



21st International Conference on

Advanced Energy Materials and Research

July 11-12, 2019 | Zurich, Switzerland

Posters

Advanced Energy Materials 2019

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Attempt to repair sanitary ware pieces by laser technology

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Traditionally, ceramic companies are completely re-fired with the ceramic pieces in order to correct small defects with few square millimetres, in sanitary ware pieces. This process represents high energy consumption, increasing the cost production. This work presents an attempt to solve this problem using a CO₂ laser technology to repair those defects, preventing the extra costs associated with a re-firing. Until now several approaches had been done using laser technology to solve the problem without success. Despite the method shows promising results, all situation led to the development of a circular crack around the defect, due to the elevated thermal gradients caused by laser radiation. A new approach was done using new materials based on sol-gel technique to fill out the cracks after laser treatment. The idea is the use of sol-gel based material and the re-firing post laser processing at lower temperature and time in order to confer the aesthetic aspect required for the commercialization of the pieces.

Recent Publications

1. K. Osvay, I. Képiró, and O. Berkesi, "Laser treatment of white China surface," *Appl. Surf. Sci.*, 2006.
2. S. Rodríguez-López, R. Comesaña, J. del Val, A. Durán, V. M. Justo, F. C. Serbena, and M. J. Pascual, "Laser cladding of glass-ceramic sealants for SOFC," *J. Eur. Ceram. Soc.*, vol. 35, no. 16, pp. 4475–4484, Dec. 2015.
3. N. B. Dahotre and S. P. Harimkar, *Laser Fabrication and Machining of Materials*. Springer, 2008.
4. J. D. Majumdar and I. Manna, *Laser-Assisted Fabrication of Materials*. 2012.
5. X. Li, J. Wang, L. L. Shaw, and T. B. Cameron, "Laser densification of extruded dental porcelain bodies in multi-material laser densification process," *Rapid Prototyp. J.*, vol. 11, no. 1, pp. 52–58, 2005.
6. N. Basile, M. Gonon, F. Petit, and F. Cambier, "Processing of a glass ceramic surface by selective focused beam laser treatment," *Ceram. Int.*, 2016.

Biography

N M Ferreira is a PhD in Physics Engineering; currently is a Researcher at i3N, Physics Department at University of Aveiro, Portugal. He had participated in several R&D projects on Material Science. He have experience as researcher in study and development of ceramics-based materials, prepared through conventional methods by melting, solid stated, with particular focus on laser processing (crystal growth – LFZ and surface sintering/modification). Present sample characterization skills include various techniques such as, electrical conductivity and magnetic properties of various oxide materials. Current focus materials are thermoelectrics, ferroelectrics and glass matrices doped with transition metals and rare earth for energy storage and conversion applications. Main expertise is related to structural, magnetic and electrical properties of materials prepared by laser processing.

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Influence of aged sol and annealing temperature on the physical properties of super-hydrophobic TiO₂ thin films

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TiO₂ thin films have a variety of applications, including electro-chromic displays, dye-sensitized solar cells, gas sensors, antireflection films, planar wave guides and optical filters. It also has environmental applications, being extensively used in the photo degradation of organic and inorganic pollutants, photovoltaic energy production and the production of hydrogen by water photo splitting. TiO₂ is currently the leading photocatalyst because it can mineralize a large range of organic pollutants. However, owing to its large band gap energy (typically <380 nm), TiO₂ can only absorb ultraviolet light but not visible light, which constitutes a proportion of solar light. The overall quantum yield rate can be influenced by the low rate of electron transfer to dissolved oxygen and a high rate of recombination between electron-hole pairs. The preparation of TiO₂ thin films has received great attention because of its remarkable optical, photocatalytic and electrical properties. TiO₂ thin films have been prepared by several techniques. In general, sol-gel methods are more flexible and offer many advantages. In this study, TiO₂ thin films were prepared by the sol-gel method using the spin-coating technique because, nanocrystalline materials have tremendous impact on various recent developments in industry and science. The annealing temperature plays an important role during the crystalline process. The influence of the aged sol and annealing temperature on the physical properties of TiO₂ thin films were investigated in this study.

Recent Publications

1. Su-Shia Lin, Chung-Sheng Liao, Sheng-You Fan, (2015), "Effects of substrate temperature on properties of HfO₂, Al and HfO₂:W films", *Surface & Coatings Technology*, 271:269-275.
2. Su-Shia Lin, Yung-Shiang Tsai, Kai-Ren Bai, (2016), "Structural and physical properties of tin oxide thin films for optoelectronic applications", *Applied Surface Science*, 380:203-209.
3. Su-Shia Lin, Chung-Sheng Liao, (2016), "Effects of the ratio of O₂/Ar pressure on wettability and optical properties of HfO₂ films before and after doping with Al", *Applied Surface Science*, 380:229-236.
4. Su-Shia Lin, Sheng-You Fan, Yung-Shiang Tsai, (2017), "Effects of annealing on wettability and physical properties of SnO thin films deposited at low RF power densities", *Ceramics International*, 43:1802-1808.
5. Su-Shia Lin, Chung-Kai Peng, Cho-Wei Li, (2019), "Wettability and optical properties of SnO-SnO₂-Sb₂O₃ thin films deposited by simultaneous RF and DC magnetron sputtering", *Journal of Alloys and Compounds*, 770:433-440.

Biography

Su-Shia Lin is Professor at Department of Applied Materials and Optoelectronic Engineering, National Chi Nan University, Taiwan. She has some research experiences in materials science. Her research work mainly focuses on electrical and optical films, optical memory and optical data storage, nanometer materials and optical design.

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Hurricane wave energy harvesting

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Global warming has triggered changes in the climate that have led to hurricanes becoming stronger and more frequent in recent years. In the past few decades, the frequency of category 4 and 5 hurricanes has increased and this trend is predicted to continue into the future. Hydrokinetic conversion devices (HCDs), which harness energy from water flow, are an already established technology, with several prototypes deployed around the world. However, these devices have a rated working velocity of only 1.5-3.0 m/s, whereas in a category 5 hurricane, wave speeds of up to 28 m/s are possible, which would render HCDs useless and even may sweep them on shore. Therefore, a novel approach to hydrokinetic conversion that offers both a sturdy design and has rated velocities to match hurricane wave speeds is required. However, energy harvesting from hurricane waves is still relatively a nascent technology and needs to be developed further in order to be implemented commercially. This project's objective is to explore the available technology options for harvesting energy from hurricane waves. If a suitable device can be designed, the enormous energy of storm waves crashing on to hurricane infested coastlines can be converted to electricity to be supplied to regions suffering from power outage as an aftermath of the hurricane. We have proposed two designs for achieving such ends. The first device uses a moving plate and bellows system attached with a hydro-power loop situated behind a seawall, which could be scaled up to become a stationary power generation system. The second design involves a composite seawall embedded with piezoelectric plates to produce electrical energy from the impact force of hurricane waves.

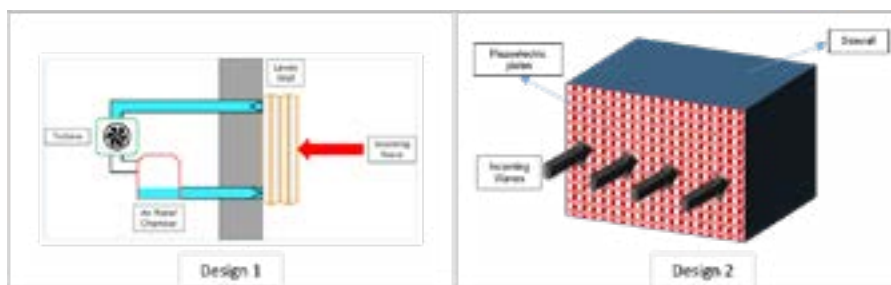


Figure: Designs proposed for harvesting energy from hurricane waves.

Biography

Mahpara Habib is a student under Dr Katherine Hornbostel's supervision at the Mechanical Engineering and Materials Science Department at the University of Pittsburgh. She is dedicated to developing materials that can harness energy from natural disasters and convert it into useful energy. At the present time, her work is focused on piezoelectric materials that can be utilized to capture energy from hurricane waves.

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Nitrogen free oxygen doped carbon nanotubes for oxygen reduction reaction

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Oxygen reduction reaction (ORR) is pivotal in renewable energy technologies such as in fuel cells and metal-air batteries. ORR is most fundamental and an important cathodic reaction of the electrochemical fuel cell. However, owing to its sluggish nature at the cathode side of proton exchange membrane fuel cell (PEMFC), there is an urgent demand for a cost-effective efficient catalyst with fast ORR kinetics. Though in practice, Pt-based electrodes and N-doped carbon material shows promising ORR activity, the durability, cost and their preparation methods restricts their wide commercialization. To address this issue, we developed metal and nitrogen-free carbon nanotubes (CNTs) through simple and mild plasma treatment. Oxygen plasma treated CNTs were used as a model for comparative study of oxygen reduction on single (SWCNT) and multi-walled nanotubes (MWCNT). Cold oxygen plasma surface modification leads to chemical doping of oxygen functionalities into the sp² carbon structure of the CNTs, charge redistribution around the doped heteroatom oxygen that promotes ORR activity. The defect sites generated owing to oxygen dopant in CNTs was confirmed by Raman spectra and X-ray photoelectron spectroscopy (XPS) surface composition. Hence, the results indicate that plasma treated SWCNT are more effective ORR catalyst compared to MWCNT due to the inherent structure of SWCNT that can access more defects and surface functional groups than MWCNT. Interestingly, for the first time we explored the comparison of oxygen functional group doped and defect induced SWCNT and MWCNT for ORR activity. Therefore, the catalytic property is dependent on the dopant (oxygenated) concentration at the wall and is related to the increase in defects as well as ORR current. The intriguing wall structure of SWCNT permits high functionality in oxygenated species and reinforce superior stability in ORR than MWCNT.

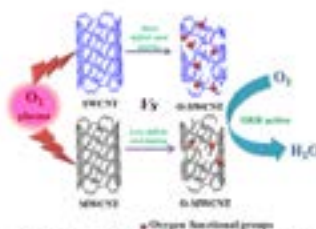


Figure 1: Low temperature oxygen plasma treatment on SWCNT and MWCNT as an active ORR electrocatalyst

Recent Publications

1. Subramanian P, Mohan R, Schechter A (2017) Unraveling the Oxygen-reduction sites in Graphitic-carbon Co-N-C Type Electrocatalyst Prepared by Single-Precursor Pyrolysis, ChemCatChem 9:1969-1978

Biography

Roopathy Mohan has pursued her Master's Degree in Chemistry from National Institute of Technology Tiruchirappalli, India. Currently, she is a Doctoral student in Fuel cell and Electrochemistry group, Ariel University, Israel under the supervision of Prof Alex Schechter. Her research work mainly focuses on the study of carbon-based oxygen reduction electrocatalysts treated by cold plasma. She has her expertise in designing plasma assisted carbon supported metal free and metal nitrogen and carbon (MNC) catalysts for electrochemical oxygen reduction reaction.

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High surface area carbon supported PtPdSn for methyl formate, methanol and formic acid oxidation

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Ariel University, Israel

Proton exchange membrane fuel cells have been investigated as an alternative power source for portable electronic devices and electric vehicles utilizing mainly hydrogen or small organic molecules (SOM) as fuel source and oxygen from air as an oxidant, at the anode and cathode respectively. The advantages of this type of fuel cells are high energy conversion efficiency directly to electricity and low operation temperatures. The slow kinetics of fuel oxidation (i.e. methanol, ethanol etc.) is the major obstacle for the commercialization of fuel cell technology based on these fuels, in addition to the high price of Pt and Pd based catalyst typically used in the anode. An addition of oxophilic second or third atom, such as Ru, Sn, Ni, etc., to Pt or Pd improves the catalytic activity and tolerance towards the presence of poisoning species during the oxidation of SOM. Carbon materials are commonly used as support materials due to their good electronic conductivity and high specific surface area that influences the properties of the catalyst, such as, charge transfer and improved dispersity of the catalyst particles. This leads to the increase in the utilization of the precious metal constituent. Ternary catalyst ($Pt_3Pd_3Sn_2$) supported on different carbon materials with different surface area (Vulcan CX72, Multi Walled Carbon Nanotubes and Black Pearl 2000 carbon) have been studied for electro-oxidation of methanol, formic acid and methyl formate. The electrochemical result shows that the MWCNT supported PtPdSn catalyst exhibits higher electro-oxidation current of methanol, methyl formate and formic acid compared to PtPdSn/XC72 and PtPdSn/BP2000.

Biography

Svetlana Lyssenko is a Master student in Fuel cell and Electrochemistry group, Ariel University, Israel under the supervision of Prof Alex Schechter. The key findings of her research work are to study the high surface area carbon supported platinum-based anode catalysts for methanol, methyl formate and formic acid electrooxidation for fuel cell applications.

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Natural plants: An efficient inhibitors of mild steel corrosion in H₂SO₄ acid

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The effect of aqueous extract of three natural plants called: *Tribulus Terrestris* (TTAE) (Inh. 1), *Vachellia Nilotica* (VNAE) (Inh. 2) and *Cymbopogon Schoenanthus* (CSAE) (Inh. 3) as inhibitors of mild steel corrosion in 1.0N H₂SO₄ acid solution at 30°C was investigated using weight loss (WL), electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization (PDP). The results showed that the three inhibitors worked well to inhibit the corrosion of mild steel in 1.0N H₂SO₄ acid, depending on the following order: TTAE> VNAE>CSAE. The addition of increasing amount of the studied inhibitors inhibit the corrosion rate of mild steel and maximum inhibition efficiency of 91.37%, 88.51%, and 87.14% respectively was obtained at 2.0 g/L⁻¹. Different adsorption isotherm models were tested and Langmuir adsorption isotherm showed best fit with the parameters. The inhibition mechanism was discussed based on adsorption on mild steel surface from 1.0N H₂SO₄ acid solution. The analysis of FTIR spectra established the formation of a strong bond between inhibitors species and mild steel surface.

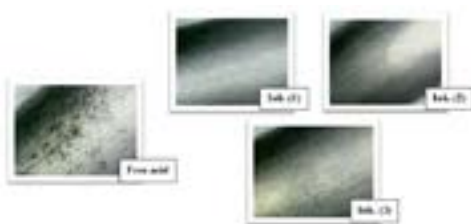


Figure 1: Macroscopic images for mild steel specimen in the absence and presence of the studied inhibitors.



Figure 2: Laboratory procedures for the preparation of the studied inhibitors

Recent Publications

1. Aisha H Al-Moubaraki, Aisha A Al-Howiti, Mervat M Al-Dailami and Enas A Al-Ghamdi (2017) Role of aqueous extract of celery (*Apium graveolens* L.) seeds against the corrosion of aluminium/sodium hydroxide systems. *Journal of Environmental Chemical Engineering* 5:4194-4205.
2. Aisha H Al-Moubaraki and Hind H Al-Rushud (2017) Anticorrosive effects of leek seeds aqueous extract (*Allium ampeloprasum* Var. *Kurrat*) on aluminum alloys 6061, 7075 and 2024 in Seawater. *Organic and Medicinal Chemistry International Journal* 3(5):1-10.
3. Aisha H Al-Moubaraki (2018) Potential of borage flowers aqueous extract, *Borago officinalis* L., against the corrosion of mild steel in phosphoric acid. *Anti-Corrosion Methods and Materials* 65:53-65.
4. Aisha H Al-Moubaraki and Hind H Al-Rushud (2018) The red sea as a corrosive environment: corrosion rates and corrosion mechanism of aluminum alloys 7075, 2024, and 6061. *International Journal of Corrosion* 1-15.

5. Ehteram A Noor, Aisha H Al-Moubaraki and Azza A Al-Ghamdi (2019) Continuous studies on using camel's urine as nontoxic corrosion inhibitor–corrosion inhibition of Al–Cu alloy in alkaline solutions. *Arabian Journal for Science and Engineering* 44(1): 237-250

Biography

Aisha H Al-Moubaraki is an Associate Professor of Physical Chemistry at University of Jeddah KSA. Her research interest are in corrosion behavior of metals in aqueous solutions-kinetic and thermodynamic studies; corrosion inhibition of metals in aqueous solutions by some organic and natural inhibitors and corrosion behavior of metals in natural environments such as soils and seawater.

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Accepted Abstracts

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Novel heterostructured nanoporous silicon (HNPS) anode for lithium ion battery: Economic prudence, system demonstration and first principle insights

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Ultra-mobile modern day lifestyle is critically powered by lithium ion battery (LIB). Since its discovery, it has come a long way to revolutionize our society and redefine our civilization. It also has huge role to play in replacing gasoline powered cars by electric cars and thereby reduce carbon foot print significantly and address a very serious global concern. At this point, one can embark onto a completely new set of technology, for example, a metal-air battery, which holds tremendous future potential but comes with serious technical challenges. However, it will be more prudent both technically and economically to realize the full theoretical potential of LIB (we are nowhere close there yet), before we change the bandwagon. Let us illustrate: pure lithium thus far could not be used as cathode in LIB and silicon, which has long been predicted to be the best element as anode material, from a pool of candidate elements spanning the entire periodic table, could not be used. Each silicon atom can theoretically hold on up to four lithium atoms in contrast to 1/6th in case of graphite, another commercially popular anode material. In this study, we focus on anode and demonstrate that how the major problems in realization of silicon anode (volume expansion and kinetic sluggishness) can be resolved by using our novel heterostructured nanoporous silicon (HNPS). We will discuss the protocol to obtain this novel HNPS from a low grade source material and compliment the understanding by first principal studies proving both thermodynamic and kinetic insights. We demonstrate lithium ion half-cell performance using HNPS. We further demonstrate the economic prudence (cost reduction by an order of magnitude) in adopting this technology commercially by comparing to a latest-model Tesla® car as a reference point.

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Photoluminescence studies of silica stabilized zirconia after CO₂ laser annealing for high temperature applications

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Laser annealing has attracted considerable attention due to its localized interaction with the treated sample and its possibility to achieve low manufacturing costs in materials processing. One of the most used sources for laser annealing is the CO₂ laser. In this research we used this type of laser for the annealing process of silica stabilized zirconia at different laser power. The effects of the annealing process and its dependence with laser annealing power were analyzed by the photoluminescence response at room temperature and with an excitation line on 488 nm. The optical response of samples annealed at different laser power is an intense double emission band centered on 694 nm, with a lower band at slightly higher wavelengths. The structure analysis by XRD shows the existence of crystalline structure at the annealed samples. The mentioned oxides alloy is a good candidate for high temperature applications.

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Architecture and interface design for ultrahigh conductivity of graphene/copper composites

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Achieving electrical conductivity to a level higher than the ultra-high conductivity of the internationally annealed copper standard (100% IACS) is the development required for copper based conductor materials for cutting-edge manufacturing and high-tech advancement. At present, the conventional refining and single-crystallization methods for improving the conductivity of metals are close to the physical limit, and the limited conductivity of materials also requires a high cost. The composite route of introducing high conductivity enhancer into the metal matrix is one of the effective ways to overcome the physical bottleneck of the conductor preparation and realize the ultra-high conductivity of the material. However, in practical preparation, it still faces the difficulty of purifying high-conductivity metallic carbon nanotubes and the difficulty of high-order ordered dispersion in metal matrix, which hinders the stable realization of ultra-high conductivity and the macro-preparation of composite materials. Graphene with a two-dimensional carbon atom structure is considered to be an excellent conductor material due to its natural zero-bandgap metallic character and ultra-high electron mobility. At present, chemical vapor deposition (CVD) has enabled large-scale preparation of graphene with high conductivity. Unlike one-dimensional carbon nanotubes, CVD graphene can be grown in situ directly on the surface of a copper substrate to form a graphene/copper heterostructure composite. The composite units are then assembled and densified. The highly oriented dispersion arrangement of graphene inside the composite material can be realized and the in-plane high conductivity property can be maximized. Our research proposed a bottom-up graphene/metal composite material preparation technology to achieve the orderly embedding of high quality graphene in a metal matrix. As a result of ultrahigh electrical conductivity of graphene (3000 times higher than copper) and corresponding graphene/metal composites (117% IACS) were obtained and the conductive mechanism were also understood by designs on architecture and interface.

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The ZnO based nanostructured anode materials for energy conversion applications @ LT-SOFC

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Introduction: Solid oxide fuel cells have got a countless consideration for the researchers in the field of energy conversion technologies due to their fuel flexibility and higher efficiency. Nanostructured materials have produced and great interest of researchers due to their vast applications in the field of chemistry, biotechnology, physics, medical science and material engineering etc. Now-a-day, the scientists attract their attention toward the nanomaterials for their use in energy conversion devices to overcome the energy crisis. Fuel cell is one of them which can fulfil energy demands. In a fuel cell device the chemical energy of fuel was converted into the electrical energy. It was composed of three components anode, electrolyte and a cathode. Among all other categories of fuel cells, solid oxide fuel cells (SOFC) were preferably used due to its reliability, flexibility of fuel, good efficiency, modularity, low emissions and environment friendliness.

Experimental: In the present research investigation, two types of ZnO based anode materials with compositions Al_{0.1}Mn_{0.1}Zn_{0.8}O (AMZ) and Al_{0.1}Mn_{0.1}Ni_{0.1}Zn_{0.7}O (AMNZ) were synthesized by solid state reaction. The phase confirmation and surface morphology of the synthesized materials were confirmed by the X-ray diffraction and scanning electron microscopic analysis, respectively. Electrical properties of the materials were also measured for energy applications.

Results and Discussion: The Scherer's formula was applied to elucidate the particle sizes of proposed materials and found to be 52 and 61 nm for AMZ and AMNZ, respectively. The maximum conductivity of AMZ and AMNZ was found to be 4.4 and 5.2 S/cm, respectively. The values of activation energy calculated by Arrhenius plot were 0.21 and 0.25 eV for AMZ and AMNZ, respectively. The fabricated materials showed both ionic and electronic conducting behaviour as confirmed by electrochemical impedance measurements. The AMNZ composition has higher value of open circuit voltage (1.01V) and power density (535 mW/cm²) in hydrogen atmosphere as compared to AMZ at 550°C indicating that the AMNZ can be used as promising anode material at low temperature for fuel cell applications. The results of measurements have been shown in figure 1

Conclusions: All these characterization results show that material is suitable for anode candidates in LT-SOFC and can be considered the new potential candidate as conventional one.

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Structural modulation and enhanced thermoelectric properties of thermoelectric thin films

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SnSe single crystals have been demonstrated to possess excellent thermoelectric properties. In this work, we demonstrate a grain size control method in growing nano crystalline SnSe thin films through a glancing angle pulsed laser deposition approach. Structural characterization reveals that the SnSe film deposited at a normal angle has a preference orientation along an axis, while by contrast, the SnSe film deposited at a glancing angle develops a nano pillar structure with the growth direction towards the incident atomic flux. The glancing angle deposition results in a reduced grain size of the thin film and enhanced thermoelectric properties with increased see beck coefficient. The enhancement of thermal power can be attributed to the increased potential barriers owing to the reduced grain size and increased grain boundaries in the film. We also demonstrated this approach in other thermoelectric thin films such as SnTe. This finding provides an alternative strategy to enhance thermoelectric performance of thin films.

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Progress into energy storage technology: About the carborundum foam ceramic structure and the fuel cells capacity

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The present research is about carborundum foam ceramic (SiC) and its huge energy storage capacity in industrial approaches. Initially observed in 1824 by Jöns J Berzelius in a synthetic diamond experience by a parasite reaction between carbon and silica, this porous material is found much utilized since the industry of 1890, reason to its precious properties, such as its powerful resistivity to thermal shocks and chemical oxidation to name but a few. SiC could be produced at various specific surfaces, as between 10 and 20 m²/g. Similarly, the granulometric composition of the used mixture powder could control its porosity. For industrial applications (as catalysts), the porosity is ranged between 37% and 45%. Regarding the permeability the key factor for most industrial applications, a large range of the latter could be denoted. Complement to these properties and following the fuel cells development in the recent years, such a material could be adopted against the storage instability problem. As observed with various fluid natures, it was established that the energy storage at low double-diffusive buoyancies consists, usually of a steady state ratio, easily controlled at pilot processes (and promotive for modest applications). By searching for a better capacity ratio, following the increase in the buoyancy impact, the fuel cell structure could become unstable, leading to a huge loss in both the process energy cost and the used materials. Facing to such a big challenge, our alternative will be thermo-mechanical. By taking the annulus shapes as an example, the generation of a high diffusive gradient between the annulus limits could increase the buoyancy efficiency and the energy ratio consequently. Of course critical situations will be reached, as the inner sub-flow regimes over the energy storage process. Against such a part, the full cell shape could light-up the perfect solution. In view of the fact that the nature of industrial processes is often non-linear, extremely complex and not sufficiently recognized, the development of primary conditions for energy storage optimization is of practical significance. As such, our presentation at Advanced Energy Materials Conference, at Zurich, Switzerland, will be undertaken to extend the optimum carborundum foam structure & buoyancy range to make accurate information about full cells stability and the evolution of the energy storage ratio during the operation time.

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Rational design of pre-intercalation electrodes for rechargeable battery

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Rational design of the morphology and complementary compounding of electrode materials have contributed substantially to improving battery performance, yet the capabilities of conventional electrode materials have remained limited in some key parameters including energy and power density, cycling stability etc., because of their intrinsic properties, especially the restricted thermodynamics of reactions and the inherent slow diffusion dynamics induced by the crystal structures. In contrast, pre-intercalation of ions or molecules into the crystal structure with/without further lattice reconstruction could provide fundamental optimizations to overcome these intrinsic limitations. In this report, we discuss the essential optimization mechanisms of pre-intercalation in improving electronic conductivity and ionic diffusion, inhibiting “lattice breathing” and screening the carriers charge. We also summarize the current challenges in pre-intercalation and offer insights on future opportunities for the rational design of pre-intercalation electrodes in next-generation rechargeable batteries.

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Sustainability in production of cement composite boards using waste and supplementary cementitious materials

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Cement Composite Board (CCB) is an important construction product, which is used for cladding as well as internal and external walls. The main components of CCB include Poly Vinyl Alcohol (PVA) fibre, Portland Cement (PC) and water. PVA fibres are expensive, not available and accessible in most of developing countries. In addition, over the past decade, to reduce the carbon emission a global movement has been begun to reduce the use of PC in construction industries due to its carbon footprint and greenhouse gas emission. In this research, an attempt has been made to manufacture CCB using the waste cardboard and supplementary cementitious materials. Cellulose fibres extracted from waste cardboard have been treated and processed by chemical solutions. A combination of fly ash and silica fume was replaced for 40% of PC. In this research, a broad range of mix proportions have been designed, made and tested based on the relevant standards. The results showed that some proposed mixes could meet the standards requirement.

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Visible-Light photoreduction of CO₂ over a cobalt porphyrin-based metal-organic framework by sacrificial electron

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This study describes the CO₂ photoreduction over porphyrin-based metal-organic framework (Co/PMOF) in the presence of triethanolamine (TEOA) as a photocatalyst and sacrificial agent, respectively, under visible light irradiation. The photoluminescence properties of porphyrin and Co/PMOF showed that the lifetime of photogenerated charge carriers in Co/PMOF is longer than porphyrin. According to Fig. 1, Co/PMOF demonstrates significant photocatalytic activity toward CO₂ reduction. The HCOO⁻ was continuously produced, the amount increasing to 23.21 μmol in 6 h. No other products have been detected in gas and liquid phases, suggesting that the Co/PMOF has highly selective toward the CO₂ reduction. For comparison, TCCP was applied as a photocatalyst for CO₂ reduction under similar condition. Only 4.56 μmol of HCOO⁻ was produced after 6 h which is confirmed the photoactivity can be significantly increased by assembling the TCPP ligand onto MOFs structure.

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Performance of dye sensitized solar cells (DSSCs) based on Cu-doped TiO₂ nanostructures photoanodes

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In this research study, Cu-doped TiO₂ nanostructures with different doping contents from 0 to 10.0% (mole fraction) were synthesized through hydrolysis at low temperature. The prepared Cu doped TiO₂ nanostructures was characterized with several techniques, X-ray diffraction (XRD) and Raman spectroscopy were used to study the morphology and structure of the nanoparticles, which confirmed the crystalline anatase tetragonal structure. The UV-Visible Spectroscopy Analysis was found that incorporation of Cu²⁺ into titanium affects the band gap of TiO₂ and extending his activity towards visible sunlight region. Scanning Electron Microscopic (SEM) analysis confirming the Cu content is incorporated into TiO₂ lattice affecting efficiency of doped samples. Further, the active specific surface area of the system was investigated employing Brunauer-Emmett-Teller (BET) measurement. Then the dye-sensitized solar cells (DSSCs) based on Cu-doped TiO₂ photoanodes were fabricated and investigated with chemically absorbed Ruthenium N3 dye electrode under light illumination with standard solar simulator (AM 1.5G, 100 mW/cm²). Results demonstrated that the 1.0% Cu-doped TiO₂ sample annealed at 773 K for 60 minutes exhibited the best photovoltaic performance of open circuit voltage ($V_{oc} = 957.5$ mV), short circuit current density ($J_{sc} = 0.795$ mAcm⁻²), and the cell efficiency was reached ($\eta = 4.524$ %), which consists 50% higher than the un-doped cell. The BET analysis was supported the founding results, indicating that the 1.0% Cu-doped TiO₂ nanoparticle presented the higher active specific surface area of 143.2 m²g⁻¹. A highest active surface area is a key parameter for solar cells effectiveness, allowing more organic dye and electrolyte to be absorbed and stored into the semiconductor that give photon from solar light energy more probability to be adsorbed which obviously led to improve global cell efficiency. This study may open up more investigated works applying Cu doped TiO₂ in photovoltaic fields.

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DFT simulations applied to multiferroic materials

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Now-a-days, superficial process is very important for chemical reactions, optical, electrical and magnetic properties. Ab-initio simulations are very specific for molecular structure, electronic density, spin, charge and others quantum information. Surface models have been developed to clarify and understand the electronic nature and properties; the Density Functional Theory (DFT) is one of more applied quantum descriptions used in surface science in molecular structure. Multiferroic materials have been researched because of its structure to represent a material with two or more properties. One special case is the electro-magnetic coupling in R3 and R3c structures as bulk superficial dimensions can contribute significantly to develop transducers and spintronic devices. Our experience in simulating multiferroic materials is presented in analysis of electronic structure directed to electronic levels and spin location from magnetic cations. However, a particular phenomenon is described in literature as the possibility to localize spin density in Ti atom became it a Ti^{3+} specie, which is very important to understand the intermetallic connection in materials with two cations, more specifically one magnetic cation and other non-magnetic cation. Such spin localization indicates band-gap reduction and spin channels from magnetic induction in a non-magnetic cation.

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Novel polyolefin-based proton exchange membranes for fuel cell applications

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A new class of polyolefin based proton exchange membranes are formed by a well-defined graft copolymer that contains a high molecular weight semicrystalline PE or PVDF backbone and several amorphous sulfonated poly(arylene ether sulfone) (s-PAES) or sulfonated polystyrene (s-PS) side chains. The suitable chemical routes will be discussed for preparing the graft copolymers with desirable backbone molecular weight, graft density, graft length, sulfonic acid concentration, etc. One example is PE-g-s-PAES copolymer that is prepared by a graft onto reaction between high molecular weight HDPE with few benzyl bromide groups and poly(arylene ether sulfone) (PAES) with two terminal phenol groups. The resulting PE-g-PAES graft copolymer was solution cast into uniform film (thickness 20–40 μm), followed by a heterogeneous sulfonation reaction to obtain PE-g-s-PAES PEMs. The unique combination of hydrophobicity, semicrystallinity and high molecular weight of PE backbone offers PEM with a stable (non swellable) matrix. On the other hand, the hydrophilic proton conductive s-PAES side chains in the PE-g-s-PAES membrane self-assemble into many conducting channels. In addition, a thin PE layer spontaneously formed on the membrane surfaces. In the bulk, these membranes show good mechanical properties (tensile strength >30 MPa, Young's modulus >1400 MPa) and low water swelling ($\lambda < 15$) even with high IEC >3 mmol/g in the s-PAES domains. Compared to Nafion 117, most PE-g-s-PAES PEMs show similar hydration numbers ($\lambda < 15$) but higher proton conductivity (up to 160 mS/cm). More interestingly, all PE-g-s-PAES PEMs show higher through-plane conductivity than in-plane conductivity. In direct methanol fuel cells, the PE surface layer also minimizes methanol cross over from anode to cathode with reduced fuel loss, and stops the $\text{HO}\cdot$ and $\text{HO}_2\cdot$ radicals, originally formed at the anode, entering PEM matrix. Overall, this newly developed PE-g-s-PAES membrane offers a combination of desirable properties, including conductivity, water uptake, selectivity, mechanical strength, and cost-effectiveness for fuel cell applications.

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Interfacial energy materials for flexible, safe batteries: Gummy electrolyte and gummy binder

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Two conformable interfacial energy materials have been designed and fabricated for battery applications, i.e. gummy electrolyte and gummy binder with a chewing gum-like appearance (thereafter called “gummy” material). Electrolytes play a very important role for battery safety and performance. The gummy electrolyte was demonstrated with beneficial properties, such as high ionic conductivity (liquid electrolyte level), good mechanical properties (solid materials level), and strong adhesion (adhesive level), as well as safety characteristics providing thermal protection for batteries. The other interfacial energy material, the gummy binder, is a dual-conductive adhesive for fabricating high performance battery electrodes. The primary function of conventional electrode binders is “binding” particles in electrodes without directly contributing to the performance of electrodes/batteries, as they cannot conduct electrons and/or ions. The gummy binder possesses high ionic and electronic conductivities, strong adhesion and appropriate mechanical/rheological properties, as well as excellent conformability and processibility. As it is a dual-conductive adhesive, the gummy binder is an effective solution to address the issues that are relevant to the interface weakness and structural instability. Firstly, the adhesive electrode matrix being the continuous phase can provide stable structures and “robust” interfaces via strong adhesion with the active electrode particles (the filler phase). The results enhance the durability of the electrodes and thus the batteries. Secondly, the continuous phase with uniform conductive interfaces provides the base for dual conductive functions (for both ions and electrons) inside the electrodes. Therefore, with such a matrix material, “robust” interfaces, which are defined as stable with high interfacial adhesion and good conductive properties for ion/electron transfer, can be built inside the electrodes. Thirdly, the gummy binder as the conductive continuous phase can also promote heating transport/releasement, thus the safety of the batteries can be improved.

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The behavior of system temperature, volume, enthalpy, and total energy of ZnO wurtzite phase under different temperature and pressure, a molecular dynamics prediction

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The dl_poly_4 software and Parallel Molecular Dynamics are investigated to analyze the behavior of system temperature, volume, enthalpy, and total energy of ZnO wurtzite phase under an extended temperature and pressure. In this work we study the effect of the temperature and pressure in the range of 300-3000K and 0-200GPa respectively on the system temperature, volume, enthalpy, and total energy. The interatomic interaction is modeled by the Coulomb-Buchingham pair potential, where we confirmed its validity. Our data are in agreement with some available results due to no more work under the previous extreme conditions of pressure and temperature. This work has great importance in pharmacy, medicine, nanotechnology industry and in geophysics, but needs confirmation in future.

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Discrete Zn, Co bimetallic sites supported on N doped carbon for high performance oxygen reduction reaction catalysis

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A new design of discrete Zn, Co bimetallic sites supported on N-doped carbon was fabricated through a competitive complexation strategy. Aberration corrected atomic resolution high angle annular dark field scanning transmission electron microscopy (HAADF-STEM) measurements combined with X-ray absorption fine structure (XAFS) reveals the existence and the structure of the Zn-Co bimetallic sites. This Zn-Co dual atom catalysts exhibit significantly improved oxygen reduction catalytic activity compared to single atom catalysts in both acid and alkaline conditions. Density functional theory (DFT) calculations reveal that the enhanced catalytic activity can significantly be attributed to the elongated O-O bond length (from 1.23 Å to 1.42 Å), and thus facilitates the cleavage of O-O bond at the ZnCoN₆(OH) sites, showing a theoretical over potential of 0.335 V during ORR process. In-situ XAS study demonstrates that Co serves as the active center during the catalysis. Furthermore, a highly active sulfur (S)-modified Zn, Co-N_x-C-S_y ORR catalyst is also developed. Besides the elongated O-O band length, the S doping can further modify the charges around Zn, Co active center and strengthen the interaction with oxygenated species by decreasing the free energy changes of $^*O_2 + e^- + H_2O \rightarrow ^*OOH + OH^-$ step. The prepared catalysts show promising potential in practical applications in both fuel cell and Zn-air batteries. Particularly, the H₂/O₂ fuel cell tests based on the Zn-Co atomic pair presents a peak power density of 705 mW cm⁻² along with excellent stability.

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