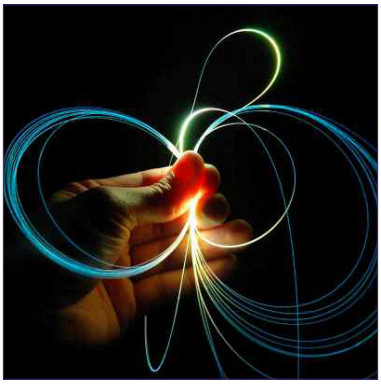
# Accepted Abstracts

## *Material Science 2019*


2nd International Conference on

# Materials Science and Engineering

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## Develop smart adaptable reinforced concrete slabs using iron based shape memory alloy

**Raafat El Hacha**
University of Calgary, Canada

In current design practice, structures are designed as passive structures. That is, they are designed to support the anticipated loads throughout their lifespan. This means, until the structure experiences the anticipated load, there is excess capacity. Smart structures are adaptive structures which have the ability to understand their condition or surroundings and react to changes in a beneficial manner using a sophisticated system of sensors, controllers and actuators. Compared to passive structures, smart structures are able to increase their capacity only when required, creating more efficient structures. Smart structures require a material that can change as required and shape memory alloy (SMA) is a potential candidate for this application. SMA has the ability to recover relatively large strains by either heating it (known as shape memory effect) or by releasing it after it's been loaded (known as pseudoelasticity). Originally discovered as a nickel-titanium (Ni-Ti) alloy in 1962; however, the special characteristics of SMA have recently been found in iron based alloys (Fe-SMA), which have significantly lower manufacturing costs than Ni-Ti making them suitable for the relatively larger structures prevalent in civil engineering. This research proposes to develop a smart concrete (RC) slab reinforced using SMA. The significance of smart slabs are that engineers can design more efficient and resilient structures. Currently, an inherent defect of RC slabs is their tendency to crack. Although it is possible to design RC structures that do not crack either with increased materials, material strength or by current prestressing techniques, this is highly impractical and results severely over designed structures. With smart slabs, the smart force can counteract loading throughout its lifespan and it would be possible to add smart force on demand before the concrete cracks. Uncracked concrete prevents moisture from contacting the internal reinforcement and is significantly more resilient to bending. The result could be more durable structures, less maintenance and strengthening and reduced need for expensive prestressing or strengthening operations potentially saving billions that would otherwise be used to repair or maintain the structure.

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## Rocking frame reinforced with superelastic Nickel-Titanium shape memory alloy

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Conventional seismic design systems rely on the inelastic behaviour of certain members to dissipate the seismic energy. This research takes a deeper look into retrofitting steel structures using the rocking structures method. This is an innovative technique where the designer is allowing for the structure to rock back and forth with the seismic loading, taking advantage of the weakening of the structure. Rocking columns reduce the strength of the structure causing it to yield sooner, thus reducing the maximum structural accelerations. However, though the maximum acceleration due to ground excitations is reduced, the rocking increases the inter-storey displacements. Shape Memory Alloys (SMA) has been attracting researchers from different fields, it is a unique class of alloy with the ability to undergo large deformations (up to 8%) and return to its original shape through stress removal. The main objective of this research is to investigate the effectiveness and feasibility of active techniques for seismic retrofitting of steel braced frames using the rocking structures combined with pseudoelastic (PE) nickel-titanium (Ni-Ti) SMA wires. To observe the behaviour of the retrofitted steel braced frame a free vibration test to determine the natural frequency of the system and a cyclic test were performed to demonstrate the effects of a rocking structure with PE Ni-Ti SMA wires to dissipate and recenter the structure when subject to an earthquake. The use of the rocking columns combined with the shape memory alloys proposed in this research not only controls where the damage occurs but limits it to be very insignificant, where no structural elements would need replacing. Results from the free vibrations test suggest that the stiffness of the system is dependent on the rigidity of the column-foundation connection than the rigidity of the cross bracing. The in-plane cyclic tests found that the Ni-Ti wires have significant pseudoelastic properties that had almost zero residual strain at 4% drift and the potential for moderate energy dissipation. Findings of this research are expected to add valuable knowledge to the field of seismic retrofitting of RC structures and widen the potential applications of the SMA in the structural engineering field.

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# The morphological evolution for composite urethane-based coating induced by photo-aging and the characterization of photo-product using FTIR-ATR and ToFSIMS

**Takato Ishida** and **Ryoma Kitagaki**
University of Tokyo, Japan

Durability is one of the most important aspects of industrial materials, and an organic-based coating is affected by outdoor conditions (e.g., ultraviolet (UV) light, heat (temperature), moisture (humidity)). Generally speaking, photodegradation is the most crucial for coating's weatherability, then, it also causes significant structural changes on exposure to UV irradiation, which causes deterioration in its physical and mechanical properties. Within degradation induced morphological changes, pore structure (including free volume) is well known as one of the most influential characteristics on macroscopic properties. Besides, regarding composite coatings (e.g., polymer matrix filled with titanium dioxide), they commonly have a layer concentrated low molecular weight component on the coating surface, this is called as 'clear layer'. The characteristics of such layer have a significant impact on surface properties. In heavily degraded case, the repairing by filling up coating binder component is one of the possible options for continuing using for degraded coatings, and then, we should choose the mending material based on the characteristics of the deteriorated coating surface. We have already found that the chemical character of surface layer should be changed depending on the degree of chain scission induced by UV irradiation, this might be because of the diffusion of low molecular weight photo-product toward the sample surface, driven by free energy gradient. Based on above consideration, in this paper, we will report the internal morphological change induced by photodegradation proved by solvent swelling behavior and the change of surface layer characteristics by using FTIR-ATR (Fourier transform infrared spectroscopy attenuated total reflection) and ToFSIMS (Time-of-Flight Secondary Ion Mass Spectrometry), moreover, their mechanisms will be discussed.

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## CVD diamond materials for high tech applications: Recent achievements and remaining challenges

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Diamond is an outstanding material that often exhibits unmatchable properties compared to other materials. Decades of research have enabled the (but not yet fully) growth understanding and coating of diamond in film form on various substrate materials. Plasma-Enhanced Chemical Vapor Deposition (PECVD) technique used to growth high quality diamond has been continuously improved over the years and allows today to address a wide range of applications based on the combination of unique and extreme properties of diamond and the variety of film properties obtainable through tuning the microstructure, morphology, impurities, and surfaces. This work introduces the latest research, recent applications, and the challenges ahead for CVD diamond films.

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## 2D semiconductor nanostructures at atomic scale

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Technology at the nanoscale has become one of the main challenges in science as new physical effects appear and can be modulated at will. Materials for spintronics, electronics, optoelectronics, chemical sensing, and new generations of functionalized materials are taking advantage of the low dimensionality, improving their properties and opening a new range of applications. As developments in materials science are pushing to the size limits of physics and chemistry, there is a critical need for understanding the origin of these unique physical properties (optical and electronic) and relate them to the changes originated at the atomic scale, e.g. linked to changes in (electronic) structure of the material. In this work, it has been demonstrated that how atomic resolution high angle annular dark field (HAADF) scanning transmission electron microscopy (STEM) can help to understand the growth mechanisms of complex 2D nanostructures such as nanomembranes, nanoflakes or nanobelts. The presentation will combine the visualization of 3D atomic models recreating the growth of these 2D nanostructures, as well as a direct correlation between their structure and chemical composition at the atomic scale, with their local properties at the nanoscale, electronic and photonic and how they can be arranged as perfect templates for quantum nanowire networks. In addition, this work shows the in-situ dynamic reconstruction processes of monolayer grain boundaries in $MoS_2$ at atomic scale under the electron beam as well as the sulfurization evolution that drive the transformation of a $MoO_2$ nanomembrane to a $MoS_2$ nanoflake.

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## Global optimization methods and techniques in Engineering design

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Traditional gradient based optimization methods and techniques are still most widely used tools in engineering design. However, the nature of the real world engineering design problems cannot be often well covered by traditional techniques due to precence of integer and discrete variables, a number of local extremes, multiple optimality criteria, etc. Global optimization methods (GOM) and techniques have property to escape the local extreme and have a better global perspective than the traditional gradient based methods. GOM allow to omit computing derivatives. The cost needed to pay for more powerfull methods is fact that the GOM manipulate with population instead of single solution leading to time consuming numerous evaluations of objective functions. Most commonly the meta-models are utilized for reducinhg computational cost. Continuous improvement of GOM methods and tools, One key issue is decomposition of complex engineering design problems into simpler sub-tasks leading as rule to reduction of complexity and computing time. In the current study are covered hierarchical multi-criteria optimization algorithms and procedures developed by workgroup for solving wide class of practical and theoretical engineering design problems like design of smart composites with structural health monitoring capabilities, design of a slotless permanent magnet generator for wind turbine, design of car frontal protection system, optimal material orientations problems for linear elastic 3D orthotropic materials, etc. These solutions are optimized taking account the features of particular problems, combining GOM tools (hybrid methods, etc.) , utilizing meta-modelling techniques (in most cases artifial neural networks).

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## Using computational simulations to support structural characterization of metals, alloys, and intermetallic compounds with solid-state NMR

**Ary R Ferreira**

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The use of solid-state nuclear magnetic resonance (ssNMR) spectroscopy in materials science has boomed in recent years. What makes it a new valuable tool for the development of the next generation of materials, providing new insights into atomic arrangement and electronic structure of solid samples. Naturally, there is no denying that this is mainly due to advances in ssNMR techniques and the high-resolution spectra that can be obtained nowadays. Nevertheless, one cannot rule out the important role of density functional theory (DFT) based computational simulations in that context. With a highlight to the gauge-including projector augmented-wave (GIPAW) method.

It is nothing new that the aid of DFT-GIPAW calculations may be crucial for unambiguous ssNMR peak assignments in a number of cases. Whether it is a matter of structural intricacy like static disorder, mixture of phases, or chemical exchange processes; or due to a combination of distinct magnetic screening mechanisms (MSMs) resulting from different aspects of the electron charge and spin densities around target nuclei. That combination of MSMs is precisely one of the biggest challenges in the interpretation of the spectra of materials in which, in the presence of the applied external magnetic field, electrons define the local environment of target nuclei behaving not only as moving charges, but also as particles with spin ½.

With a focus on the 27Al nuclide in weakly magnetic intermetallic compounds and in a bulk glass alloy, the aim of the current research is to show that DFT-GIPAW calculations of orbital and Fermi-contact shifts can not only promote a less unbiased interpretation of the respective ssNMR spectra, but also demonstrate the possibility of expanding out the applicability of that type of spectroscopy to a new class of materials.

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## Synthesis and electrochemical performances of polyanionic compounds for Na-ion batteries anodes

**Zeyu Wang, Yue Zhao** and **Zhuo Deng**
Soochow University, China

Polyanion compounds possess many advantages as Na-ion batteries anodes. For example, various crystal structures with open channels for Na-ions are available, and the polyanion compounds are believed to have high thermal stabilities due to strong covalent bonding of oxygen atom in the polyanion polyhedral. Furthermore, the reaction potentials of the compounds in the process of charging and discharging are influenced by the environment around the polyanion themselves, so we can adjust the structure of polyanion to change the reaction routes and improve the electrochemical performance. $Na_3V_2(PO_4)_3$ is a promising cathode material for Na-ion batteries due to the unique NASICON framework and excellent ionic conduction. On the other hand, the conductivity of $Na_3V_2(PO_4)_3$ is poor due to the presence of $PO_4^{3-}$, therefore many works were done to improve the electro chemical performance of materials through coating amorphous carbon layer on $Na_3V_2(PO_4)_3$ particles or synthesizing composite with conductive graphene and soon. This work aims to seek a simple and safe route to synthesis $Na_3V_2(PO_4)_3$/C composite and $NaVPO_4$ F/C composite by introducing the $F^-$ and to investigate their electrochemical performances.

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# Synthesis and controllable time and feed ratio of organic-inorganic hybrids with near infrared absorption for solar cells

**Nahla Omer, Fayin Zhang, Gang Zhao, Shanyi Guang** and **Hongyao Xu**
Donghua University, China

Nowadays organic dyes materials have been receiving more interested in solar cell due to improved solution process ability, scalable synthesis, tunable chemical and physical properties via molecular design and low cost. However, the compatibility and aggregation of squaraine dye limited broad application. In this study, we designed a system contend of octavinyl-polyhedral oligomeric silsesquioxane OV-POSS which used to solve these problems. These is the first time designed a novel hybrids large broad absorption visible to near infrared transient absorption spectroscopy, prepared by OV-POSS with 6-Bromoquanaldine and Squaric acid (semisquaraine (SSQ) squaraine (SQ)) H2 their light properties a broad spectral coverage in a big region from 400 to 800 nm. Our systems were characterized by Fourier Transform Infrared Spectroscopy FTIR, 1HNMR, UV-Vis-Spectra, Water contact angle images and FE-SEM properties, and when a combination our system dyes with N719 as co-sensitization in photovoltaic performance using Ti foil-based solar cell DSSC. From a solar simulator hence exhibited good performance in solar cell application.

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# Investigation of the electronic structures and photoelectrical properties of cyanoacrylic dye on $ZnTiO_3$ perovskite for dye-sensitized solar cells

**Ali Cheknane**[1] and **Kacem Cherifi**[2]

[1]Université Amar Telidji de Laghouat, Algeria

[2]University of Tlemcen, Algeria

The aggregation of sensitizers on a semiconductor is crucial for determining the light-harvesting efficiency of dye sensitized solar cells (DSSCs). The interfacial properties of dyes adsorbed on a $ZnTiO_4$ film, such as adsorption configurations and adsorption energy, can impact the total amount of dye sensitizers that loads and the stability of a DSSC device.

In this work $ZnTiO_3$ perovskite was selected as a photoanode for DSSC. First principal calculation study based on the DFT method has been used to study the adsorption energy of the Cyanoacrylic dye onto $ZnTiO_3$ (101) and (110) surfaces. The electronic structures and photoelectrical properties of cyanoacrylic at $ZnTiO_3$ complex are performed using the generalized gradient approximation approach (GGA-PBE), in order to treat the vend-wells interaction, DFT-D approach was applied in CASTEP code.

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## An integrated application of natural geomaterials for heavy metals removal in aqueous system

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The present work has been conducted to evaluate the potential application of natural geomaterials, from Tunisia, in removing toxic metals from aqueous solutions in mono- and multiple-elements systems. Adsorption experiments were performed using batch sorption methodology as an appropriate technique in the current study. The chemical and mineralogical characterizations showed that limestone samples from southern Tunisia contained up to 99.6% calcium carbonate with small amounts of clay minerals, including smectite, kaolinite and illite. The characterization of the collected samples allowed the selection of the most auspicious sites that could be excavated for use as adsorbent. We examined the effects of impurities in limestone on its capacity to retain several selected heavy metals. The experimental data showed highly efficient materials in the removal of heavy metals (Pb, Cd, Cu and Zn). Kinetic data demonstrated a high degree of fitness to the pseudo-second order and intra-particle diffusion models. The selectivity sequence of the studied metal was Pb(II) > Cu(II) > Zn(II) ≈ Cd(II) in single and mixed systems. The applicability of Tunisian natural clays, from Gabes and Gafsa areas, in the removal of several metal ions was also evaluated. Mineralogical and spectroscopic characterizations indicated that the clay of Gabes area was mainly montmorillonite whereas the sample collected from Gafsa district contained high amount of carbonates. From the adsorption studies, it was concluded that both smectitic and calcareous clays could be used for the removal of several metal cations in aqueous systems. The sequence of heavy metals adsorption in single and multi-element systems onto the studied clays was: Pb(II) > Cu(II) > Zn(II) > Cd(II). In the mixed systems, the adsorption capacity decreased for each metal due to the competitive effect. Such findings are contingent upon some physical properties of the studied metals (i.e., relative binding strength, hydrated radius, electronegativity and hydrolysis constant).

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## Advanced composites in defence and space industries

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This review aims to summarize the available and promising applications of advanced composites structures in defence and space industries. Advanced composite materials and especially nanocomposites being multi-functional, which can have enhanced mechanical, thermal and electrical properties all at once thanks to recent research on nano additives. Multi functional materials bring added advantages other than their well known low structural weight thus they are further attractive in applications where weight and functional properties are critical. Structural health monitoring and self healing/reparing technologies involving nano composites are adapted to many parts which have long service life and damage problems under severe environments. Therefore, several sectors such as defence, aerospace, and transportation accelerated their research on advanced composite materials. This effort led to increased industrial applications which in turn gave rise to several startling side effects such as effects on occupational health and safety. Use of nano particles in industrial environments require special caution especially in case of long term exposure due to their unique properties.

In this review, the influence of nano particles such as carbon nanotubes, graphenes and nanosilica on the properties of composites, nanocomposite production methods, difficulties in integration into conventional and advanced composite production techniques will be discussed. The main focus will be on promising applications in defence and space industries will be discussed.

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## Stress effects on structural, elastic and electronic properties of bulk $MoS_2$

**Chorfi H[1,2], Salvado M A[1], Franco R[1], Fahima B[2]** and **Recio J M[1]**

[1]University of Oviedo, Spain

[2]University of Constantine, Algeria

The stability limit of crystalline $MX_2$ laminar materials under variable stress conditions is of capital interest for their technological applications. Quantum-mechanical simulations can provide useful and accurate information on this limit. In this contribution we perform first-principles density functional theory calculations to quantitatively evaluate the behavior of bulk molybdenum disulfide under general stress conditions. We show the anisotropy of the crystalline structure along principal crystallographic directions and the Van Der Walls nature of the inter-layer forces, we determine a complete, consistent set of accurate values for lattice and elastic constants. We also elucidate the change in material properties that occur when hydrostatic pressure (HP), normal compression (NC), biaxial tensile (BT) and biaxial compression (BC) are applied. The compression ratio, the transition from semiconductor to semi metal, the pressure dependence of the elastic constants and the nature (direct versus indirect) of the band gap are discussed. Deformation potentials that quantify these changes are reported. The good agreement with experiments for small strain validates our methodology and our calculated values.

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## Statistical analysis of fatigue test in jute reinforced polyester composites using Weibull distribution

**Djeghader D**
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In this research, the unsaturated polyester resin (polylite 420-852) is used in combination with bidirectional jute fiber to generate composites materials by a contact molding technique. The parameter which was carried out on the prepared samples was impact test to plot the S-N curve, which is based on Wöhler equation. Two-parameter Weibull probability was used for analysis statistically the fatigue life results of composite jute/polyester samples. Weibull graphic was plotted for each loading level using fatigue data. Then, S–N curves were drawn for different reliability levels (Ps=99%, Ps=90%, Ps=50%, Ps=36.8% and Ps=10%) using Weibull data. These S-N curves were introduced to the identification of the first failure time as reliability and safety limits of the material.

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## Making non-fired brick using induction furnace and electric arc furnace steel slag

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Slag is a major waste product in steel industries. It is considered as hazardous waste that requires a large place for dumping. Induction furnace slag and electric arc furnace slag were used in this study for making bricks. Cement, lime, gypsum and water were used along with the crushed dried slag for making the bricks. Without firing, they were produced only by applying forming pressure of 1000 psi, 2000 psi and 3000 psi and cured under water for different time period of 7 days, 14 days and 28 days. Also the slag percentage was varied to 0%, 10%, 25% and 50%. Their compressive strength, water absorption, porosity and density were measured. The compressive strength of different compositions showed ten to twelve times higher result compared to the conventional burnt clay bricks. In comparison, electric arc furnace slag bricks revealed higher compressive strength than the induction furnace slag bricks. Water absorption percentage was also very low compared to conventional clay bricks. They showed results with high density with low porosity. Our main purpose in this research was to prevent environment pollution and utilize a waste product as a recycling element.

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## Synthesis of $Mg_2Si$ magnesium matrix in-situ composites

**Asrafuzzaman** and **K M Shorowordi**
Bangladesh University of Engineering and Technology, Bangladesh

During the past decade, considerable research effort has been directed towards the development of in-situ metal matrix composites (MMCs), especially in Magnesium Metal Matrix Composites in which the reinforcements are formed in-situ by exothermal reactions between elements or between elements and compounds. SiC can be used as a reinforcement which takes part in in-situ reaction with Magnesium. The main objective of this experiment was to produce magnesium silicide ($Mg_2Si$) since this gives better microstructural and mechanical properties than the magnesium alloy itself. For better results, SiC was heat treated at different temperatures for a different amount of times to remove any contaminations on the SiC particles and make the surface properly active. SiC mixed with pure magnesium chips and magnesium alloy blocks and heated in the furnace with argon gas to prevent oxidation of the magnesium. Heating of the mixture was done at different temperatures for different time periods. Among the trials, pure Mg and Mg alloy combined with SiC produced mentionable result at 900˚C for 1 hour time period.

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## Comparison of corrosion behavior and effects of corrosion on TMT and 60 grade steel bars

**Kazi Faiza Amin** and **Humayra Bushra**
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Steel reinforcement bars are used extensively in construction industries. Bars used in underwater or marine structures are subjected to corrosion which can change the properties of the reinforcement over time. Thermo-Mechanically Treated (TMT) bars have gained popularity in the recent decades in construction industries. Corrosion behavior of the TMT steel bars and 60 grade steel bars were studied by accelerated corrosion test by impressing a DC voltage between steel bars (anode) and Stainless Steel plates (cathodes) in a 5% NaCl bath for specific time periods ranging from 10 minutes to 40 minutes at an interval of 10 minutes and one at 135 minutes. The samples were tested to determine the effect of corrosion time on weight loss, corrosion rate, mechanical properties, fracture mode and microstructure. Both types of steel exhibited decreasing corrosion rate with time but the TMT steel exhibited a greater weight loss and corrosion rate than the 60 grade steel. TMT steel lost a significant amount of the outer case with increased corrosion time. The microstructures of both of the steels were unchanged after corrosion. The effects on the mechanical properties and fracture mode were not significant at such corrosion time. Corrosion tests with longer time duration are needed to observe the effects on the mechanical properties

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# One simple and facile synthesis of different phase of vanadium di-oxide ($VO_2$) via hydrothermal route

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Among all these vanadium dioxide phases, $VO_2$ (B) and $VO_2$ (M) are especially interesting due to their layered structure, good energy capacity with high potential and promising applications in the field of energy conversion. $VO_2$ (B) is used as cathode material for Li-ion batteries, it is also used as precursor for the synthesis of $VO_2$ (M/R). $VO_2$ (M) is useful as a coating on smart windows, electrical and optical switching devices etc. In the past few decades, a lot of research work has been done in the area of synthesis of $VO_2$ (B) and $VO_2$ (M). But the synthesis of $VO_2$ (M) in a single step without doping is still rare. Here, we have reported the successful facile synthesis of $VO_2$ (B) and $VO_2$ (M) in one step by hydrothermal method.

**Methods:** The different phase of $VO_2$ has been synthesized by varying molar ratio of reducing agent (citric acid monohydrate, $C_6H_8O_7.H_2O$) to vanadium source (vanadium (V) oxide, $V_2O_5$) at an autoclave temperature of 230°C for 24hr by hydrothermal method. Six samples were synthesized with corresponding variation in molar ratio of vanadium (V) oxide to citric acid monohydrate as 1:1, 1:1.5, 1:2, 1:3, 1:4, 1:5 respectively.

**Results:** The synthesized nanoparticles were characterized by XRD for phase identification and comparison done with simulation also. SEM and TEM were performed for morphology and, UV-Vis and FTIR for other physico-chemical information. Electrical conductivity studies were carried out against temperature, and thermal properties were measured using a STA. Single phase $VO_2$ (B), $VO_2$ (M) and amorphous $VO_2$ can be synthesized by the mere variation of reducing agent relative concentrations.

**Conclusion:** A simple, one-step procedure is sufficient to produce pure phases without the use of inert environment or post-synthesis heat treatments. In addition, the crystal size mode is found to be sub-10 nm

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