



4<sup>th</sup> International Conference on **Electrochemistry**

June 11-12, 2018 | Rome, Italy

# Posters

Electrochemistry 2018

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**Computational modeling and studies of hydroxyapatite with defects of the oxygen vacancy type providing its photocatalytic activity**Vladimir S Bystrov<sup>1</sup>, Jose Coutinho<sup>2</sup>, Leon A Avakyan<sup>3</sup>, Anna V Bystrova<sup>1</sup>, Ekaterina V Paramonova<sup>1</sup> and Yuri D Dekhtyar<sup>4</sup><sup>1</sup>Keldysh Institute of Applied Mathematics RAS, Russia<sup>2</sup>University of Aveiro, Portugal<sup>3</sup>Southern Federal University, Russia<sup>4</sup>Riga Technical University, Latvia

A new model of the structure of hydroxyapatite (HAP) with defects of the oxygen vacancy type and hydroxyl group vacancy type has been developed. The model made it possible to explain the change in the optical properties of the HAP and provide for the mechanism of its photocatalytic activity. The obtained new results and knowledge allow us to already purposefully change the optical properties of HAP (introduction of the necessary type of the defects) and control the photocatalytic activity of HAP, which is extremely important for many practical applications (in the cleaning the environment, including the water from harmful impurities and components, in the chemical photocatalytic synthesis, in the antimicrobial treatment, etc.). The model is developed on the basis of several new approaches to the density functional theory (DFT) with combined application of the various hybrid and exchange-correlation functionals, and also taking into account the Coulomb shielding of the defect charge, which allows made more exact and accurate calculation of structural, optical and other properties of HAP materials. These approaches continue to develop on some new more complex models of the super-cells of HAP, which will allow us to obtain a number of even more highly accurate results of calculations of the HAP properties for both pure and with different defects. The computed properties of HAP material with super-cell model (2x2x2 - 8 unit cell) are considered using semi-local (PBE potential) and hybrid exchange-correlation functionals with different fraction of exact exchange contribution. The excitation properties are compared with the results of GW-approximation method for calculation of quasi-particle band structure. It was shown that optical properties of bulk HAP are best described using B3LYP exchange-correlation functional and for pure HAP have band gap  $E_g \sim 7.3$  eV, while with O vacancy it is lowered.

**Recent Publications:**

1. Bystrov V S, Coutinho J, Bystrova A V, Dekhtyar Y D, Pullar R C, Poronin A, Palcevskis E, Dindune A, Alkan B, Durucan C and Paramonova E V (2015) Computational study of hydroxyapatite structures, properties and defects. *J. Phys. D: Appl. Phys.* 48:195302.
2. Bystrova A V, Dekhtyar Yu D, Popov A I, Coutinho J and Bystrov V S (2015) Modified hydroxyapatite structure and properties: modeling and synchrotron data analysis of modified hydroxyapatite structure. *Ferroelectrics* 475(1):135-147.
3. V S Bystrov, C Piccirillo, D M Tobaldi, P M L Castro, J Coutinho, S Kopyl and R C Pullar (2016) Oxygen vacancies, the optical band gap ( $E_g$ ) and photocatalysis of hydroxyapatite: comparing modelling with measured data. *Applied Catalysis B: Environmental*. V 196:100-107.
4. V Bystrov, A Bystrova and Yu Dekhtyar (2017) HAP nanoparticle and substrate surface electrical potential towards bone cells adhesion: Recent results review. *Advances in Colloid and Interface Science* 249:213-219.
5. V S Bystrov et al. (2017) Surface modified hydroxyapatites with various functionalized nanostructures: computational studies of the vacancies in HAP. *Ferroelectrics* 509:105-112.

**Biography**

Vladimir S Bystrov has completed PhD, Dr. Habil.Phys. Dr.Sci. Phys. & Math. from Russian Academy of Sciences. Since 1993, he has his expertise in various fields of computational molecular modeling, computational exploration and computer simulation of nonlinear multifunctional nanomaterials and different organic & bio-molecular nano-structures such as: bioferroelectric & polymer PVDF/PVDF-TrFE thin ferroelectric films, graphene/oxide graphene and related polar composite nanomaterials; amino acids (glycine, etc.), peptides nanotubes, thymine & DNA; hydroxyapatite (HAP) & nanoparticles, etc. Computational studies of nanostructures were made using the molecular mechanics, quantum-chemical calculations (ab initio, DFT, semi-empirical methods), molecular dynamics (MD) on the base of various software (HyperChem, AIMPRO, VASP, etc.) and clusters in Russia IMPB & KIAM, Linux cluster in University of Aveiro, Portugal. He is a Head of the Group for Computer Modelling of Nanostructures and Biosystems of IMPB-KIAM RAS, Pushchino.

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**Electrochemical control of the oxide film growth on niobium**

Michał Stępień and Krzysztof Fitzner

AGH University of Science and Technology, Poland

Depending on the thickness of the oxide layer on niobium different properties of this material can be obtained, which can be exploited in sensing, decorative materials, electronic paper and displays. The aim of this work is to produce the oxide layer in the controlled way utilizing electrochemical experiment. The layer of the oxide will be formed by anodization of Nb electrode in acidic aqueous solution. Then, the electrochemical impedance spectrometry (EIS) is used to control the thickness of the growing layer due to the relation:  $C = \frac{\epsilon_0 \epsilon_r A}{d}$  where:  $\epsilon_0$  – permittivity of the vacuum;  $\epsilon_r$  – permittivity of the oxide film; A – geometric area of the oxide; d – barrier oxide thickness; C – capacitance obtained from EIS after proper choice of the equivalent circuit. However, successful control requires exact knowledge of dielectric constant of niobium oxide. Depending on oxidation conditions, different values of  $\epsilon_r$  can be obtained. Therefore, this value will be verified by using simultaneously EIS and ellipsometric measurements.

**Recent Publications:**

1. Arsova I et al. (2006) Electrochemical formation of anodic oxide films on Nb surfaces: ellipsometric and Raman spectroscopical studies. *Journal of Solid State Electrochemistry* 11(2):209-214.
2. Komatsu I et al. (2016) Color change mechanism of niobium oxide thin film with incidental light angle and applied voltage. *Thin Solid Films* 603:180-186.
3. Potucek R K et al. (2006) Impedance characterization of anodic barrier Al Oxide film beneath porous oxide layer. *Journal of the Electrochemical Society* 153(8):B304.
4. Richter F et al. (2001) Optical properties and mechanical stress in SiO<sub>2</sub>/Nb<sub>2</sub>O<sub>5</sub> multilayers. *Thin Solid Films* 389:278-283.
5. Szymanowski H et al. (2005) Optical properties and microstructure of plasma deposited Ta<sub>2</sub>O<sub>5</sub> and Nb<sub>2</sub>O<sub>5</sub> films. *Journal of Vacuum Science & Technology A* 23(2):241-247.

**Biography**

Michał Stępień graduated MSc from the AGH University of Science and Technology in 2010. He received his PhD degree in 2015 (Synthesis of oxides nanostructures on the surface of selected transition metals) under the guidance of Professor Krzysztof Fitzner. His research interests are based on synthesis and surface modification oxides nanotubes. Now he is a Research Worker in AGH in Department of Physical Chemistry and Metallurgy of Non-Ferrous Metals.

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**Influence of the dopant concentration on photoelectrochemical behavior of Al-doped TiO<sub>2</sub>**Anna A Murashkina and Alexei V Emeline  
Saint Petersburg State University, Russia

Titanium dioxide is the most extensively studied photoactive material since the discovery of water photo-assisted electrolysis with titanium dioxide photo-anode. Materials based on titanium dioxide can be used in photocatalytic systems for water and air purification, formation of self-cleaning and antibacterial coatings, in solar cells and sensors. Titanium dioxide possesses a sufficiently high photochemical (photocatalytic) activity, good chemical stability and non-toxicity and low cost of its production. In the present study we explored the effect of Al dopant concentration within the range <1.1 wt.% on the photoelectrochemical activity of Al doped TiO<sub>2</sub> photo-anode. The experimental dependencies of photoelectrochemical efficiency on Al dopant concentration indicate that there is an optimal Al concentration 0.5 wt.% corresponding to the highest photo-activity. The analysis of the spectral dependencies of the photocurrent confirms that 0.5 wt.% of Al provides the highest activity at photoexcitation in both intrinsic and extrinsic absorption spectral range. It was also shown that Al doping does not affect the optical band gap of TiO<sub>2</sub>. The dependence of photoelectrochemical activity on Al concentration correlates with the corresponding dependencies of the flat band potential and work function indicating the shift of the Fermi level toward the conduction band for the Al concentration <0.5 wt.% and toward the valence band for the Al concentration >0.5 wt.%. Such alteration of the Fermi level position is explained in terms of alteration of the type of major compensating intrinsic defects for Al concentration <0.5 wt.% acting as shallow traps, to Al concentration >0.5 wt.% acting as deep traps. Transformation of compensating defects from shallow traps which are ineffective in charge recombination processes to deep traps which act as effective recombination centers is responsible for the optimal dopant concentration, 0.5 wt.%, to achieve the higher photoelectrochemical activity of Al-doped TiO<sub>2</sub>.

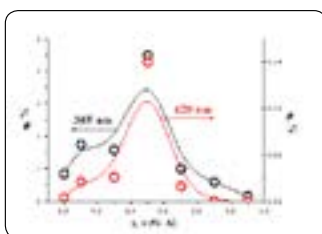


Figure 1: The dependence of IPCE on Al-dopant concentration at 365 and 420 nm.

**Recent Publications:**

1. Nakata K, Ochiai T, Murakami T and Fujishima A (2012) Photoenergy conversion with TiO<sub>2</sub> photocatalysis: New materials and recent applications. *Electrochimica Acta* 84:103-111.
2. Fujishima A, Zhang X and Tryk D A (2008) TiO<sub>2</sub> photocatalysis and related surface phenomena. *Surf. Sci. Rep.* 63:516-582.
3. Henderson M A (2011) A surface science perspective on TiO<sub>2</sub> photocatalysis. *Surface Science Reports* 66:185-29.
4. Robertson P, Robertson J and Bahnemann D (2012) Removal of microorganisms and their chemical metabolites from water using semiconductor photocatalysis. *Journal of Hazardous Materials* 211– 212:161–173.
5. Asahi R, Morikawa T, Ohwaki T, Aoki K and Taga Y (2001) Visible-light photocatalysis in nitrogen-doped titanium oxides. *Science* 293:269-271.

**Biography**

Anna A Murashkina has her expertise in the development and investigation of semiconductors for the solar energy conversion into the chemical energy. These semiconductor materials can be used in photocatalytic systems for water and air purification, formation of self-cleaning and antibacterial coatings, in solar cells and sensors.

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**Study on the spontaneous generation of electrostatic potential gradient in an electrolyte due to the presence of a static magnetic field and its applications in construction of analogous voltaic, daniel and concentration cells magnetolysis: An alternative to electrolysis**Rajatava Mukhopadhyay and Debosmita Pathak  
Jagadis Bose National Science Talent Search, India

Electricity and magnetism were considered as separate identities until late 19th century, when people like Maxwell, Faraday came to the forefront to change the idea.

Classical electromagnetic theory of Maxwell, with the help of certain experiments, disclosed that current electricity and magnetism at two opposite faces of the same coin, that is, they are different approaches to the same aspect of physics. Electromagnetism is one of the most important aspects of physics, since it broke the jinx of classical physics and paved the way to the beginning of research about structure of matter and consequently to the foundation of quantum mechanics.

An electric current can induce a magnetic field, and vice-versa. So, electricity and magnetism should, so to say, be interchangeable, which is the main idea we have tried to implement.

Electrolysis is something we are all familiar with. In electrolysis, electricity flows due to a potential difference developed across the two electrodes of a cell, due to differential reduction potential at the two terminals.

*So, can this potential difference be induced using a magnet too?*

Surprisingly, yes.

Replacing the cathode and anode of an electrolytic cell with the north and south poles of a magnet (respectively), we get the exact same result as that expected from electrolysis.

Cations get attracted to the north and anions to the south pole. Electrons flow from the south to the north pole through the magnet (analogous to anode to external circuit to cathode) and current from the north to the south, on completing the circuit (for a half-cell setup).

Moreover, a magnetolytic cell can be recharged by simply reversing the polarity of the two half-cells, by exchanging the magnetic poles immersed in them.

So, to conclude, lysis and current flow with the help of magnets ---- '*magnetolysis*', maybe a viable, sustainable and economic alternative to electrolysis in the near future. *All practical applications of an electrolytic cell can be realised through an analogous magnetolytic cell.*

All the experimental data, associated graphs and data are stored for future reference.

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**Synthesis of quinone derivatives and its application to redox electrode****Bong Ho Lee and Yeajoon Bon**  
Hanbat National University, South Korea

Physical mixing of activated carbon (AC) and a quinone derivative, 2, 5-bis (pro-2-ny-1-ylamino) cyclohexa-2, 5-diene-1, 4-dione (coded HBU-281) was used to design a composite electrode for supercapacitors. The process proves to be simple and cost-effective because it demands only the initial synthesis of the organic additive. The electrode properties were probed in terms of composite composition, redox behavior, specific capacitance, and cycle life. The capacitance performance of the AC electrode is enhanced due to the extra redox reaction of hydroquinone/quinone couple of HBU-281. AC facilitated electron distribution to the HBU-281 making pronounce its redox activity. The composites due to the synergistic effect of AC and HBU-281 gave higher capacitance and indicating excellent cycle stability than the individual electrodes. These findings led to the conclusion that physical mixing of AC and HBU-281 can be adopted to design cheap and excellent composite electrodes for supercapacitor.

**Biography**

Bong Ho Lee have been studying electrical energy storage materials including electrolytes and electrodes based on organic and inorganic chemistry for many kinds of batteries and supercapacitors.

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**Lithium bis(oxalate)borate electrolyte salt for supercapacitors in elevated temperature applications****Jang Myoun Ko** and **Choong Sup Yoon**  
Hanbat National University, South Korea

The electrolyte plays one of the most significant roles in the performance of electrochemical supercapacitors. Most liquid organic electrolytes used commercially have temperature and potential range constraints, which limit the possible energy and power output of the supercapacitor. The effect of elevated temperature on a lithium bis(oxalate)borate (LiBOB) salt-based electrolyte was evaluated in a symmetric supercapacitor assembled with activated carbon electrodes and different electrolyte blends of acetonitrile (ACN) and propylene carbonate (PC). The electrochemical properties were investigated using linear sweep voltammetry, cyclic voltammetry, galvanostatic charge–discharge cycles, and electrochemical impedance spectroscopy. In particular, it was shown that LiBOB is stable at an operational temperature of 80°C, and that, blending the solvents helps to improve the overall performance of the supercapacitor. The cells retained about 81% of the initial specific capacitance after 1000 galvanic cycles in the potential range of 0–2.5 V. Thus, LiBOB/ACN:PC electrolytes exhibit a promising role in supercapacitor applications under elevated temperature conditions.

**Biography**

Jang Myoun Ko have been studying electrical energy storage materials including electrolytes and electrodes based on organic and inorganic chemistry for many kinds of batteries and supercapacitors.

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**Notes:**

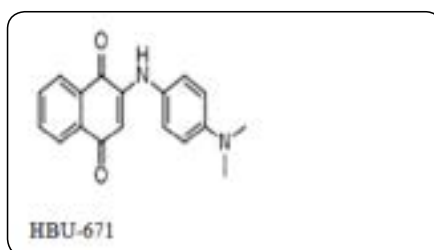


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**Naphthalene derivative supported activated carbon composite electrode with enhanced capacitance and potential window for supercapacitor****Jeong H Park and Isheunesu Phir**  
Hanbat National University, South Korea

A derivative of 1,4-Naphthoquinone coded HBU671 is synthesized and used in addition to activated carbon as composite electrode for supercapacitor application. From the electrochemical properties analysis, a specific capacitance of about 300 Fg<sup>-1</sup>, almost double the specific capacitance of activated carbon was obtained for the composite electrode at a scan rate of 100 mV s<sup>-1</sup> and a potential window of -0.2~1 V. This improvement is due to the inherent redox reaction in HBU671. Cycle test also proved that this new composite is still stable even after 1000 cycle within the applied potential window and it is highly recommended for practical application.

**Biography**

Jeong H Park has his expertise in Organic Synthesis. He synthesizes novel organic compounds and tries to apply them to electro-material and other fields.

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**Notes:**

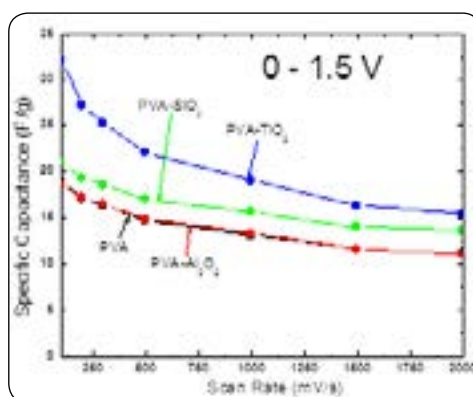
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**Flexible poly(vinyl alcohol)-ceramic composite separators for supercapacitor applications****Sang Hern Kim**

Hanbat National University, South Korea

Electrochemical characterization was conducted on poly(vinyl alcohol) (PVA)-ceramic composite (PCC) separators for supercapacitor applications. The PCC separators were fabricated by mixing various ceramic particles including aluminum oxide ( $\text{Al}_2\text{O}_3$ ), silicon dioxide ( $\text{SiO}_2$ ), and titanium dioxide ( $\text{TiO}_2$ ) into a PVA aqueous solution. These ceramic particles help to create amorphous regions in the crystalline structure of the polymer matrix to increase the ionic conductivity of PVA. Supercapacitors were assembled using PCC separators with symmetric activated carbon electrodes and electrochemical characterization showed enhanced specific capacitance, rate capability, cycle life, and ionic conductivity. Supercapacitors using the PVA- $\text{TiO}_2$  composite separator showed particularly good electrochemical performance with a 14.4% specific capacitance increase over supercapacitors using the bare PVA separator after 1000 cycles. With regards to safety, PVA becomes plasticized when immersed in 6 M KOH aqueous solution, thus there was no appreciable loss in tear resistance when the ceramic particles were added to PVA. Thus, the enhanced electrochemical properties can be attained without reduction in safety making the addition of ceramic nanoparticles to PVA separators a cost-effective strategy for increasing the ionic conductivity of separator materials for supercapacitor applications.



**Figure 1:** The plot of specific capacitance versus scan rate for various PVA-ceramic composite separators

**Biography**

Sang Hern Kim has his expertise in polymer synthesis. He synthesized novel polymers and tried to apply them to electro-material and other fields.

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**Preparation of surface modified nanosalts and its application to an organic electrolyte additive**

Yong Joo Kim and Sang Jun Kim

Hanbat National University, South Korea

Lithium sulfonyl silica (LSS) was synthesized by replacing the surface -OH group in fumed silica with  $(\text{CH}_2)_3\text{SO}_3\text{Li}$  and adopted as electrolyte additive for lithium ion battery. 3 wt.% of the synthesized particles in 1 M  $\text{LiPF}_6$  (EC/DMC=1:1) showed improved ionic conductivity and potential window over the pristine electrolyte. The discharge capacity of the  $\text{LiCoO}_2$ /graphite is particularly enhanced with the addition of LSS at higher C-rates due to the enhanced ionic conductivity at room temperature. The  $\text{LiCoO}_2$ /graphite cells using 1.0 M  $\text{LiPF}_6$ /EC/DMC (1:1) and 1.0 M  $\text{LiTFSI}$ /EC/DMC (1:1) with the additive also showed superior performance for the self-discharge test carried out at 45 for 200 days. These positive impacts of LSS on  $\text{LiCoO}_2$ /graphite cells warrant its use in lithium ion batteries.

**Biography**

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Notes:

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**The novel hydroelectrometallurgical technology of simultaneous production of metallic manganese, electrolytic manganese dioxide and manganese sulfate monohydrate****G Tsurtsunia, D Shengelia, N Koiava, T Lezhava, D Gogoli, L Beriashvili and S.Suladze**  
Ivane Javakishvili Tbilisi State University, Georgia

The novel hydroelectrometallurgical technology is developed to simultaneously production of electrolytic metallic manganese, electrolytic  $\gamma$ -MnO<sub>2</sub> and MnSO<sub>4</sub>·H<sub>2</sub>O in one technological cycle. The united, complex technological scheme consists of two technological lines. One of these lines is designed for: By sulfuric acid leaching of MnO containing primary products formed by high thermal reduction of manganese oxide ores; Purification from Fe<sup>3+</sup>, Ni<sup>2+</sup>, Co<sup>2+</sup> and other heavy metals cations by hydrolysis (pH<sub>4</sub>) and adding Na<sub>2</sub>S into the MnSO<sub>4</sub> solution; Crystallization of MnSO<sub>4</sub>·H<sub>2</sub>O after treatment of concentrated MnSO<sub>4</sub> solution in autoclave under high temperature condition; Supply of hot, autoclave outlet solution of MnSO<sub>4</sub> to anodic area (anodic area is separated by anionic membrane to prevent flow of NH<sub>4</sub><sup>+</sup> into anolyte) where  $\gamma$ -MnO<sub>2</sub> is deposited on the anode. The second technological line is designed for: Purification of solution prepared from MnSO<sub>4</sub>·H<sub>2</sub>O produced in the autoclave and technical (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub> by (NH<sub>4</sub>)<sub>2</sub>S and supply of purified solution to the cathodic area of the same reactor where metallic Mn is deposited on the cathode. In accordance with presented technological scheme, optimal technological parameters are determined for MnSO<sub>4</sub>·H<sub>2</sub>O and 50-55 g·l<sup>-1</sup> Mn<sup>2+</sup>-containing solutions obtained by autoclave treatment of concentrated clean solution of MnSO<sub>4</sub> (115 g·l<sup>-1</sup> Mn<sup>2+</sup>) produced after processing of manganese oxide ore. The technological novelty also is exploitation of heat pump to maintain 35-380C in catholyte and 92-940C in anolyte in an electrochemical reactor working under 20A load and divided by anionic membrane (AMI 7001S). As a cooling agent of heat pump, R-600a (isobutane) was chosen. The evaporator of the heat pump was immersed into the catholyte and the condenser - into the anolyte. The effectiveness of heat pump was also determined.

**Recent Publications:**

1. G. Tsurtsunia, D. Gogoli, N. Koiava, I. kakhniashvili, N. Jokhadze, T. Lezhava, N.Nioradze, D.Tatishvili. (2017) Electrodeposition and Characterization of Mn-Cu-Zn Alloys for Corrosion Protection Coathing. IOP Conf. Series: Earth and Environmental Science 95 042035.
2. P. Nikoleishvili, G. Gorelishvili, V. Kveselava, G. Tsurtsunia, N. Nioradze, R. Kurtanidze, D. Dzanashvili. (2017) Hydrogen generation by reforming of sodium hypophosphite on cobalt-boron oxides containing catalyst. Green and Sustainable Chemistry, 7, pp. 85-93.
3. G. Tsurtsunia, N. Koiava, D. Gogoli, I. Kakhniashvili, T. Lejava, N. Jokhadze, E. Kemoklidze. (2016) Study of the Influence of the Electrolysis Parameters on Mn-Zn, Mn-Cu, Mn-Cu-Zn Alloys Coatings from Electrolytes Containing Complexing ligands. J. Chem. Chem. Eng. 1 13-27.
4. G. S. Tsurtsunia, N. S. Koiava, N. S. G. G. Gogishvili, I.T.Zaridze, I. B. Kakhniashvili, G. G.Gorelishvili, V. M. Kveselava, P. N.Nikoleishvili. (2015) Simultaneous Production of Electrolytic Metallic Manganese and Electrolytic Manganese Dioxide in an AMI 7001S Anion Exchange Membrane Electrochemical Reactor. J. Electrochemical Society, 162, (8) E96-E103
5. P.O. Nikoleishvili, G.S. Tsurtsunia, V.M. Kveselava, G.G. Gorelishvili, R.R. Kurtanidze, D.T. Sharabidze, and D. I. Dzanashvili. (2015) Using Hydrogen Obtained by Reforming of NaBH<sub>4</sub> on Modified Cobalt Catalyst in Hydrogen-Oxygen Fuel Cell. Russian J. Electrochemistry, Vol. 51, No. 7, pp. 665-671.

**Biography**

Gigla Tsurtsunia got his PhD from Karpov Physico-Chemical Institute in 1977, Moscow, Russia. His interest is related to electrochemical technology of production of manganese and its compounds, electrodeposition of alloy coatings and fuel cells. He published more than 40 papers and got 6 patents.

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# Accepted Abstracts

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**Advances in non-aqueous oxygen electrochemistry, in connection to developing rechargeable Li and Na –oxygen batteries**Aurbach D<sup>1</sup> and Sun Y K<sup>2</sup><sup>1</sup>BINA - Bar-Ilan University, Israel<sup>2</sup>Hanyang University, South Korea

Rechargeable Li-oxygen and Na-oxygen batteries if successful and practical can rival internal combustion engines in terms of very high energy density and enable highly competitive electrochemical propulsion for electric vehicles. These systems however, are very problematic. So far, we do not have electrolyte solutions that are stable enough towards the active metals and also towards the oxygen reduction moieties which are superoxide and peroxide species. These oxide moieties are reactive towards all relevant polar-aprotic solvents, especially in the presence of Li ions, which are highly electrophilic Lewis acids in aprotic solutions. Oxygen reduction in the presence of Li ions usually forms solid  $\text{Li}_2\text{O}_2$  as a final stable product. We can control its formation and deposition mechanism through the properties of the electrolyte solutions, as mentioned in the attached image. We can promote fast Li-peroxide precipitation as thin films on the cathode (bottom-up mechanism) or as thick deposits (top-down mechanism). There is a dilemma what should be preferred, because fast deposition may mean low retention time for side reactions (higher stability). Oxidation of Li-peroxide upon charging may require too high over-potentials which endanger the anodic stability of the electrolyte solutions and cathode materials. We know today to overcome this problem by the use of catalysis by redox mediators. We developed new solvents that can be better protected against attacks by oxygen reduction species. We explored alternative anodes which should be less reactive than lithium or sodium metals. In order to explore properly and optimize electrolyte solutions and cathode materials we developed a new methodology in which Li or Na –oxygen cells are explored with bi-compartment cells that completely avoid any chemical communication between the anode and the cathode side, except Li or Na ions exchange. We will discuss the true practical horizons of these battery systems.

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**Nanowire arrays for selective and durable CO<sub>2</sub> reduction****David P Fenning**

University of California, USA

The rapid changes in the global climate during the last century have been extensively ascribed to anthropogenic CO<sub>2</sub> emissions caused by the combustion of fossil fuels. Efforts are then required to decrease the consumption of fossil fuels and to develop methods to produce renewable carbon-based fuels. One promising approach is artificial photosynthesis, a process in which solar energy is used to drive the reduction of CO<sub>2</sub> to fuels or valuable chemicals. A pressing need exists to develop an efficient, robust, selective and earth-abundant catalyst for the CO<sub>2</sub> reduction reaction (CO<sub>2</sub>RR), which can be used directly as a cathode in a photovoltaic-electrolyzer system or coated on an efficient light absorbing photocathode material in a photoelectrochemical (PEC) cell. Copper (Cu) is a non-toxic and earth-abundant catalyst for the CO<sub>2</sub>RR, and there are facile and scalable methods to make its nanostructures, etc. and as such it is arguably the best-studied catalyst for the CO<sub>2</sub> reduction. However, its reported performance (considering selectivity, durability, and efficiency) so far is too low for practical applications. Herein, we present our efforts to nanoengineer efficient CO<sub>2</sub>RR catalysts. Among them, I will highlight our production of Cu(OH)<sub>2</sub> nanowire arrays, synthesized by a facile and scalable solution growth method, for selective and durable CO<sub>2</sub> reduction. The Cu(OH)<sub>2</sub> nanowire array shows selective CO<sub>2</sub> reduction to C<sub>2</sub>-C<sub>3</sub> products, with a faradaic efficiency of ~40% for C<sub>2</sub><sup>+</sup> products. The catalysts exhibit durable CO<sub>2</sub> reaction of over 24 hours with a minimal change in faradaic efficiency of each gas/liquid product and total faradaic efficiency.

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**Python script in the processing of electrochemical impedance spectroscopy and current transient measurements for the determination of the chemical capacitance****Daniel Andres Triana Camacho**

Universidad Industrial de Santander, Colombia

**B**ig data is defined in a variety of ways, including the search and retrieval of information to make decisions and; the science behind the data when these are used to respond any question. On other hand, chemical capacitance (a fundamental thermodynamic quantity related to charge accumulation at an electronic conductor/ionic conductor interface), is conventionally obtained by electrochemical impedance spectroscopy (EIS). Herein, current transients (CT) are proposed as an alternative measurement to determine the chemical capacitance. Thus, we describe a Python script to evaluate whether chemical capacitance can be obtained by CT collected at multiple potentials. The experimental procedure was performed with the redox pair  $\text{Fe}(\text{CN})_6^{3-}/\text{Fe}(\text{CN})_6^{4-}$ , a model one electron outer sphere process, and applied to the derivation of the chemical capacitance of the redox-active species on a Pt electrode. To validate the methodology here proposed is necessary to organize, process, and matching between these two different types of measurements, like so display information in the form of mathematical models, plots and files. Hence, we develop a protocol to analyze and compare a large amount of data irrespective of time scale. Usually, the experimental data for CT and EIS are analyzed independently and in different ways by computational programs, for instance, repeating the sampling process for different times yields a family of curves named “sampled current-voltammograms”, one for each time scale. In addition, EIS data may be presented in several types of plots (e.g., Bode or Nyquist), which increase the volume of information obtainable from these measurements. Therefore, a `getData` class was created to get and process the experimental data from CT and EIS measurements. To process the experimental data a Python script was used to instantiate two objects: `input` and `data` objects. An `input` object is a javascript object notation (JSON)-like object where the file name and the potential for experiment data are defined, thereby JSON object was implemented as a Python dictionary. A `data` object is the instantiated `getData` object with the information contained in the data files referenced in the `input` object. A Python script containing the `input` and `data` objects was created to process experimental data of  $\text{Fe}^{III}/\text{Fe}^{II}$  redox pair in solution. A total of 64 data files were obtained with NOVA 2.0 software for electrochemistry. Each CT data file contains approximately 15000 experiment numbers, and EIS, 305. With instantiate `getData` object the capacitance curves against potential from EIS and CT was constructed and compared in an easier way than process data with traditional tools used in electrochemistry. It is concluded that at a specific condition of time scale, the integral of CT and EIS measurements give similar results of capacitance.

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# 4<sup>th</sup> International Conference on **Electrochemistry**

June 11-12, 2018 | Rome, Italy

## Forest of structured nanowires for energy storage and production

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The storage and production of electrical energy is a major issue of the 21<sup>st</sup> century. Many methods are developed today for embedded systems in the range of small storage. In this context, the development of nanoscale 3D structures makes it possible to considerably increase the specific area of the material. By working on this surface increase but also on its reactivity we can considerably increase the performances of the devices. We have developed in our laboratory electrochemical methods for the production of ultra-dense align nanowires and nanotubes embedded in nanoporous alumina membrane with various materials like metals (Cu, Au, Ni, Pt), semiconductors (Si, Ge) or dielectrics (TiO<sub>2</sub>, polymers) for their integration into electrical devices in partnership with companies in link with industrial issue. We will present some of our results in various fields of electricity production such as PtCu and/or PtNi nanotubes fuel cells, Si nanowires solar cell and thermoelectric devices. We will also present their applications for electrical storage: 3D metal-insulator-metal capacitors, electrolytic capacitors, and supercapacitors. Electrochemical elaboration as well as electrochemical operation will be presented.

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June 11-12, 2018 | Rome, Italy

**Moving beyond lithium-ion batteries****John Muldoon**

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Without a doubt the Holy Grail of battery research is the development of a post lithium ion technology. This may require a shift towards batteries containing a pure metal anode. Li metal is an attractive metal anode in part due to its high volumetric capacity ( $2062 \text{ mAh cm}^{-3}$ ), a high reductive potential of  $-3.0 \text{ V}$  vs. normal hydrogen electrode (NHE) and the wide availability of lithium electrolytes. However, its deposition occurs unevenly with formation of dendrites which leads to safety concerns during cycling. In contrast to lithium metal, magnesium metal deposition is not plagued by dendritic formation. However, magnesium has a reductive potential of  $-2.36 \text{ V}$  vs. NHE and has a unique electrochemistry which prohibited the use of magnesium analogues of lithium electrolytes. Since the oxidative stability of electrolytes governs the choice of cathodes it is of paramount importance to develop non-corrosive magnesium electrolyte with wide electrochemical windows which will permit discovery of high voltage cathodes. I will present the latest developments and future challenges which must be overcome. Elemental sulfur is a very attractive cathode for the post Li ion battery since the sulfur has high theoretical capacity of  $1672 \text{ mAh/g}$ . Despite these attractive properties, practical application of Li-S battery is still unrealized due to some big challenges for the sulfur cathode such as high resistance, low loading of active material and dissolution of the intermediate polysulfide into the electrolyte during charge and discharge. These issues cause low columbic efficiency, fast capacity fade and self-discharge of the Li-S battery. In order to suppress the dissolution of the intermediate polysulfides and minimize the addition of conductive carbon; our group has created a controlled nano-architecture template in which sulfur nanoparticles encapsulated with the conductive polyelectrolyte nanomembranes coated with nanocarbon. The findings of this work will be discussed.

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**Electrochemical deposition of artificial recognition unit for gluten epitope selective determination**Zofia Iskierko<sup>1</sup>, Piyush S Sharma<sup>2</sup>, Alessandra Maria Bossi<sup>1</sup> and Włodzimierz Kutner<sup>1,3</sup><sup>1</sup>University of Verona, Italy

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Gluten, which chemically corresponds to storage proteins deposited in the starchy endosperm cells of the developing grain, is the allergen that triggers autoimmune reactions in people suffering from celiac sprue (CS). It is estimated that CS affects 1-2% of the European population with direct healthcare costs estimated at about 3 bn EUR/year. The only effective therapy is strict dietary abstinence from gluten. In fact, even a small contamination of food with gluten can cause serious adverse reactions from digestive system. Food considered as gluten-free, thus safe for CS suffering people, should contain less than 20 mg/kg of gluten. Molecularly imprinted polymers (MIPs) are artificially made receptors with the ability to bind reversibly and therefore, to recognize the target analytes. The fabrication of MIPs against small molecules or peptides is now straightforward whereas imprinting of large molecular structures, such as proteins, is still challenging. A possible solution is to imprint just defined epitopes instead of the whole protein. In the present study, a toxic gluten epitope, PQQFPQQ, was chosen as a template for imprinting. The MIP film was prepared by electrochemical polymerization of bis(bithiophene) derivatives, bearing either cytosine or carboxylic acid substituent, in the presence of the template and a cross-linker. After deposition, the template was extracted from the polymer film. Subsequently, the film composition was characterized by x-ray photoelectron spectroscopy (XPS) as well as its morphology and thickness was studied by atomic force microscopy (AFM). Performance of this chemical sensor was tested under laboratory conditions. Extended-gate field-effect transistor (EG-FET) sensor signals were measured for an aqueous solution of the PQQFPQQ analyte, as well as its interferences with 1 or 2 mismatched amino acids. Moreover, the sensor responses were measured toward the PQQFPQQ analyte in gluten samples digested with pepsin at pH  $\approx$  2. Finally, analytical parameters of the devised chemosensor were evaluated.

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4<sup>th</sup> International Conference on **Electrochemistry**

June 11-12, 2018 | Rome, Italy

**Electrochemical reduction of carbon dioxide to value-added chemicals using copper-based catalysts****Dan Ren**

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New energy technologies have attracted unprecedented research attention since the start of this century, as they will assist in reducing our dependence on fossil fuels. Meanwhile, the increase of the atmospheric carbon dioxide concentration, which caused severe climate changes, forces us to seek for solutions to alleviate carbon emissions. One promising technology is to design systems that convert carbon dioxide to carbon-containing fuels or chemicals using renewable energy sources, such as solar or wind. Among these systems studied, electroreduction of carbon dioxide driven by photovoltaics has achieved the highest efficiency so far. While many metals could reduce carbon dioxide to formate or carbon monoxide, copper is the only metal that catalyzes the formation of hydrocarbons and alcohols such as ethylene and ethanol, with appreciable amounts. However, the selectivity is rather poor. Here, we investigate different copper structures for the selective reduction of carbon dioxide to ethylene, ethanol and n-propanol. With the aid of operando Raman spectroscopy and extensive surface characterizations, we are able to reveal the active sites for the formation of different products and offer new insights into the mechanism. While CO dimerization is the key step for the formation of ethylene, a CO-insertion mechanism is proposed to be one of the possible routes to the formation of ethanol and n-propanol. Apart from the effect of surface structures, the influence of electrochemical factors such as overpotential and the mass transport of carbon dioxide on the catalysts' selectivity are also illustrated. We find that the selectivity of copper catalysts are largely dependent on the applied potential and limiting current of the system, by analyzing 24 different copper catalysts reported by >10 research groups worldwide, including metallic, oxide-derived and chloride-derived copper particles. These studies help us design better catalysts for this catalytic reaction. A prototype device combining a solar panel with an optimized electrolyzer will be introduced as well. This device is demonstrated to produce ethylene under the intermittent natural sunlight.

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**Activated carbon felt and graphite felt as efficient electrode materials for sulfide removal from waste water streams**N Sergienko<sup>1</sup>, O Gutierrez<sup>1</sup>, I Rodriguez Roda<sup>1,2</sup> and J Radjenovic<sup>1,3</sup><sup>1</sup>Catalan Institute for Water Research, Spain<sup>2</sup>LEQUIA - University of Girona, Spain<sup>3</sup>Catalan Institution for Research and Advanced Studies, Spain

Sulfide, a by-product of many industrial processes, causes a wide number of environmental problems. Electrochemical treatment is one of the most emerging techniques used for its removal nowadays since it offers low cost treatment that allows robust removal of sulfide *in situ*. In this study we evaluated the efficiency of low cost electrode materials such as activated carbon felt (ACF) and graphite felt (GF) and proposed the mechanism of sulfide removal. In order to avoid electrode passivation with sulfur, different electrode regeneration strategies were evaluated. Both materials enabled complete removal of sulfide, with ACF requiring lower energy, i.e.,  $4.6 \times 10^{-3}$  Wh/L compared to GF ( $11 \times 10^{-3}$  Wh/L). Also, the mechanism of sulfide removal on ACF and GF was different. Sulfide removal on ACF occurred mostly due to its rapid chemisorption, as a result of which pre-adsorbed HS reacted with oxygen functional group on the ACF surface and formed elemental sulfur. The resulting sulfur was incorporated into the ACF matrix and therefore it was not available for recovery. As for GF, chemisorption also occurred, but it was slower and less efficient due to the smaller surface area of the material, lower concentration of oxygen functional groups at its surface and higher GF hydrophobicity. In addition to chemisorption, other processes contributed to sulfide removal, including electrochemical oxidation of sulfide to elemental sulfur and indirect oxidation to sulphate with oxygen produced on the anode due to parasitic reaction. To recover the GF electrode, electrodeposited sulfur was successfully reduced *in situ* to sulfide/polysulfides. In this study, we confirmed that adsorption governs the process of sulfide removal when ACF is used as an anode, while electro-oxidation likely plays a minor role. GF could be successfully applied for anodic oxidation of sulfide present in wastewater. Moreover, the possibility of *in situ* regeneration of GF electrodes prolongs the lifetime of an electrode and makes its application more sustainable..

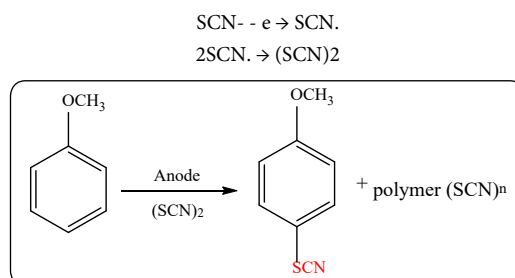
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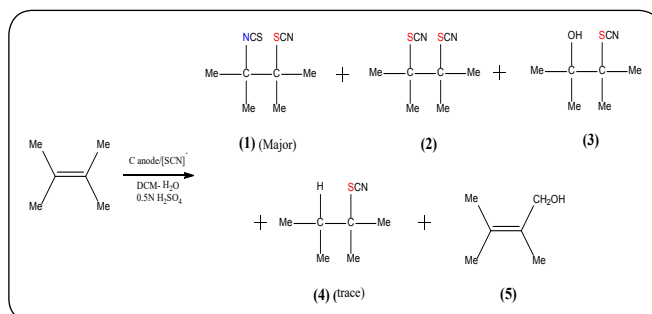
June 11-12, 2018 | Rome, Italy

**Electrochemical thiocyanation of aromatic and alkene derivatives**James Y. Becker, Avishai Levy and Anna Gitkis  
Ben-Gurion University of the Negev, Israel

The anodic thiocyanation of aromatic compounds [1, 2] showed both regio- and isomer- selectivity. For example, the para-thiocyanate isomer was formed exclusively:



The one-pot anodic thiocyanation and isothiocyanation of alkenes in both acidic two-phase (water-dichloromethane) and homogeneous one-phase (water-acetonitrile) media will be described too [3, 4]. A selected example of type of products obtained is illustrated in the scheme below:



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**Determination of lead in gunshot residue using anodic stripping voltammetry****Magdalena Wajrak**

Edith Cowan University, Australia

Lead is a naturally occurring element in the Earth's crust, which is known to negatively affect human health and can destroy ecosystems. Lead enters the body primarily through inhalation of lead containing dust and accidental ingestion. One common source of lead in the environment is from gunshot residue. The gunshot residue is a by-product of the reaction in the primer mix. The primer mix in bullets contains lead styphnate, barium nitrate, antimony sulphide, and these chemicals are all present in gunshot residue. Environments with high levels of gunshot residue, like shooting ranges, contain high levels of lead, and so measuring the lead in these environments is essential. Currently lead in gunshot residue can be determined by inductively coupled plasma (ICP) and scanning electron microscopy (SEM), however, these instruments are all laboratory based and significantly expensive. A portable instrument that can quickly and accurately assess gunshot residue samples in the field would be a useful tool in reducing the risk of lead exposure. Voltammetry can be a solution to this problem. This investigation compared ASV technique to ICP-MS in order to validate the ASV as a potential method for lead detection in gunshot residues. The linearity, repeatability and limit of detection that were determined pertained to the accuracy and precision of the instrument; only creating a 1% error of uncertainty, having a linear correlation which has an R<sup>2</sup> of above 0.999 and being able to detect lead as low as 0.01 ppb concentration. Gunshot residue samples were analysed by both ICP-MS and ASV, and this created a correlation of 0.995 for all samples. ASV is a suitable method in determining the concentration of lead in gunshot residue.

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**Sodium vs. lithium co-intercalation with diglyme electrolyte into graphite anodes: Evidence from multi-nuclear solid state NMR spectroscopy****Nicole Leifer, Miryam Fayena Greenstein, Albert Mor, Gil Goobes and Doron Aurbach**  
Bar Ilan University, Israel

The growing need for cost-effective batteries for large scale energy storage is motivating sodium-ion battery (SIB) technology development, especially in applications where energy density/weight is not crucial. However, the performance of intercalation compounds as viable electrodes for SIB has not matched the success of Li-ion batteries (LIBs). Graphite, as the most widely used anode material in current commercial LIBs, exhibits very low capacities (<35 mAh/g) as an anode material in SIBs, as compared to 372 mAh/g for Li. This has been attributed to the instability of the Na ions intercalated into graphite, unlike Li ions. By using diglyme as the electrolyte solvent, however, reversible Na intercalation in graphite was achieved with capacities reaching 80 mAh/g for up to 1000 cycles and >99% reversible capacity. The good recyclability and limited capacity fade was attributed to the concomitant intercalation of the alkali ions with coordinated diglyme molecules (co-intercalation), i.e. the formation of ternary (t)-GIC complexes upon discharge. Analogous studies with Li gave inferior results, with exfoliation of the graphite layers upon extended cycling. Computational studies suggest that the Na-diglyme complex intercalates and binds quite differently than Li-diglyme complex in the graphite. However, experimental evidences of co-intercalation are only indirect and so is their relation to the disparate electrochemical behavior of Na vs. Li. This study examined the graphite anode material, diglyme molecules and the alkali ions upon electrochemical cycling against Na or Li metal in a diglyme-based electrolyte solution via solid-state NMR spectroscopy. Direct evidence for co-intercalation, as well as qualitative and quantitative comparisons of the details of the ion-solvent-graphite interactions, are provided via <sup>23</sup>Na, <sup>7</sup>Li, <sup>1</sup>H and <sup>13</sup>C NMR measurements. The conclusion from this work should prove useful for improving the performance of other higher capacity carbon based anodes for SIBs.

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**Electrochemical determination of caffeine content in Ethiopian coffee samples using lignin modified glassy carbon electrode****Meareg Amare and Senait Aklog**  
Bahir Dar University, Ethiopia

Lignin film was deposited at the surface of glassy carbon electrode potentiostatically. In contrast to the unmodified glassy carbon electrode, an oxidative peak with an improved current and overpotential for caffeine at modified electrode showed catalytic activity of the modifier towards oxidation of caffeine. Linear dependence of peak current on caffeine concentration in the range  $6 \times 10^{-6}$  to  $100 \times 10^{-6}$  molL<sup>-1</sup> with determination coefficient and method detection limit (LoD=3 s/slope) of 0.99925 and  $8.37 \times 10^{-7}$  molL<sup>-1</sup>, respectively, supplemented by recovery results of 93.79–102.17% validated the developed method. An attempt was made to determine the caffeine content of aqueous coffee extracts of Ethiopian coffees grown in four coffee cultivating localities (Wonbera, Wollega, Finote Selam, and Zegie) and hence to evaluate the correlation between users preference and caffeine content. In agreement with reported works, caffeine contents (w/w%) of 0.164 in Wonbera coffee; 0.134 in Wollega coffee; 0.097 in Finote Selam coffee; and 0.089 in Zegie coffee were detected confirming the applicability of the developed method for determination of caffeine in a complex matrix environment. The result indicated that users' highest preference for Wonbera and least preference for Zegie cultivated coffees are in agreement with the caffeine content.

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**Two-dimensional metal chalcogenides analogous NiSe<sub>2</sub> nanosheets and its efficient electrocatalytic performance towards glucose sensing****Sukanya Ramaraj, Sakhivel Mani and Shen Ming Chen**  
National Taipei University of Technology, Taiwan

Recently, 2D layered transition metal dichalcogenide materials have received great consideration because of their unique electronic properties, large surface area and high electrocatalytic activity. In this connection, for the first time the similar nanostructured material of NiSe<sub>2</sub> nanosheets (NiSe<sub>2</sub>-NS) has been synthesized by a facile hydrothermal method for electrocatalytic applications. Scanning electron microscopy (SEM), transmission electron microscopy (TEM), x-ray photoelectron spectroscopy (XPS), energy dispersive x-ray analysis (EDX) and x-ray diffraction spectrum (XRD) results confirmed the formation of NiSe<sub>2</sub>-NS with required stoichiometry and morphology. Electrochemical impedance spectroscopy (EIS) data indicate that electron transfer is facile at the NiSe<sub>2</sub>-NS modified glassy carbon electrode (GCE). It has been an electrode modifier for glucose sensing applications. The electrochemical studies were performed for NiSe<sub>2</sub>-NS modified GCE using cyclic voltammetry (CV) and Amperometric i-t techniques. The results are suggesting the effective response of NiSe<sub>2</sub>-NS/GCE with a very low limit of detection (LOD) and sensitivity of 23 nM and 5.6  $\mu\text{A } \mu\text{M}^{-1}\text{cm}^{-2}$  respectively. Moreover, the selectivity data exhibited excellent anti-interference property of NiSe<sub>2</sub>-NS/GCE towards glucose in the presence of possible interfering agents viz. ascorbic acid, dopamine, and glucose.

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**Equilibrium electro-osmotic instability in concentration polarization at a perfectly charge-selective interface****Isaak Rubinstein**

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**E**quilibrium electroosmotic instability in concentration polarization at a perfectly charge-selective solid, such as ion-exchange membrane or metal electrode, previously deemed impossible, is possible if one takes into account the finite electrical conductivity of the solid. A simple model for electro-convective diffusion of ions in the depleted diffusion layer predicts a supercritical transition to instability in the vicinity of the limiting current, as opposed to the subcritical transition for the previously studied non-equilibrium instability related to the extended space charge. The linear stability analysis in this model yields the division of the parameter space into domains in which each instability mechanism with its characteristic signatures dominates. Identification of the particular instability mechanism for a given system requires a detailed experimental study of the vicinity of the instability threshold in terms of both the voltage versus current dependence and flow visualization.

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**Advanced carbon materials for energy storage****Vinod Nair**

Farad Power Inc., USA

Farad Power is engaged in developing new methods for making activated carbon with a higher surface area, pore volume and specific capacitance values compared to the coconut shell based carbons. This talk will present some of the recent results obtained from these new carbon materials. Carbon for supercapacitors: With our carbons, we have achieved 30% improvements in capacitance over the industry-standard carbon used today with better resistance. I expect another 40-50% improvement by electrode density optimization (including jet-milling, which we had not done for our measurements). This will give specific capacitance of 150 F/gm (compared to the industry standard of 100 F/gm); Hard Carbon for LiB & SiB batteries: This product is used as an anode material in lithium-ion and sodium-ion batteries (e.g. in a typical Tesla car today, about 58 Kg of anode carbon is used). We have characterized the materials with x-ray diffraction and Raman spectroscopy and it has better parameters than other hard carbons we have evaluated; Carbon for LiB & SiB cathodes: We have developed a carbon with pores less than 1 nm using a new chemical activation method. This material is being evaluated for lithium batteries (with sulfur and selenium cathodes) with very high energy densities (>500 Wh/Kg), for a potential EV battery application; Carbon Enhanced Lead-Acid Batteries: Replacing partially or completely the lead electrodes in lead acid batteries to reduce the sulfation problems and enhancing the charge acceptance, power density and cycle life of conventional lead acid batteries; Meso porous carbon: This is a carbon material with large quantities of mesopores (2-3 nm range) for gasoline vapor emission control. This material can reversibly adsorb and desorb gasoline vapors so that the evaporative loss during parking can be virtually eliminated.

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4<sup>th</sup> International Conference on **Electrochemistry**

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**Enzyme engineering in bioelectrochemical systems****Lital Alfonta**

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Coupling between redox enzymes and electrodes relies first and foremost on a successful interfacing between the enzymes and the inorganic surfaces with which they interact. An interface that allows from one hand a specific analyte recognition and on the other hand an efficient signal transduction. Some of the challenges in interfacing between biological molecules and inorganic materials stem from wrong orientation of the enzyme towards the interface and from the need to use mediated electron transfer with a diffusional redox mediator due to a difficulty in relaying a signal from a redox center that is deeply buried inside the protein matrix. Using genetic code expansion tools, and genetic engineering approaches we were able to modify redox enzymes and surfaces for biosensing and biofuel cell applications so they could have superior properties over native enzymes. In my talk, I will demonstrate how does site-specific wiring of redox enzymes which is genetically encoded, can improve electron transfer due to controlled and short electron transfer distances and due to proper enzyme orientation. I will also demonstrate how a rational genetic engineering of an enzyme gives it superior properties and activity, compared to those of the native enzyme.

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**Development of multilayered porous composite silicon/graphite/metal oxide thin film anodes for Li – ion batteries****V Madhusudhan Rao<sup>1</sup>** and **M Venkateswarlu<sup>2</sup>**<sup>1</sup>Vignan's University, India<sup>2</sup>Amara Raja Batteries Ltd., India

Multilayered porous composite silicon/graphite/metal oxide thin films are produced using chemical vapour deposition (CVD) and sputtering techniques as potential anode material for lithium-ion batteries. The x-ray diffraction (XRD) and Fourier transform infrared spectroscopy studies confirmed the phase and structural co-ordination. The formation of uniform silicon and graphite layers are confirmed by high resolution transmission electron microscopy (HRTEM) and energy dispersive x-ray spectroscopy (EDS). Li insertion/extraction evaluation was performed mainly with cyclic voltammetry (CV) and constant current charge discharge cycling. The cycleability and Li ion accommodation capacity were found to depend on the film thickness. Film of thickness upto 500 Å gave charge capacity over 4100 mAh g<sup>-1</sup> and maintained upto 100 cycles, while a 1000 Å and more thick films were able to give capacity upto 2500 mAh. g<sup>-1</sup>. The performance of thin films of thickness less than 500 Å (Sample 1), less than 1000 Å (Sample 2) and more than 1000 Å is shown in the graph .

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