Energy Storage Discussion 2019

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Book of abstracts

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Program

Monday, October 14th		Tuesday, October 15th		Wednesday, October 16th		Thursday, October 17th	
Time		Time		Time		Time	
10:00 - 14:00	Invitational "Supercapacitors" workshop for experts	08:30	Registration to the conference			11:00 - 14:00	Invitational "Simulation of batteries" workshop for experts
		09:00	Opening ceremony				
		09:20	Keynote talk "**Carbon Nanotubes for Capacitive Electrodes**" By Prof. George Chen	09:20	Keynote talk "**Role of spectroscopic techniques in characterization of electrode/electrolyte interface reactions in Li-ion batteries**" by Dr. Jolanta Swiatowska		
		10:20	Oral Session 1	10:20	Oral session 3		
		11:20	Poster session with coffee break	11:20	Coffee break		
				11:40	Keynote talk "**Uncovering the properties of cathode materials for rechargeable Li, Na, Mg and Ca-ion batteries by computational means**" by Dr. Ma. Elena Arroyo		
				12:40	Oral session 4		
		13:20	Pause	13:40	Pause		
		16:00	Keynote talk "**Towards Developing High Performance Li-batteries: Advanced Experimental and Simulation Techniques** " By Dr. Mahbub Islam	16:00	Round Table: "**Present and prospectives of Energy Storage**"		
		17:00	Oral session 2	17:30	**Closing ceremony**		
		18:00	Coffee break	17:40	Coffee break		
		18:20	Talk "**the potential of energy storage in the national electricity system**" by Dr. Roberto U. Ruiz-Saucedo	18:00	Closed Meeting of the Technical-Academic Committee of the mexican Energy Storage Network		
		18:50	Talk "**The Energy Storage Network and the National Lab for Energy Conversion and Storage**"				
		19:20	Concluding remarks of day 1				

Oral session 1		**Tuesday, October 15th, 10:20-11:20 Chairman: Dr. Raúl Lucio Porto (UANL)**
ID	**Name of the work**	**Authors**
Cap_11	Sustainable production of bio-derived carbons using concentrated solar energy for their use in Supercapacitors	Ana Karina Cuentas-Gallegos, Diana C. Martínez-Casillas, Diego R. Lobato-Peralta, Alejandro Ayala-Cortés, Heidi I. Villafán-Vidales, Camilo A. Arancibia-Bulnes, Víctor H. Sánchez-Ramos, Daniella E. Pacheco-Catalán.
Cap_06	Synthesis of nanoporous carbon from red onion waste: evaluation of the catalytic activity for the oxygen reduction reaction and the capacitance	P.C. Meléndez-González, O.J. Duarte-Urbina, F. Fernández-Luqueño, B. Escobar-Morales, P. Quintana, F.J. Rodríguez-Varela, I.L. Alonso-Lemus
Oral session 2		**Tuesday, October 15th, 17:00-18:00 Chairman: Dr. Ignacio González Martínez (UAM)**
ID	Name of the work	Authors
Sim_03	A kinetic and model approach to describe the intercalation and de-intercalation of Li+ in an electrode for Ion lithium battery.	I. O. Santos-Mendoza, G. Aparicio-Mauricio, J. Vazquez-Arenas, C. O. Castillo-Araiza
Sim_01	Quantum Capacitance Beyond the Rigid Band Approximation in N doped Graphene	Álvaro Ochoa-Calle, Alfredo Guevara-García, Jorge Vazquez-Arenas, Ignacio González, Marcelo Galván
Oral session 3		**Wednesday, october 16th, 10:20 - 11:20 Chairman: Dr. Eduardo M. Sánchez Cervantes (UANL)**
ID	Name of the work	Authors
Bat_01	From Materials design to pouch cells applications at electrochemical Energy laboratory UAM	M. Oliver-Tolentino, G. Ramos-Sánchez, G. Guzman, E. J Canto-Aguila, J. Alcaraz, R. Suarez, A. Guevara-García, M. Martínez-Cruz, C. Juarez-Yescas, C. Islas-Vargas, S.N. Arellano-Ahumada, C. Moreno-Crespo, T. Paulino, C.I. Lopéz, M. Galvan, M. Vera, F. González, D. Ramírez-Rosales, I. Padilla-Martinez, E. Haro, A. Manzo-Robledo, H. Pfeiffer, I. Gonzalez
Bat_06	Effect of Na-preconditioning of silicon anodes for Li ion batteries	E. Espinosa-Villatoro, J.S. Ko,J.L. Nelson-Weker, E. Quiroga-González
Oral session 4		**Wednesday, october 16th, 10:20 - 11:20 Chairman: Dr. Jorge G. Vazquez Arenas (UAM)**
ID	Name of the work	Authors
Bat_19	Effect on the thermal treatment on the Anatase to Bronze conversion of TiO_2 and its electrochemical performance as a cathode for hybrid Li+/Mg^{+2} ion batteries	Edgar González-Juárez, Rubí A. Hernández-Carrillo, Fabiola García-Gutiérrez, Nayelly Pineda-Aguilar, Domingo I. García-Gutiérrez, Lorena Garza-Tovar, Eduardo M. Sánchez

Oth_16	Manufacturing Zn^{2+} ion secondary batteries from recycling exhausted Zn/C primary cells	J.C. Calva-Yañez, M.T. Oropeza-Guzmán, O.A. Jaramillo-Quintero, M. Solís de la Fuente, M.E. Rincón

Poster session		**Tuesday, October 15th 11:20 - 13:20**
ID	**Name of the work**	**Authors**
Bat_02	Influence of electron conductive additives in electrochemical performance of Lithium-Sulphur Batteries	A. González[1], M. Pineda[1], T. Paulino[1], J. Flores[1], H. Ávila[1], I. González[2], G. Ramos[2], G. Guzmán[2]
Bat_03	Synthesis and characterization of lithium ferrite (Li_5FeO_4) for lithium ion battery application.	F. Reséndiz-Marco1, G. I. Espinoza-Salgado1, C. Juarez-Yescas, I. González1 and G. Ramos-Sánchez1,2
Bat_04	Si nanowalls as anode for lithium ion batteries	V. Aca-López[1], E. Quiroga-González[2], J. Światowska[3], E. Gómez-Barojas[1] and A. Luna-López[1]
Bat_05	Onyx anodes for Li-ion batteries	E. Morales-Merino1, E. Quiroga-González2
Bat_07	Transition metal hexacyanocobaltates for potassium storage applications	E. J Canto-Aguilar1, M. A. Oliver-Tolentino1, I. González-Martínez1
Bat_08	Ionic liquid effect on MoS_2 synthesis and its behavior as anode material for lithium ion batteries	R. Briones Martínez1, S. M. de la Parra Arciniega1, L. L. Garza Tovar1, R. M. Jiménez Barrera2, E. M. Sánchez Cervantes1
Bat_09	Synthesis of Reduced Graphene oxide/TiO_2 composites as anode material of lithium ion batteries	G. Santamaría-Juarez[1], E. Gómez-Barojas[1], E. Quiroga-González[2], E. Sanchéz-Mora[2] and J. D. Santamaría Juarez[3]
Bat_10	Solvothermal synthesis of Sb_2S_3 and its application as anode for Li-ion battery	O.E. Gutiérrez-Garza1, E. Quiroga-González2 and L.L. Garza-Tovar1
Bat_11	Implementation of in situ X-Ray Diffraction studies for lithium Ion battery materials	Miguel Ángel Martínez-Cruz1, C. Juarez Yescas1, Ignacio González1, Miguel Ángel Oliver-Tolentino1,3, Guadalupe Ramos-Sánchez1, Federico González1
Bat_12	Macroporous Si decorated with TiO_2 nanoparticles as anode material for lithium ion batteries	E. Gómez-Barojas1, G. Santamaría-Juárez1, E. Quiroga-González2, and E. Sanchéz-Mora2
Bat_13	High energy density Pouch cell design and manufacture based on $LiCoO_2$ cathodes	Carlos Iván López-Vicente1, Tomasa Paulino-Segundo1, Guadalupe Ramos-Sánchez1

Bat_14	Separators for ion intercalation batteries based on biopolymers modified by ceramic nanoparticles addition	K. Y. Martínez-Paredes1, I. I. Leal-Villanueva1, D. Burgos1, G. Ramos-Sánchez1,2, H. J. Ávila-Paredes1, I. González3 and G. Guzmán-González1, 2
Bat_15	Role of metal ion on the distribution of charge density in metal organic frameworks used as anodes in lithium ion batteries	S. N. Arellano-Ahumada1, M. A. Oliver-Tolentino2, G. Ramos-Sánchez2, C. E. Moreno-Crespo1, I. I. Padilla-Martínez3, I. González4. D. Ramírez-Rosales1
Bat_16	Impedance spectra analysis of $LiFePO_4$ by means of EEC in a three-electrodes set up cell	Ruben Suarez1, Ignacio Gonzalez1, Guadalupe Sanchez1 and Gregorio Guzman1
Bat_17	Study of the SbxSbySz/carbon nanofibers composite as anode of sodium ion batteries	L.A. Rodríguez-Guadarrama1, J. Escorcia- García2, E. Quiroga-González3, J. Campos-Álvarez4 y I.L. Alonso-Lemus5.
Bat_18	Diffusion of lithium in porous germanium for lithium-ion battery applications	A. N. Sosa, A. Trejo, M. Cruz-Irisson
Bat_20	Sulfured Multiwall Carbon Nanotubes as Cathode for Li ion batteries using a chitosan-starch based electrolyte	Y. Estévez-Martínez1, L. Rángel-Ángel1, E. Quiroga-González2 and V.M. Castaño-Meneses3
Bat_21	Preparation of Graphene Aerogels with MnO_2 Nanorods and Polivinylidene Fluoride for Li-ion Battery Applications	Ortiz-Rodríguez, J. C.1, Ku-Herrera J. J.2, Acosta-Ortiz, R.1, Ramos-Sánchez G.3, Guzmán-González, G.4, Jiménez-Barrera R. M2
Bat_22	Study of composite material of SnO_2/PANI/ RGOODA for their application in Li- battery	L. Solís-Méndez[1], J.M. Baas-López[2], E. Enrique Quiroga-González[3], J. A. Uribe-Alonso[1], D. Pacheco-Catalán[2]
Cap_01	Supramolecular assembly of nanostructured conducting polymer hydrogels by hydrotropic agents for energy storage applications	José J. Alcaraz-Espinoza[1], Gregorio Guzmán-González[2], Guadalupe Ramos-Sánchez[2] and Ignacio González[1]
Cap_02	Thin-film YSZ electrolyte on all solid state Nanosupercapacitor based on Symmetric Ru electrodes for mild temperatures	J.L. Vazquez[1], O. Romo[1], C. López[1], R. López-Noda[2], F. Solorio[3], E. Lizarraga[1], H. Tiznado[1] and J. Read[4]
Cap_03	Chemical vapor deposition few layer graphene films for microsupercapacitors	G. Moreno-Muñoz[1], J. M. Baas-Lopez[1], D. E. Pacheco-Catalán[1]
Cap_04	Performance as a supercapacitor under potentiostatic floating tests of carbon electrodes prepared from avocado stones	A.G. Sánchez Valdez[1], L.L. Garza Tovar[1], E.M. Sánchez Cervantes[1], D.E. Pacheco Catalán2 and L.C. Torres González1

Cap_05	Bimodal mesoporous carbons - PMo$_{12}$ composites for supercapacitor	E. Fuentes Quezada[1], D. C. Martínez Casillas[2], E. de la Llave[3], A. K. Cuentas Gallegos[2]
Cap_07	Nanostructured VOPO$_4$ for Electrochemical Capacitors	Jorge Zuñiga Martínez[1,2], Sara Elena González Náñez[1,2] , Raúl Lucio Porto[1,2,] Thierry Brousse[3], Iván Eleazar Moreno Cortez[1,2], Luis Alberto López Pavón[1,2].
Cap_08	$Mn_3(PO_4)_2\cdot 7H_2O$ as Electrode Material for Electrochemical Capacitors	Karla Cristina Alanís Estrada[1,2], César Iván García Guajardo[1,2], Jorge Alexis Zúñiga Martínez[1,2], Valeria Elizabeth Ulloa Zúñiga[1,2], Raúl Lucio Porto[1,2,*], Thierry Brousse[3], Iván Eleazar Moreno Cortez[1,2], Luis Alberto López Pavón[1,2]
Cap_09	MnHPO$_4$ as Electrode Material for Electrochemical Capacitors	Elaine Stefany Jara Arreozola[1,2], César Iván García Guajardo[1,2], Jorge Alexis Zúñiga Martínez[1,2], Valeria Elizabeth Ulloa Zúñiga[1,2], Raúl Lucio Porto[1,2,*], Thierry Brousse[3], Iván Eleazar Moreno Cortez[1,2], Luis Alberto López Pavón[1,2]
Cap_10	Green supercapacitors assembled with activated carbons obtained from Agave residues by solar pyrolysis	D.R. Lobato-Peralta[1], D. C. Martínez-Casillas[1], H.I. Villafán-Vidales[1], C.A. Arancibia-Bulnes[1] and A.K. Cuentas-Gallegos[1]
Oth_02	Magnesium alloys for hydrogen storage	M. Osorio-García1, O. Hernández Silva1, C. Casas Quesada2, J.M. Cabrera2, A. Tejeda Ochoa3,4, J. M. Herrera-Ramírez3, Y. Todaka4, K. Suárez-Alcántara5, J. L. Carrillo-Bucio5, J. G. Cabañas Moreno1
Oth_03	Synthesis of vanadium oxide as phase change material for mitigate energy use in buildings	C. Y. Fragoso F.[1], M. Z. Figueroa -Torres.[1], J. R. Gonzalez-López.[1], A.A. Zaldívar-Cadena[1]
Oth_04	Synthesis of nanohybrid aerogels based on GO-TiO$_2$/PVDF for energy storage applications	Durón-Sánchez, L. H. I1, Jiménez-Barrera, R. M.2, Soriano-Corral, F.1, Soria-Arguello, G.2, Rodríguez-Ortíz, J.C.1, Ku-Herrera J. J.2
Oth_05	Effect of dispersion on the average intercalation voltage in Prussian Blue Analogues	C. Islas-Vargas1, A. Guevara-García2, M. Oliver-Tolentino2, G. Ramos-Sánchez2, I. González1 and M. Galván1
Oth_06	Synthesis of LiMn$_{1.5}$Ni$_{0.5}$O$_4$ (LMNO) high voltage spinel cathode	J. Olmedo-González1,2,3, O. F. Plascencia-Hernández3, H. Pfeiffer3, R de G. González-Huerta1, G. Ramos-Sánchez2
Oth_07	Study of gases generation in Li2CuO$_2$ cathode through Differential Electrochemical Mass Spectrometry in situ (DEMS-in situ)	C. Juarez-Yescas[1], J. Olmedo-González[1,2], M.A. Oliver Tolentino[1], A. Manzo-Robledo[2], R de G. González-Huerta[2], I. González[1], G. Ramos-Sánchez[1,3]
Oth_08	Fungi-derived hierarchically porous carbon for energy storage application	P.N. García Hernández[1], J.M. Baas López[1], T. Thompson[1], R. A. Valdez-Ojeda[1], D. Pacheco-Catalán[1]
Oth_09	Cerium oxide thin films as electrolyte in SOFC	U. Garduño[1], M. García[1], I. Zumeta[1] and E. Espinoza[2]

Oth_10	Cerium oxide films for photoelectrocatalytic applications	Gabriela Mariela Reyes Chaparro[1], Inti Zumeta Dubé[1], José Manuel García Rangel[2], Mario Fidel García Sánchez[1]
Oth_11	Transition metal pentacyanoferrates: a new family of materials for energy storage in aqueous solutions	Grisel Hernández-Cortés1, Juvencio Vazquez-Samperio 1,2 , Ariel Guzmán-Vargas 2, Edilso Reguera-Ruíz 1, Próspero Acevedo-Peña3
Oth_12	Mathematical modeling for the adjustment of parameters of a battery Title of the abstract	M. Villegas1, M. Camas1 and A. Coronado1
Oth_13	From gasifier residue to useful material for energy storage	Diana C. Martínez-Casillas[1,2], I. Mascorro-Gutierréz[1], María L. Betancourt-Mendiola[3], Gabriela Palestino [3], Enrique Quiroga-González[4], and A. Karina Cuentas-Gallegos[1]
Oth_14	Immobilization of POMs on carbon nanotubes for the development of Negative electrodes for hybrid energy storage devices	C. Medrano[1] and A.K. Cuentas[1]
Oth_15	Sb/Sb_2O_3/carbon nanocomposites for Li-ion storage: Effect of the carbon matrix dimensionality	O.A. Jaramillo-Quintero[1], J.L. García-Ocampo[2] and M.E. Rincón[2]
Oth_17	Improving the Electrochemical Behavior of Layered Cobaltous Terephtalate by Co-Co Interaction Through Pyrazine Linker	J. Vazquez-Samperio[1,2], P. Acevedo-Peña[3], M. Oliver-Tolentino[4], I. Padilla-Martinez[5], M. Gonzalez-Montiel[3], A. Guzmán-Vargas[2], E. Reguera-Ruíz[1]
Oth_18	Protocol for evaluation of the ionic conductivity in alkaline anion exchange membranes	Elvia Palacios L.[1], Consolación Medrano V.[1], Tatiana Romero C.[1], J. Roberto Flores H.[1]
Oth_19	New generation GDLs´performance characterization for fuel cell technology	I. Lorena Albarrán S.[1], Irati Azkona B.[1], Tatiana Romero C.[1], J. Roberto Flores H.[1]
Oth_20	Adsorbed Methane Molecules in a Heteroestructured System	Jade A. Galicia1, Ana A. Lemus-Santana1, Benjamín Portales M1., Erick A. Juarez-Arellano2, Edilso Reguera1
Sim_02	Ab initio calculation of the effect of M-N (M= Fe, Ni, Co) on the stability and catalytic activity for the Oxygen Reduction Reaction in Metal-Air batteries	Deysi Gómez-Cholula[1], Guadalupe Ramos-Sánchez[1,2], and Ignacio.González[1]
Sim_02	Hydrogen storage on Mg and Ca-functionalized siligene: A DFT study	B.J. Cid[1], J.E. González[1], M.C. Crisóstomo[2], A. Miranda[1], M. Cruz-Irisson[1]

Bat_23	Probe Lithiation Behavior of Conversion-type Anode Materials Using Synchrotron Chemical Microscopy	Yang Ren[1,2]* Jesse S. Ko[1], Robert M. Kasse[1], Bor-Rong Chen[1] Xuefeng Song[3], Michael Toney[1], and Johanna Nelson Weker[1γ]

Keynote Talks

K1

Role of spectroscopic techniques in characterization of electrode/electrolyte interface reactions in Li-ion batteries

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Understanding the electrode processes occurring at the electrode/electrolyte interfaces and in the bulk electrode materials is necessary for development of high energy density batteries (lithium-ion, sodium-ion or sulfur batteries) for portable and transport applications. The main electrode processes in Li-ion batteries (LIB) are insertion/extraction reactions that induce chemical and morphological changes in the positive and negative electrode materials. These reactions are accompanied by decomposition of electrolyte that leads to formation of passive layer. The passive layer formed on the negative electrode material, widely known as a solid electrolyte interphase (SEI) layer [1], strongly influences the battery performance and cycle life of battery. Much thinner passive layer named as a solid permeable interphase (SPI) layer [1], can be formed on the positive electrode material. The mechanism of electrode passivation is even more complicated if the electrode material is not stable during the process of lithiation/delithiation and cycling and undergoes the volume changes expansion/shrinkage. The strong electrode modifications occur in the case of high capacity alloying or conversion-type electrode materials, such as Si-based or transition metal oxide/sulfide-base materials, respectively [2, 3].

To have a better insight into these different reactions induced by electrochemical processes the advanced surface-sensitive techniques: X–ray photoelectron spectroscopy (XPS) and time-of-flight secondary ion mass spectrometry (ToF-SIMS) are particularly suitable for characterization of chemical modifications of electrode materials. Apart the chemical composition of the surface SEI layer, a dynamic increase/decrease of SEI upon lithiation/delithiation, and the irreversible chemical and volume modifications of electrode materials upon cycling evidenced by ToF-SIMS ion depth profiles will be discussed. Using ToF-SIMS ion depth concentration profiles the ionic transport properties of different electrode materials can be estimated [4]. The ionic transport of Li can be limited by Li trapping in the bulk of electrode material, at the interfaces, formation and growth of the SEI layer.

References

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K2

Carbon Nanotubes for Capacitive Electrodes

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Nano-structured carbon materials including carbon nanotubes (CNTs), graphenes and activated carbons (ACs) of high specific surface areas play an important role in electrochemical energy storage (EES) technologies, particularly for supercapacitors [1a]. Whilst ACs have been commercially exploited widely, graphenes are on the top of list of EES research activities. However, CNTs are in fact advantageous in several aspects compared with ACs and graphenes. CNTs have higher conductivities than ACs, and can be utilised as filler and scaffolder for composite materials. Unlike graphenes which are thin layers and stack up readily (face-to-face) in parallel to the electrode surface, and hence block ion movement through the layers, CNTs can pack naturally in random orientations, or grow aligned in perpendicular to the electrode surface, constructing hierarchically porous structures that are highly beneficial to ion movement. Interfacial conjugation between CNTs and conducting polymer also helps increase the charge storage capacity [1b]. There is however a challenge to use catalytically produced commercial CNTs which are long and curved and hence highly entangled [1c], making it difficult to disperse in a liquid medium for further processing. In laboratory practice, entangled CNTs are partially oxidised in mixed sulfuric and nitric acids, producing very effectively shortened and anionised CNTs that disperse in aqueous solutions easily [2a]. Using such processed CNTs for supercapacitor application was very successful in laboratory [1a, 2b, 2c]. Unfortunate, with nitric acid as an oxidant, emission of nitrogen oxides (NOx) is inevitable, preventing commercial application. This presentation analyses the roles of CNTs in composite materials for supercapacitor electrodes, and also new and cleaner approaches for NOx-free oxidation of CNTs [3].

References

[1] (a) C. Wei, B. Akinwolemiwa, L. Yu, D. Hu, G. Z. Chen, in *Polymer Composites with Functionalized Nanoparticles* (Eds: K. Pielichowski, T. M. Majka), Elsevier, New York (2019) 211–248. (b) G. Z. Chen, *Prog. Nat. Sci.-Mater. Int.* 23 (2013) 245. (c) H. G. Tennent, *US Patent 4663230*, 1984.

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[3] C. H. Wei, B. Akinwolemiwa, Q. F. Wang, L. Guan, L. Xia, D. Hu, B. C. Tang, L. P. Yu, G. Z. Chen, ***Adv. Sust. Sys.*** (2019) 1900065 (7 pages).

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K3

Uncovering the properties of cathode materials for rechargeable Li, Na, Mg and Ca-ion batteries by computational means

M.E. Arroyo y de Dompablo[1]

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Electrochemical energy storage systems are one of the key energy-storage technologies. Among them, lithium-ion batteries (LIB) are used in portable electronic devices, and may offer a possible near-term solution for environment-friendly transportation and energy storage for renewable energies sources. The functioning of LIB is based on the use of cathode materials reacting through Li intercalation reactions. Many electrode characteristics of Li-intercalation materials can be anticipated and investigated in depth using computational techniques at the Density Functional Theory (DFT). The success of such approach has been extensively demonstrated in the last two decades [1]. The general strategy is firstly to calculate average voltage and volume changes associated to the Li insertion reaction. Further, DFT could be applied to gather additional information regarding electronic and ionic conductivities, crystal structure of intercalated phases and precise voltage-composition-curves at various temperatures. Importantly, there are no restrictions for the DFT exploration of either existing or virtual materials (i.e. materials not having been achieved experimentally) and this paves the road to the discovery of electrode materials for battery technologies based on the intercalation of metal-ions other than Li. In this communication we will present an overview of the field including Li, Na, Mg and Ca-ion intercalation cathode materials.

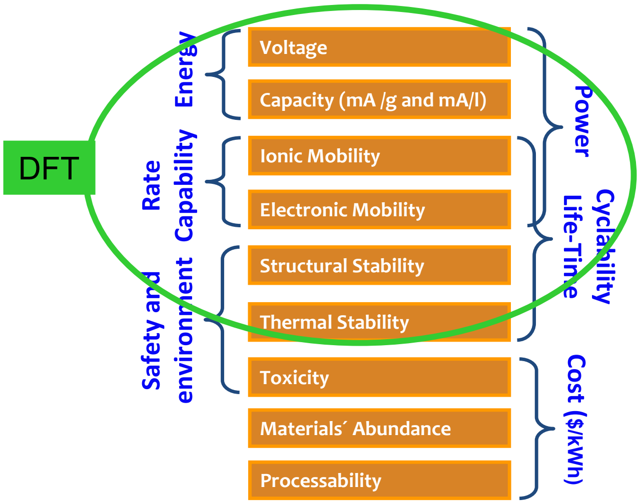

Fig. 1: Relevant cathode properties manageable by DFT methods [1].

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[1] Y.S. Meng and M.E. Arroyo-de Dompablo, *Accounts of Chemical Research* 46 (2013) 1171

K4

Towards Developing High Performance Li-batteries: Advanced Experimental and Simulation Techniques

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Rechargeable lithium-sulfur (Li-S) batteries exhibit tremendous potential as an alternative to the current lithium-ion batteries, however, the challenges such as low cycle life, poor coulombic efficiency, and high self-discharge hinders their commercial applications. Conventional carbon materials have poor adsorption towards polysulfide thus possesses limitations in trapping polysulfides within the cathode material to prevent their shuttling. Therefore, a quest for alternative sulfur-hosting materials has received significant research thrust in the Li-S battery field. Transition metal dichalcogenides (TMDs) are promising as catalyst at the cathode surface to stabilize polysulfide shuttle process along with enhancement in its redox kinetics. The interaction between catalyst and polysulfide has been evaluated from the *in situ* spectro-electrochemical studies. The introduction of catalyst-based cathodes in the Li-S system is expected to open a new avenue for improving electrochemical performance. Addition to the experimental studies, first-principles based atomistic modeling is playing an increasingly important role in the design and understanding the battery chemistry. The molecular dynamics (MD) simulations are employed to examine the mechanistic details of the degradation of lithiated sulfur cathode materials at nanoscale during battery operation. Finally, atomistic scale simulations to address the grand challenges in understanding complex interfacial chemistry in Li-ion batteries will also be presented.

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Oral

Cap_11

Sustainable production of bio-derived carbons using concentrated solar energy for their use in Supercapacitors

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Bio-derived carbons are carbon-based products obtained from pyrolysis of biomass, and if they show the adequate structural and chemical properties they can be applied as electrodes in supercapacitors. Solar pyrolysis is of great interest due to the environmental advantages, where pyrolysis operation parameters such as temperature, heating rate, and solar radiation affect the physicochemical properties of the obtained bio-derived carbons. Our work is focused on the influence of solar pyrolysis operation parameters and biomass composition in the physicochemical properties of carbons, and how these properties influences the energy storage properties in supercapacitor cells of carbons obtained from agave angustifolia, pecan nutshell, and tomato pruning wastes. The different biomasses were first characterized, to quantify their lignin, cellulose, hemicellulose, and ash composition. Bio-derived carbons were obtained by solar pyrolysis in the 25kW IER-UNAM solar furnace, using temperatures from 500ºC up to 1600ºC, and heating ramps between 4 and 30 C/min. Structure of bio-derived carbons were characterized by physisorption, XRD, SEM, and RAMAN spectroscopy. Surface chemistry was determined from elemental analysis, EDS, and Infrared spectroscopy for all carbons. In addition, electrochemical energy storage mechanisms were determined in aqueous electrolytes by cyclic voltammetry in 3-electrode cells, obtaining a capacitive behavior with minor pseudocapacitive contribution from heteroatoms. Specific capacitances up to 80-115 F/g for carbons from agave angustifolia, 90-190 F/g from tomato pruning residues, and 100-160 F/g for H_3PO_4-activated carbons from pecan nut shell were obtained. The best bio-derived carbons were used to assemble 2-electrode supercapacitor cells, and studied by galvanostatic charge-discharge cycles. The best performance in supercapacitor cells from these bio-derived carbons resulted in 20-40 F/g with cycling stability up to 5000 cycles, with specific energy of 5-9 Wh/kg and specific power of 200-1000 W/Kg.

Cap_06

Synthesis of nanoporous carbon from red onion waste: evaluation of the catalytic activity for the oxygen reduction reaction and the capacitance.

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Red onion rubbish, a world-wide available abundant waste, is a potential source of carbon containing several chemically active heteroatoms. In this work, novel red onion-waste derived self-doped porous biocarbons were successfully obtained by a simple thermochemical process. The effect of heat treatment temperature on their structural features, porous complexity and carbon chemistry were analyzed. In addition, these properties of the biocarbons, used here as electrocatalysts, were correlated with their catalytic activity for the Oxygen Reduction Reaction (ORR) and specific capacitance, both evaluated in alkaline media. The most active metal-free electrocatalyst, labelled as RWB800, has a remarkable high catalytic activity for the ORR, with an onset potential of 0.97 V vs. RHE, a number of electrons transferred of 3.9 and a percentage of hydrogen peroxide between 1.2 and 12 %. Moreover, RWB800 showed a high specific capacitance of up to 309 F g^{-1}. In addition, the process to produce the biocarbons proposed in this work can be easily scalable, thus offering a sustainable alternative for the use of onion wastes in the large-scale production of low-cost electrodes for electrochemical devices, employed for clean energy generation and storage such as anion exchange membrane fuel cells and supercapacitors.

Sim_03

A kinetic and model approach to describe the intercalation and de-intercalation of Li^+ in an electrode for Ion lithium battery.

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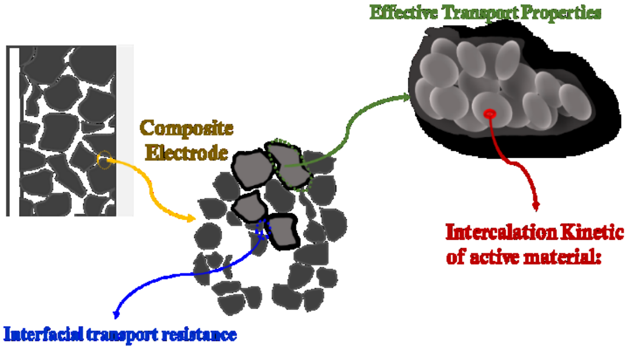
Two main criticisms have been claimed regarding the actual models (first principle) for Li-ion batteries: the lack and intricacy of experimental techniques to determine isolated transport parameters [1], and the formalism to explain the interactions arising between active and inactive components of the composite (i.e. pseudo-2D model) with the intercalation/de-intercalation mechanism of Li^+ ions in very complex geometries (i.e. porous composite) [2–5]. Therefore, a new model is proposed describing the electrode based on the kinetic approach of the coverage of Li^+ and the maximum thermodynamic capacity of Li^+ at several C-Rates, obtained with an experimental design. The kinetic model is coupled to the cell model without the typical particle conception for active material, while a continuum medium with effective transport parameters was considered for the electrode; the model also accounts for the interfacial transport between solid and liquid phases.



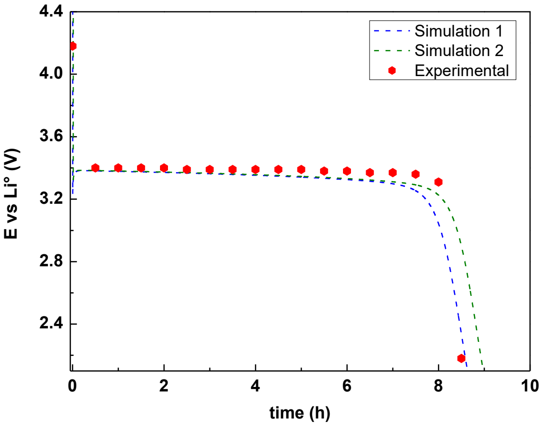


Fig. 1: Conceptualization of the electrode and experimental and model results comparison.

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Sim_01

Quantum Capacitance Beyond the Rigid Band Approximation in N doped Graphene

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Quantum capacitance is evaluated within the context of the Grand Canonical Kohn-Sham formalism by using Joint Density Functional Theory (JDFT) [1], in order to propose a strategy to estimate the relative capacitance capabilities of pristine and N doped graphene. The connection of the total capacitance with the chemical softness [2] is discussed; that connection allows identifying local capacitance, a concept introduced by Szarek, [3] as a property easy to evaluate in the JDFT formalism; in addition, the analysis of regional capacitances performed in this work is intended to characterize the relative impact of different forms of N doping in the capacitance of graphene. Also, a comparison between this new method and the rigid band procedure is conducted.

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Bat_01

From Materials design to pouch cells applications at electrochemical Energy laboratory UAM

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The electrochemical Energy laboratory at UAM, was created in 2014 with the firm intention to perform basic and applied research in the energy production and storage sector, especially to impulse the utilization of renewable clean energy. In this context, our group is working in different areas related to alkali ion batteries using, Lithium, Sodium and Potassium.

Our main motive is the development of applied science in Mexico with emphasis on the understanding of the basic principles and mechanisms occurring at the molecular for a further science guided modification of the materials and process and application in the very specific conditions of Mexico. To do so, the initial part of the process is the first principles guided synthesis of materials using abundant metals in Mexico, this process has allowed us to expect the effect of certain dopants and modifications at the atomic level. A combined machinery of chemical/structural characterization techniques employing X-ray Diffraction, Raman spectroscopy, Infrared spectroscopy, Nuclear Magnetic Resonance and Electronic Paramagnetic Resonance have helped to create a library of the main characteristics of the materials and their main effect on the electrochemical properties. Moreover, the electrochemical evaluation using standard methods such as galvanostatic experiments and Electrochemical Impedance Spectroscopy, is widely utilized with more than 50 channels readily available for characterization. During the last years, in-situ and in-operando monitoring by X-ray Diffraction, differential electrochemical mass spectrometry, Raman spectroscopy and Electronic Paramagnetic Resonance, macroscopic have helped to determine the changes occurring during cycling. Leading to full prototype scaling. studying both anodes, cathode, binder, polymer electrolytes and the assembly of the devices, with the aim to improve the electrochemical performance and manufacture of pouch cells made in México.

In particular, it has been found that pure Li_2CuO_2 is uncapable of fully attain its theoretical capacity due to the impossibility to form stable CuO structures, only when the potentials lower than 3.8 are utilized the oxygen evolution is abated. Ab initio calculations then demonstrated the possibility of cation doping, being the most favorable dopants Ni and Co; experimentally Ni doping was possible up to 5%at while higher amounts lead to the formation of phase mixtures; however, both, doped and phase mixtures leads to better electrochemical properties. On the other hand, anionic doping (Fluorine) also resulted in a phase with lower tendency towards the oxygen evolution. It was found by insitu techniques that phase mixtures interaction leads to a higher durability related to the stabilization of one phase at the expenses of the other (in situ X-Ray analyzes and the avoided oxygen evolution at higher potentials (DEMS).

Bat_06

Effect of Na-preconditioning of silicon anodes for Li ion batteries

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Due to the nowadays' huge energy demand of different applications, it is extremely important to create batteries with a performance far superior to current Lithium-ion batteries (LIBs) [1]. A great effort has been made in the research of several materials for possible use as anode for new generation of LIBs. Among them, Si has proven to be the best candidate to replace graphite as the anode of a LIB. Graphite has a gravimetric capacity of 372 mAhg^{-1}, much lower than that of Si, of 4200 mAhg^{-1} [2]. In addition, it is the second most abundant element in the earth's crust, is environmentally friendly, and has a low electrical potential *vs* Li [3]. Although Si offers many virtues, these are accompanied by some drawbacks. The insertion/extraction of Li$^+$ to/from Si causes a large volume change in its structure (>300%). If it is used as a bulk, it fractures and pulverizes after a few charge/discharge cycles causing loss of contact, which subsequently leads to capacity fade [4]. Additionally, if it is not cycled properly, its solid electrolyte interface (SEI) is not stable [5]. To overcome these drawbacks and improve the stability of Si anodes, several studies have been carried out, e.g. to mix it in composites (with metals, polymers, carbon) to improve its conductivity, and to nano- or micro-structure it (as nano-/micro-wires, nano-/micro-particles, etc.) to improve its mechanical stability. It has also been demonstrated that cycling (charge/discharge) very slowly (in 10 h or slower) for 3-5 cycles before the normal use, helps for the mechanical stability, since Si becomes porous and does not expand/contract anymore after this treatment [2, 6, 7]. This is a kind of pre-conditioning process. In view of the latter approach, in this work an electrochemical preconditioning process of Si anodes with Na, for their use in Li ion batteries, is proposed. As is the case of Li, Na also creates alloys with Si [8]. Considering that the de-sodiation process may also leave pores behind, these pores may be wider than the ones obtained with Li (Na has an atomic radius larger than the one of Li). At SSRL we were able to use synchrotron radiation to observe in greater detail the modifications caused in the Si anodes through the Na preconditioning process. With XRD (with a wavelength of 0.9744 Å in BL11-3 at SSRL) we could observe the structural changes in Si throughout the cycling process. The morphology changes were tracked with TXM (BL6-2 at SSRL) and Ptychography (BL7.0.1 at ALS). Additionally, soft X-rays were used for XAS, providing insight of the evolution of the SEI layer formed at the Si anode after being precondictioned with Na and after using the anodes in a LiB. Impedance spectroscopy and cyclic voltammetry were used to analyze the electrochemical processes in the anodes, and evidence the effect of the preconditioning in the performance of the anodes in a LIB.

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Oth_16

Impedance spectra analysis of $LiFePO_4$ by means of EEC in a three-electrodes set up cell.

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Lithium-ion batteries (LIB) is the most efficient energy storage device available on the market. Nowadays they dominate the portable electronics sector, providing energy to laptops, cell phones, electric bicycles, and electric vehicles among others. However, some challenges need to be overcome to enhance their characteristics, one of them is the development of new materials possessing high energy density and high capacity at high charge-discharge rates, using low cost precursors and possessing term durability. On the other hand, these materials should be characterized by affordable techniques, among them, Electrochemical Impedance Spectroscopy (EIS) is employed as a powerful tool to analyze hidden reactions occurring at the electrode/electrolyte interface and within the porous structure of the active materials. There are many reports in the literature related with the study of LIBs using EIS analysis but these has been mainly performed in a two-electrode setup; thus, the obtained impedance spectra is overall and gives information of the changes occurring in the full cell. In this work, EIS is applied to investigate the changes and behavior of the well-know $LiFePO_4$ and the influence of the binder using a novel three-electrode setup cell, which allows analyzing the contribution of both anode and cathode individually. The impedance spectra were obtained at different electrochemical potentials in the charge and discharge process at C/20 and analyzed by means of Equivalent Electrical Circuits (EEC). Besides, the deconvolution method was used to distinguish the contributions of each element in the circuit. In order to relate the changes in durability to the specific changes in the impedance spectra of the active material the analysis and fit with EEC allowed to determine the parameters involved in the reactions occurring inside of the LIB, i.e.: The solution resistance R_s, charge transfer resistance R_{ct}, double layer capacitance C_{dl}, C_{li} Lithiation capacitance, Lithiation resistance R_{lr}, chemical capacitance C_μ, Warburg diffusion W, and others. The analysis of the trends and corresponding correlations will be performed to understand the behavior of the battery and thus maximize the performance and durability of the electrodes.

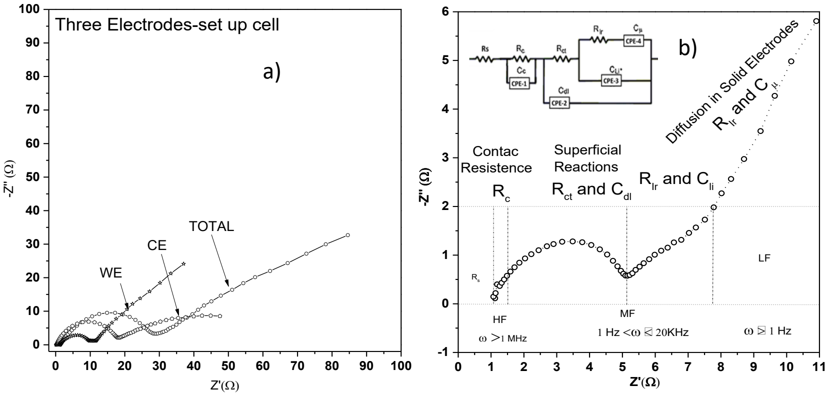

Fig. 1: Nyquist Diagrams. a) Contribution of electrodes, b) EEC Model

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Poster

Bat_02

Influence of electron conductive additives in electrochemical performance of Lithium-Sulphur Batteries

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Lithium sulphur batteries (LiSB) have theoretical specific capacity and energy density of 1675 mAh g^{-1} and 2600 Wh kg^{-1}, respectively [1]. Due to these reasons and to the fact that they have multiple oxidation states that allow 2 Li^+ ions per each sulphur atom (S). LiSB have become an important option to provide energy to mobile devices such as electric vehicles. In addition, they represent a better technological option than other storage technologies based on Li^+ intercalation, mainly due to their relative natural abundance and the low environmental impact of the battery components [2]. On the other hand, sulphur is an insulating material which during the reduction/oxidation process produces species that can dissolve in the electrolyte. Therefore, developing materials that improve conductivity and prevent dissolution of sulphur compounds is a priority. In the present work, it is reported a study focusing on the design and synthesis of new cathode materials (sulphur as active material, conductive additive and polymeric binder) that can enhance the electronic conductivity, which allows to increase the electrochemical performance and the life time of the LiSB. In addition, different electrolytes are tested in order to avoid the dissolution of lithium polysulphides and in general, improve the overall performance of the LiSB [3]. Therefore, electrochemical performance of different cathodes for LiSB was evaluated. Considering the effects generated by the use of different conductive additives (CA), thermal conditions for preparation of compound electrodes and the use of different electrolytes. The results (Fig 1) indicate that electron conductive additive affects the initial capacity but the oxygen functional groups are capable to decrease the capacity fade.

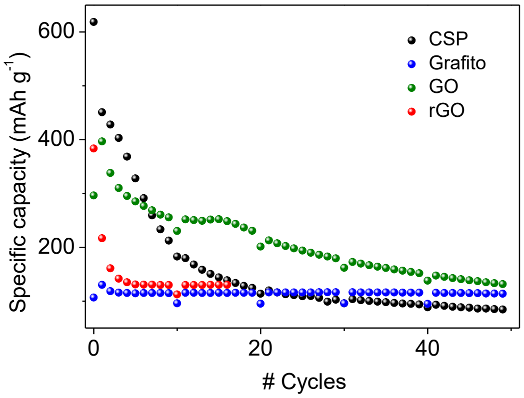

Fig. 1: Discharge capacity of BLi-S cathode electrodes (70% sulphur, 20% conductive additive and 10% binder) at 50 cycles

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Bat_03

Synthesis and characterization of lithium ferrite (Li_5FeO_4) for lithium ion battery application.

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In an effort to shift lithium ion battery technologies to more cost effective and greener alternatives, new chemistries are being studied to replace current cobalt and nickel-based systems. Some research has focused on using copper-based systems, as is in the case of Li_2CuO_2[1]; however, other iron-based materials could prove to be promising. Li_5FeO_4 has previously been studied and proven to be an effective CO_2 captor, showing high structural stability even at high temperatures [2]. Its high lithium content as well as its structural stability make it an attractive candidate for lithium ion batteries as an intercalation cathode. Pentalithium ferrite was synthesized by a solid-state reaction using lithium oxide (Li_2O) and iron oxide (Fe_2O_3) at 850 °C for 20 h. The material was successfully synthesized and characterized by x-ray diffraction, Fig. 1.

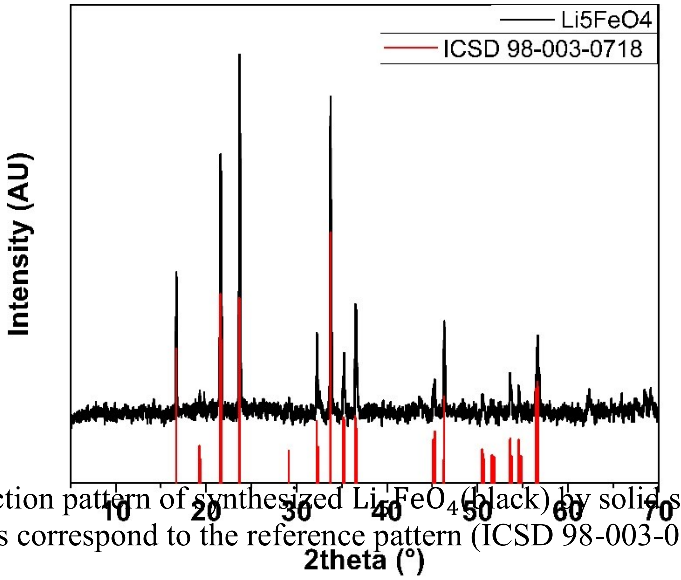

Fig. 1: X-ray diffraction pattern of synthesized Li_5FeO_4 (black) by solid state reaction. The red lines correspond to the reference pattern (ICSD 98-003-0718).

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Bat_04

Si nanowalls as anode for lithium ion batteries

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Keywords: Si nanowalls, Si battery anode

Silicon as anode material for Li ion batteries (LIBs) offers a nominal Li storage capacity of 4200 mAh/g, more than ten-fold that of standard graphite anodes (330 mAh/g) [1]. In spite of this advantage, bulk Si is not used as anode material, because it pulverizes due to the volumetric expansion/contraction generated during insertion and extraction of Li ions. Furthermore, bulk Si has additional disadvantages, such as low diffusivity of Li ions and low electronic conductivity. To overcome these disadvantages, it has been proposed to micro- or nano-structure Si in order to minimize the mechanical stress generated by volume expansion [2], and to use highly doped Si substrates to improve the electronic conductivity [3]. In this work, we propose the use of Si nanowalls as superior Li ion battery anode. We report on the optimization of the Metal Assisted Chemical Etching (MACE) process for the micro-structuring of Si substrates with different doping level and their performance as anode in LIBs. Even when it is desired to have highly doped walls to use them in batteries, the etching process is tricky for highly doped substrates.

A set of boron-doped <100> Si substrates, but with two different resistivities (0.0005-0.0007 Ω·cm and 15-25 Ω·cm) have been micro-structured by MACE. First, silver particles were chemically deposited on the Si substrates to act as catalyst in the etching process. Then MACE was performed, optimizing the composition of the etching solution (that contained HF, H_2O_2 and H_2O) for each resistivity of Si, in order to have similar morphological structures. The obtained Si nanowalls have been used as anodes in half cell batteries. Galvanostatic lithiation/delithiation cycles have been carried out and the changes in the chemical composition of the set of anodes have been analyzed by X-ray Photoelectron Spectroscopy. This technique has been useful in elucidating the effect of the resistivity of the Si substrates on the performance of the anodes.

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Bat_05

Onyx anodes for Li-ion batteries

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The increased demand of high-energy, high-power density, high capability and low cost lithium ion batteries is one of the motivations to look for new active materials for their electrodes. Silicon is an attractive anode material for Li ion batteries, as it has a capacity of 4200 mAh/g, more than ten times higher theoreorical capacity than its counterpart, graphite, the most common anode material implemented in commercial Li-ion batteries [1, 2].

Although a large number of micro and nano silicon structures have exhibited excellent electrochemical performance as anode materials, their practical application in batteries is difficult because their manufacturing processes are not completely scalable. Another possible constraint is that their production cost is high, both because of the precursors and because of the necessary equipment to produce the material at the gram and kilogram level [2].

In the quest of solutions for Si anodes, some researchers have proposed the use of materials that contain a high percentage Si, instead of using pure Si, to avoid the expensive (economically, energetically and environmentally) purification process. SiO_2 in the form of quarz or as silicates is one of the most promising options, with capacities of up to 1960 mAh/g. In the present work, we propose the use of Onyx as a source of SiO_2, since it represents 76.52% of its composition [3].

One of the reasons why choosing Onyx, is the fact that Puebla is one of the main producers of this mineral. The idea is to use Onyx residues left by the artisans in the elaboration of their handcraft, thus having a sustainable vision.

For this project, we got Onix residues n the form of powder from an artisan from the region of Puebla. Raman and infrared spectroscopy, as well as X-ray powder diffractometry were used to identify the components of the mineral. An strategy is being developed to eliminate the most of the components, except SiO_2. Subsequently, the material will be impregnated with an organic source of carbon, to carbonize it afterwards, so that the conductivity of the material improves.

It is expected to obtain a good performance of the prepared materials as anode for Li ion batteries, competing with the performance of other SiO_2 anodes, reaching around 800 mAh/g [1]. This value doubles the capacity of graphite anodes. With the new anodes we may solve the problem of the high costs of Li-ion batteries and improve their storage capacity, while taking care of the environment.

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Bat_07

Transition metal hexacyanocobaltates for potassium storage applications

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The coverage of our energy consumption through renewable sources stablish the challenge to develop more efficient energy storage technologies, especially based on abundant materials. Electrochemical lithium-ion batteries (LIBs), for storage of electrical energy, have partially satisfied these needs. However, the concern about its abundance has motivated research on other metals such as sodium and potassium, which are shown as strong candidates to replace it [1,2].

In the past, potassium-ion batteries (KIBs) have not been attractive systems due to the relative larger atomic mass and ionic radii of potassium. However, recent investigations have revealed characteristics that make energy storage potassium-based systems promising alternatives to the Li-based ones, as the more negative potential of the K/K^+ couple in organic solvents (-0.09 V vs Li/Li^+ in PC) and the smaller Stroke´s radii it possess comparing to Li^+ and Na^+ ions [3].

Different to the observed for LIBs and NIBs, the progress on KIBs has been relatively slow and especially limited for the materials able to host the larger potassium ions. Related to that, prussian blue analogues (PBAs), a class of metal organic frame works, have shown a superior K-ion storage capacity, due to the large cavities formed between the ion-metals and the cyano groups in the crystal lattice, leading to specific capacities as high as 324 mAh g^{-1}[4].

This work aims to evaluate the performance of a series of Prussian blue analogues (PBAs) based on hexacyanocobaltates of transition metals, as negative electrodes for K-ion based energy storage devices. We have electrochemically characterized these materials by cyclic voltammetry and different spectroscopic techniques as infra-red (FTIR), Raman and X-ray diffraction, at specific working potentials, in order to correlate the changes on composition with the reversible and irreversible electrochemical processes observed, to get a better insight on the still non-clear ion storage mechanism involved on the high capacities of these materials.

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Bat_08

Solvothermal synthesis of Sb_2S_3 and its application as anode for Li-ion battery

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Sb_2S_3 material has been considered a competitive candidate to be used as anode material in high performance lithium ion batteries (LIBs), due to its high theoretical specific capacity ~ 946 mAh g^{-1}, significantly higher than that of the widely used graphite (372 mAh g^{-1}) [1-4].

In this work, rod-bundles of antimony trisulfide (Sb_2S_3) have been successfully synthesized via solvothermal method. For this purpose, antimony potassium tartrate $C_8H_{10}K_2O_{15}Sb_2$ and carbon disulfide (CS_2) have been used as precursors, and ethylene glycol as solvent. The synthesis was performed at 180°C for different times from 24 to 72 h. However, the size and morphology of the samples did not change after 24h.

XRD diffractograms confirm that the samples are Sb_2S_3 with orthorhombic structure. SEM micrographs of the samples indicate the rod-bundles structure, with the diameter of the rods ranging from 0.7 µm – to 1 µm (see Fig. a) and b)). The samples are currently under progress also tested as anode in half battery cells, using Li metal as counter electrode.

Galvanostatic test as anode for Na batteries of single and interconstructed Sb2S3 materials

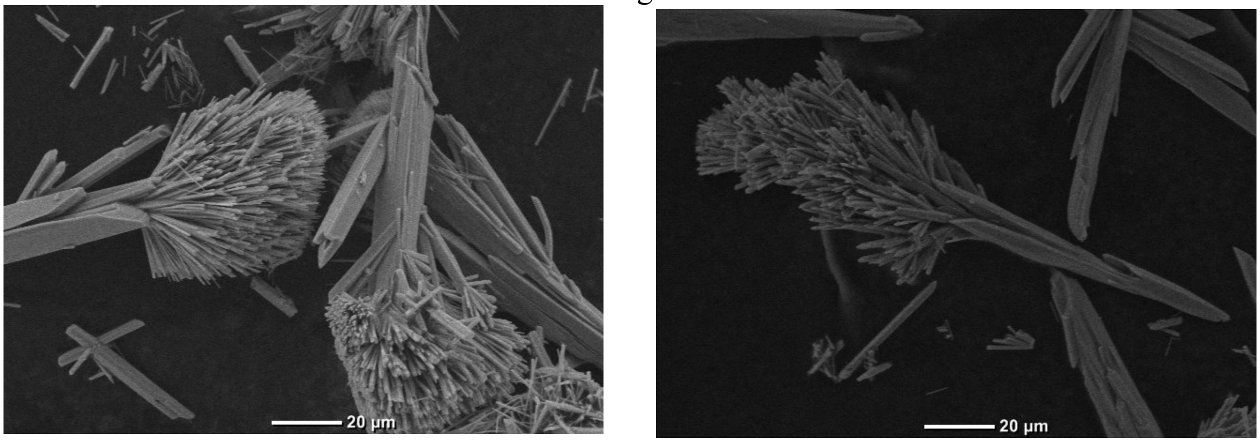

Fig. 1: SEM micrograph of Sb_2S_3 rod-bundles prepared solvothermally at 180 °C for a) 24 h and b) 72 h.

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Bat_09

SYNTHESIS OF REDUCED GRAPHENE OXIDE/TIO$_2$ COMPOSITES AS ANODE MATERIAL OF LITHIUM ION BATTERIES

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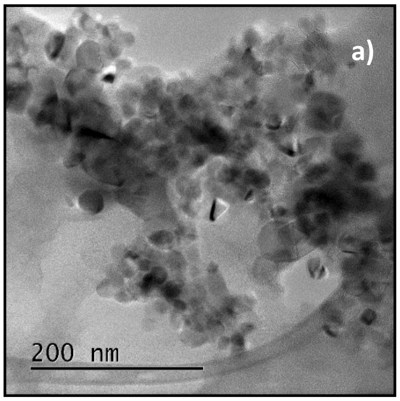
It this work we report on the synthesis of graphene oxide (GO) and reduced graphene oxide/titanium dioxide composites (rGO/TiO$_2$) as possible high-performance anode material for Li-ion batteries. GO is synthesized from graphite powder using a modified (by us) Hummer's method. Commercial TiO$_2$ nanoparticles (P25 TiO$_2$, Degussa) have been pre-treated thermally at 550 °C for 2 h to obtain a clean TiO$_2$ surface. rGO/TiO$_2$ nanocomposites have been synthesized by the solvothermal method at 150 °C for 5 hrs. The rGO/TiO$_2$ ratio in the composite was varied in proportions 1:1 and 1:2 wt%. TEM micrographs show TiO$_2$ nanoparticles homogenously dispersed onto the GO sheets (see **Fig. 1a**). The Raman spectrum of GO contains the D and G lines at 1344 and 1591 cm^{-1} assigned to the first-order scattering of E_{2g} phonons by sp$_2$ carbon atoms and the breathing mode of κ-point photons of A_{1g} symmetry, respectively [1]. In the Raman spectra of the rGO/TiO$_2$ nanocomposites the D band is broadened and shifted with respect to that of GO (see **Fig. 1b**). Once the synthesis of the rGO/TiO$_2$ nanocomposites has been achieved, hopefully this composite may present an enhancement in the Li-ion insertion/extraction cycling performance and in the electronic conductivity, compared to pure TiO$_2$ anodes containing carbon black. The characterization results suggest that the incorporation of TiO$_2$ with rGO could facilitate the electron transfer and the electrical conductivity enhancing the Li-ion insertion/extraction cycling performance of batteries, compared to the one of just TiO$_2$ mixed with carbon black anodes.



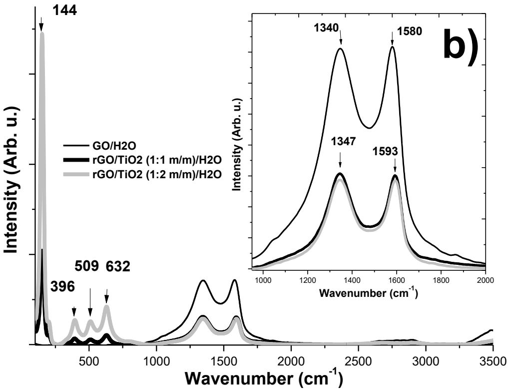


Fig. 1 a) Typical TEM micrograph of rGO/TiO_2 composites in proportion 1:1 and **b)** overlapped Raman spectra of GO, rGO/TiO_2 composites 1:1 and 1:2 wt %.

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Bat_10

Solvothermal synthesis of Sb_2S_3 and its application as anode for Li-ion battery

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XRD diffractograms confirm that the samples are Sb_2S_3 with orthorhombic structure. SEM micrographs of the samples indicate the rod-bundles structure, with the diameter of the rods ranging from 0.7 µm – to 1 µm (see Fig. a) and b)). The samples are currently under progress also tested as anode in half battery cells, using Li metal as counter electrode.

Galvanostatic test as anode for Na batteries of single and interconstructed Sb2S3 materials

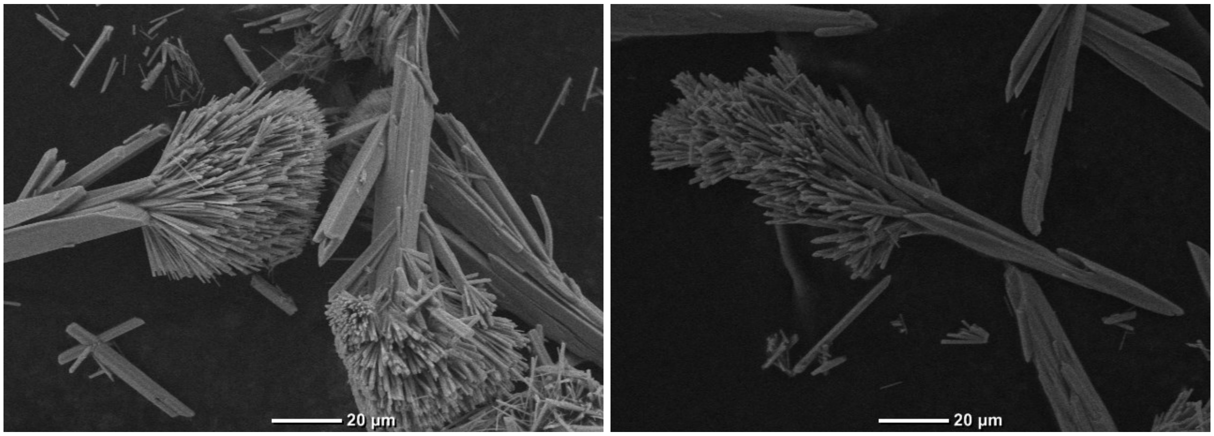

Fig. 1: SEM micrograph of Sb_2S_3 rod-bundles prepared solvothermally at 180 °C for a) 24 h and b) 72 h.

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Bat_11

Implementation of in situ X-Ray Diffraction studies for lithium Ion battery materials

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One of the main problems related to the identification of the process occurring during Lithium Ion battery charging/discharging processes is related to the lack of tools capable to determine in a simple manner the changes occurring inside the cell [1]. On the one hand, the initial analysis of the samples can only identify the chemical/structural properties, on the past the development of new materials only rely on these properties; however the cycling process can alter the chemical/structural properties in unpredictable manners. The post-mortem analysis can be influenced by several reactions in which Li takes place and the conditions after disassembling can be totally different. On the other hand, the electrochemical analysis, although a powerful tool (including electrochemical impedance) is incapable to relate any specific redox process with a change occurring within the cell. Thus, the combination of electrochemical cyclic with in situ analysis can lead to interesting analysis which can help to develop new material.

In this work, we present the implementation of the in situ XRD technique and the analysis of several materials possessing interesting structural changes, single phase materials, solid solutions and phase mixtures (Figure 1).

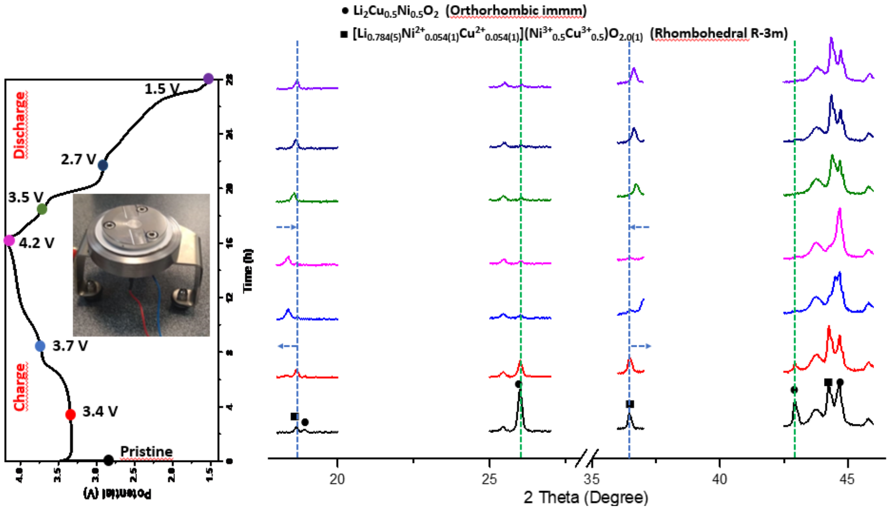

Fig. 1: In situ X-Ray analysis of $Li_2Cu_{0.5}Ni_{0.5}O_2/LiCuNiO_2$ phase mixture during battery charging.

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Bat_12

MACROPOROUS Si DECORATED WITH TiO_2 NANOPARTICLES AS ANODE MATERIAL FOR LITHIUM ION BATTERIES

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Recently, three-dimensional macroporous structure materials used in Lithium ion batteries (LIBs) have attracted great attention due to their special features: 1rst, the wall thicknesses are of the order of nanometers which shorten both electronic and ionic pathways and 2nd, macropores with a size range of micrometers enable easy infiltration of electrolyte and fast liquid-phase Li ion diffusion, reducing the concentration polarization and increasing rate performance and capacity of the cell [1]. This is the case of macroporous Si, with gravimetric storage capacity of 4200 mAh/g. On the other hand, TiO_2 has been recently reported as a good candidate to be used as anode, due to its mechanical stability for hundreds of cycles, and its high cycling rate capability; however it shows low storage capacities. A synergy may be present combining the aforementioned materials. Here we report about the synthesis of macoporous Si (macro-PSi) decorated with TiO_2 nanoparticles, and the preliminary results of using the composite as anode in a Li ion battery.

A set of macro-PSi layers were grown electrochemically in p-type crystalline Si <100> substrates with 10-15 Ω·cm resistivity, using HF diluted in DMF as electrolyte. The samples were oxidized at 500 °C for 5 min under 10 mL/min of oxygen flux. Then, they were silanized by dipping them into an MPTS solution (10 % v/v of water) and rinsed with propanol. Later on, the samples were dipped into a suspension of TiO_2 nanoparticles (particle size = 25 nm) in water (1mg/mL). They were let dry and the residual TiO_2 was washed away with a buffer phosphate solution. Scanning electron microscopy (SEM) images of the PSi samples show a porous surface morphology with pores diameters of 1-2 µm (see **Fig. 1a**) and the cross section SEM images show an array of parallel pores with length of 7-8 µm (see **Fig. 1b**). The SEM micrographs of the composites (not shown here) showed a macro-porous morphology of the PSi layers decorated with TiO_2. Electrochemical characterization of the anodes show promising results.

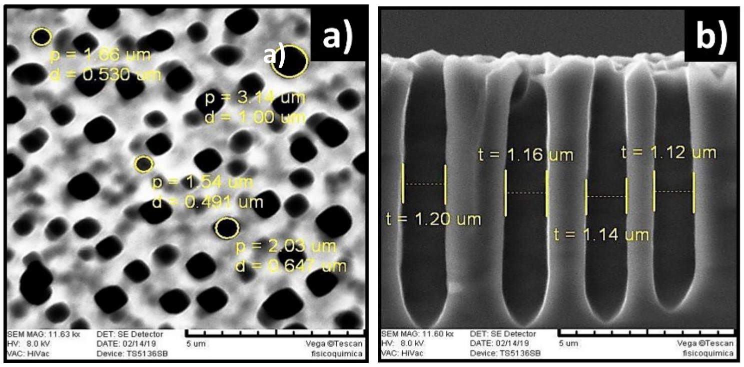

Fig. 1 SEM micrographs of an as grown macro-PSi layer showing: **a)** the surface morphology and **b)** its cross section.

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Bat_13

High energy density Pouch cell design and manufacture based on $LiCoO_2$ cathodes.

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Lithium-ion batteries (LIB) research at the materials level has increased a lot during last years; however, LIB research at the device level hasn´t gain momentum, especially in Mexico. The production of small devices is important to start creating collaborations with the industrial sector. The design and manufacture of pouch cells has been encouraged by its compact form and versatility.

In this work we demonstrate the viability to manufacture a 2 Ah at the laboratory level subjected to the condition of 6x5 cm area for high energy density applications. The cell was proposed to contain lithium cobaltate ($LiCoO_2$) [1] and graphite as cathode and anode respectively. Due to the proposed scheme to possess high energy density in a compact design, the pouch cells were forced to contain the maximum amount of active material to meet the expectations. The manufacturing process consisted of five stages, electrode processing, cutting, assembly, sealing and welding, electrochemical tests. The cathodes were made of a measure of 46 x 58mm coated with active material on both sides and anodes capable of satisfying the energy density of $LiCoO_2$. An important point was to determine the conditions for the cells to have the expected specific capacity and to push them towards their prompt implementation in renewable systems.

This work was possible thanks to the financial support from project SECITI/080/2017

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Bat_14

Separators for ion intercalation batteries based on biopolymers modified by ceramic nanoparticles addition

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Battery systems based on Alkaline Ion intercalation processes are one of the best alternatives for energy storage, due to their versatility allowing vast utilization in several electronic devices [1]. Most of the LIB properties rely on the electrodes properties [2]; however, characteristics such as ionic conductivity and lithium transfer number, which depend on the intrinsic characteristics of the electrolytes and separators or both, can cause a more drastic effect on the BILs electrochemical performance [3]. The separators commonly used in LIB are non-biodegradable membranes of polypropylene and polyethylene, whose structural characteristics do not modify the intrinsic properties of liquid electrolytes, such as ionic conductivity and cation transfer number. Therefore, there exist a number of possibilities to modify both: a) the polymer used as separator, utilizing biodegradable non-toxic monomers, and b) modify the separator chemical structure to enhance the Ion transport properties.

In this work, new membranes based on Carboxymethylcellulose and Methylcellulose are reported as a new alternative for new green separators; the processing variables and properties are analyzed. Moreover, the biopolymers are modified by incorporating nanoparticles of ceramics (TiO_2, SiO_2 and ZrO_2) and the modification of the ionic transport properties (ionic conductivity, cation transfer number and electrochemical stability window) in liquid electrolytes is evaluated for Li^+, Na^+ and K^+ electrolytes.

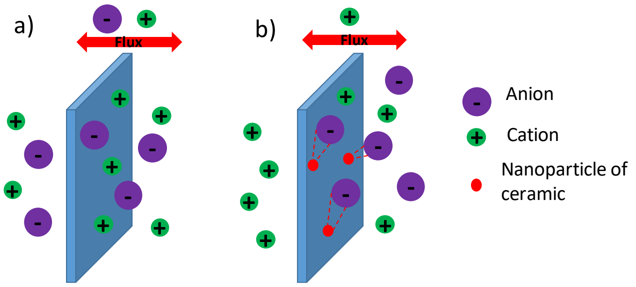

Figure 1. Cation transport mechanism on separator for IIB; a) conventional separators and b) biopolymers modified by incorporating nanoparticles of ceramics.

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Bat_15

Role of metal ion on the distribution of charge density in metal organic frameworks used as anodes in lithium ion batteries

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The world's demand for electricity is constantly growing and is predicted to increase by 50% from 2015 to 2040. As a result of man-made climate change, there is increasing focus on clean renewable energy sources. While solar, wind and wave energies are important, they are inherently variable and a range of energy storage technologies will be required for these renewable energy sources to reach their full potential. Within the energy storage technologies, batteries are likely to play a vital role.

Lithium-ion batteries (LIBs) consist of lithiated Co, Ni, Mn oxides as positive electrodes (cathodes), various carbonaceous composites as negative electrodes (anodes), and lithium- bearing salt in organic solvents or polymer gels as electrolytes. The development of LIBs is closely associated with the use of new electrode materials and electrolytes. In this context the use of Metal−organic frameworks (MOFs) has been recently reported and used as anode. MOF is built by a metallic ion center coordinated to an organic ligand, so the metallic site is susceptible to redox processes, nevertheless, different authors suggest that there are no changes in the oxidation state of the metal ion, during charge/discharge process, associating the efficient charge transfer to the organic ligands, which play a key role in the excellent Li storage mechanism. However, the effect of the metal ion on the distribution of charge density on the organic binder and its participation in the intercalation of lithium during Charge/Discharge process has not been discussed.

In the present work three MOF were synthetized, using terephthalic acid as laminar and pyrazine as a pillar linker, with different metal ion center: manganese, cobalt and zinc. Electrochemical properties during charge/discharge process are correlated with the effect of metallic center over organic linker, this interaction is evaluated by Raman spectroscopy and Electron Spin Resonance (ESR), which helps to elucidate the lithium intercalation mechanism.

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Bat_16

Impedance spectra analysis of $LiFePO_4$ by means of EEC in a three-electrodes set up cell.

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Lithium-ion batteries (LIB) is the most efficient energy storage device available on the market. Nowadays they dominate the portable electronics sector, providing energy to laptops, cell phones, electric bicycles, and electric vehicles among others. However, some challenges need to be overcome to enhance their characteristics, one of them is the development of new materials possessing high energy density and high capacity at high charge-discharge rates, using low cost precursors and possessing term durability. On the other hand, these materials should be characterized by affordable techniques, among them, Electrochemical Impedance Spectroscopy (EIS) is employed as a powerful tool to analyze hidden reactions occurring at the electrode/electrolyte interface and within the porous structure of the active materials. There are many reports in the literature related with the study of LIBs using EIS analysis but these has been mainly performed in a two-electrode setup; thus, the obtained impedance spectra is overall and gives information of the changes occurring in the full cell. In this work, EIS is applied to investigate the changes and behavior of the well-know $LiFePO_4$ and the influence of the binder using a novel three-electrode setup cell, which allows analyzing the contribution of both anode and cathode individually. The impedance spectra were obtained at different electrochemical potentials in the charge and discharge process at C/20 and analyzed by means of Equivalent Electrical Circuits (EEC). Besides, the deconvolution method was used to distinguish the contributions of each element in the circuit. In order to relate the changes in durability to the specific changes in the impedance spectra of the active material the analysis and fit with EEC allowed to determine the parameters involved in the reactions occurring inside of the LIB, i.e.: The solution resistance R_s, charge transfer resistance R_{ct}, double layer capacitance C_{dl}, C_{li} Lithiation capacitance, Lithiation resistance R_{Ir}, chemical capacitance C_{μ}, Warburg diffusion W, and others. The analysis of the trends and corresponding correlations will be performed to understand the behavior of the battery and thus maximize the performance and durability of the electrodes.

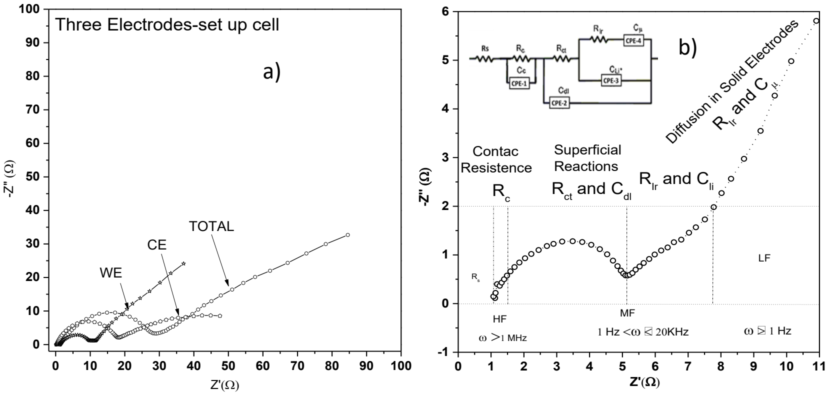

Fig. 1: Nyquist Diagrams. a) Contribution of electrodes, b) EEC Model

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Bat_17

Study of the $Sb_xSb_yS_z$/carbon nanofibers composite as anode of sodium ion batteries.

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Energy storage play a key role for improved quality of life. In this regard, lithium-ion batteries (LIBs) are widely used for portable devices and electric vehicles. However, it is estimated that global lithium reserves will not meet market demand. Therefore, sodium-ion batteries (SIBs) have emerged as a promising alternative for energy storage. In this work, it has been synthesized for the first time a composite material of $Sb_xSb_yS_z$/ carbon nanofiber (CNFs) using low-expensive synthesizing methods. First, CNFs have been obtained by electrospinning method with subsequent calcination at 700°C.Afterward, a Sb_xSb_yS thin coating is deposited on the CNFs by chemical bath deposit technique to obtain the $Sb_xSb_yS_z$/CNF. In order to promote the crystallization of $Sb_xSb_yS_z$ material, the composite is heated at 300 °C in nitrogen atmosphere. The evaluation of the resulting composite as the anode in SIBs has a reversible discharge capacity of 261.18 mAh g^{-1} and a columbic efficiency of 61.4% after 9 cycles, achieving and high stability and excellent cycling performance. On the other hand, the electrical conductivity of the composite increases from $8.72x10^{-3}$ to $1.31x10^{-2}$ S due to the incorporation of $Sn_xSb_yS_z$ nanoparticles in the CNFs. Finally, an easy and inexpensive route has been proposed for the synthesis of $Sb_xSb_yS_z$/CNF composite with great potential for its use as an anode material for BIS.

Bat_18

Diffusion of lithium in porous germanium for lithium-ion battery applications

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Porous Germanium (pGe) has shown promise for the development of new generation Li ion batteries; however the effect of Lithium in its properties has not been studied extensively. In this work the effect of surface and interstitial Li on the electronic properties of pGe was studied using a first principles density functional theory scheme. The porous structures were modelled by removing columns of atoms in the [001] direction [1] and the surface dangling bonds were passivated with H atoms, and then replaced with Li atoms [2]. Also, the effect of a single interstitial Li in the Ge was analyzed. The transition state and diffusion barrier of the Li in the Ge structure was studied using a QST scheme [3]. The results show that the energy band gap decreases with increasing concentration of Li at the surface, thus increasing the electronic conductivity and favoring the electronic conduction in the nanostructure, while the interstitial Li creates effects similar to an N doping where the Fermi level shifts to the lower end of the conduction band, and creates metallic states. The results show as well, that, the Li diffuses through a trajectory from Td-Hex-Td interstitial sites. These results could prove useful for the development of new anode materials in lithium-ion batteries.

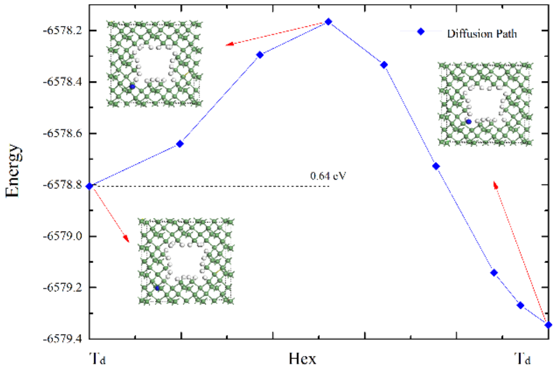

Fig.1: Diffusion energy for a Li dopant along the Td–Hex–Td pathway.

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Bat_19

Effect on the thermal treatment on the Anatase to Bronze conversion of TiO_2 and its electrochemical performance as a cathode for hybrid Li^{+}/Mg^{+2} ion batteries

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Abstract

Recently, Li^{+}/Mg^{2+} hybrid-ion batteries (LMIBs) have attracted interest as a new electrochemical energy storage device and have emerged as an alternative to solve problems associated with the formation of lithium dendrites and as a reduction of lithium metal cost. LMIBs bottom cells were fabricated using TiO_2-B as cathode, Mg metal as anode and APC/LiCl (APC= All-phenyl complex) as electrolyte. TiO_2-B was prepared by controlled heat treatment of TiO_2 anatase nanorods at 450°C up to 4 hours. Samples were extracted 1h intervals and were characterized by SEM, TEM, DRX and Raman spectroscopy; electrochemical tests were performed by cyclic voltammetry and galvanostatic charge/discharge test. Raman analysis indicates a higher proportion of TiO_2-B with percentages of 95, 79, 67 and 29% at 1, 2, 3 and 4h of thermal treatment, respectively. Stability tests for 80 cycles on TiO_2-B 1h show greater stability and cyclicity with a 72% discharge retention capacity. On the other hand, battery performance was carried out by charge/discharge tests at different C rates, in a range of 0.01-2V Mg/Mg^{+2}. The results showed a discharge capacity for TiO_2-B 1h of 3,30 mAh/g.

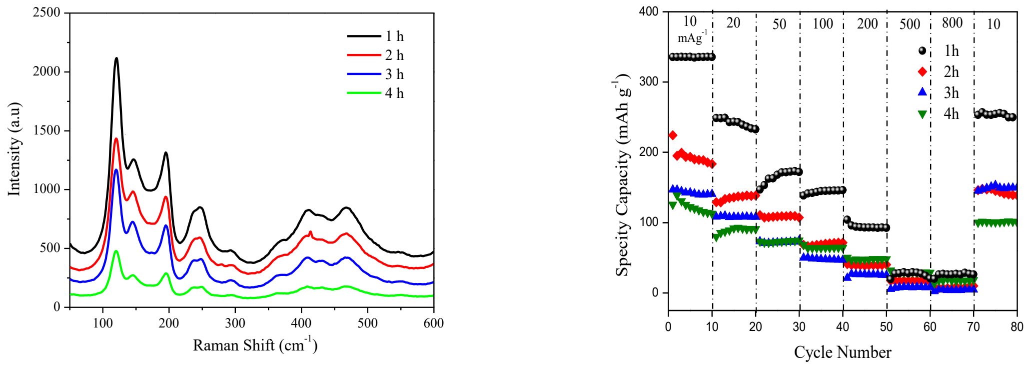

Figura 1. a) Raman spectrum for the determination of TiO_2-B b) Rated capability test.

Bat_20

Sulfured Multiwall Carbon Nanotubes as Cathode for Li ion batteries using a chitosan-starch based electrolyte

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Nowadays, it has been reported that solid electrolytes are considered promising materials in-store energy field, due to their unique properties such as high ionic conductivity, physical flexibility and their ability to provide good electrode/electrolyte contact [1]. Compared to the liquid state, the production of leak and gas formation during the decomposition of the solvent is avoided, in addition to being small, lightweight and safe [2].

In this work is reported the synthesis and the physical and electrochemical characterization of chitosan-starch polymers modified with sulfured multiwall carbon nanotubes. For obtain, the structural and physicochemical properties of polymers were used the techniques of FTIR and Raman spectroscopy. The electrical and electrochemical properties were determined by using Electrochemical Impedance Spectroscopy and Conductivity Measurements. The results obtained indicate that the polymeric material is a viable candidate to be used as an electrolyte for lithium batteries.

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Bat_21

Preparation of Graphene Aerogels with MnO_2 Nanorods and Polivinylidene Fluoride for Li-ion Battery Applications

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Over the last decade, interest in the development of new materials for lithium ion (Li-ion) batteries has been increasing drastically due to population growth and global energy demand [1]. In this regard, nanostructured graphene aerogels for Li-ion batteries have recently been investigated as an alternative to conventional graphite-manufactured anodic materials. Due to their high porosity, low-density, and large surface area, graphene aerogels can facilitate Li^+/electron transport, accelerate diffusion kinetics, and improve cycling stability. On the other hand, the addition of metal oxides such as MnO_2 in carbon-based aerogels can also improve electrochemical performance by increasing the space between graphene sheets and storage capacity [2].

In this work, reduced graphene oxide (rGO) aerogels with MnO_2 nanoparticles and polivinylidene fluoride (PVDF) were prepared via hydrothermal method. Aerogels were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). Photograph (**Figure 1a**) and SEM image (**Figure 1b**) show the low density and high porosity of the obtained graphene aerogels. Formation of MnO_2 nanorod-like morphology is confirmed with SEM and TEM analyses (**Figure 1c** and **d**, respectively). The preparation route represents a useful methodology for the design of new three-dimensional graphene materials with potential applications in electrochemical devices.

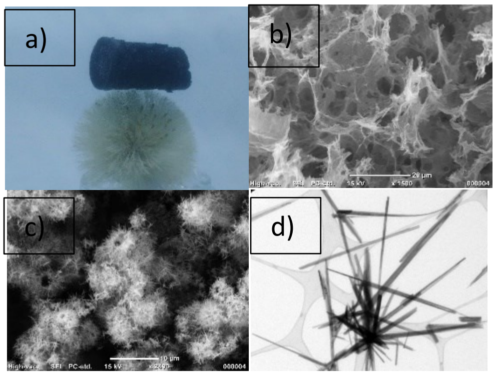

Figure 1. a) Image of rGO aerogel, b) SEM image of rGO aerogel, c) SEM image of MnO_2 nanorods, and d) TEM image of MnO_2 nanorods.

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Bat_22

Study of composite material of SnO_2/PANI/ RGOODA for their application in Li- battery

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Lithium-ion batteries (LIB's) are today one of the primary sources of energy for many of the electronic and electrical devices. However, there are many industries, such as the automotive industry, which requires developing batteries that have a balance between high power density, high capacity, and high cyclability. So, the development of new batteries or the improvement of existing ones is a relevant issue today.

In this work, a commercial LIB model with graphite anode was used as a reference, whose theoretical specific capacity is 372 $mAhg^{-1}$ (LiC_6). In the literature, there are reports of works that have tried to replace graphite with other materials with higher theoretical capacity, such as metal oxides, but which have lower electrical conductivities and lower cyclability (20-50 cycles). It was proposed to improve the anode of a LIB with a ternary composite material of SnO_2, PANI and a functionalized and chemically reduced graphene oxide with octadecylamine and hydrazine (RGOODA), respectively. The three materials were synthesized separately, obtaining PANI fibers and sheets of SnO_2 and RGOODA, with the aim of reducing the volumetric expansion presented by pure Sn ($\Delta V=260\%$) in the redox cycles, improving the electrical conductivity of the electrode and increases the contact and intercalation surface of lithium ions in charge/discharge cycles. Then, the effect of the concentration of PANI and SnO_2 on electrochemical properties such as capacity or cyclability is studying

The scope of this work includes the physicochemical characterization of the three materials through analytical and instrumental techniques such as XRD, XPS, RAMAN, FTIR, BET, TGA, and SEM. These materials will be to assemble the electrodes to different compositions and characterize the materials through electrochemical techniques as: CV, charge-discharge cycles at current constant and EIS.

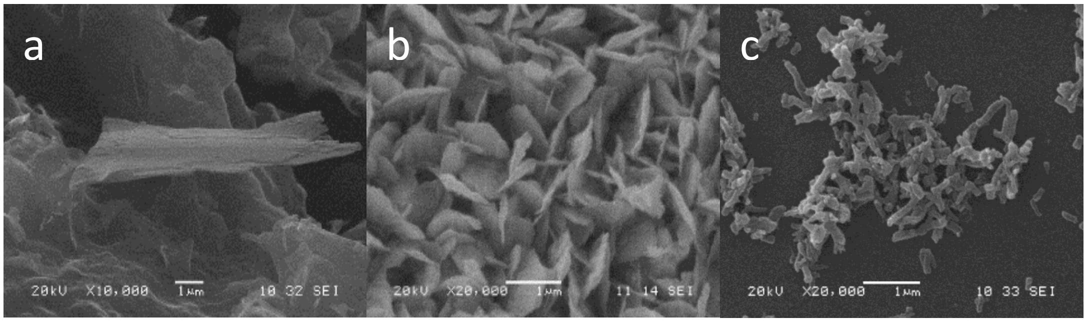

Fig. 1: SEM images of materials obtained: a) RGOODA, b) SnO_2 y c) PANI

Bat_23

Probe Lithiation Behavior of Conversion-type Anode Materials Using Synchrotron Chemical Microscopy

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Next generation Li-ion batteries (LIBs) boast high gravimetry and volumetric capacities, but require significant improvements to their cycling rate in order to meet future demands on large scale applications such as electric vehicles and power storage for smart-grids [1]. Conversion-type anode materials (CTAMs) are attractive anodes for next-generation LIBs because of higher specific capacity and better safety than intercalation-type materials [2]. However, this lithiation-delithiation cycle cannot be repeated indefinitely with its irreversibility originating from the relatively large volume expansion during phase transition and poor electronic/ionic conductivity dominated by the diffusion limited transfer of lithium across the phase boundary [3–5]. These leads to capacity fade.

In this study, we investigate the phase transition behavior with an advanced Synchrotron-based X-ray microscope at SSRL (SLAC) with nano-sized chemical resolution [6-7], to gain a better understanding of the lithiation/delithiation kinetics of the conversion reaction across electrode scale. By using hierarchical and porous nanostructures NiO (HPN-NiO) with orderly constructed primary nanoparticles as a proof-of-concept, we provide fundamental understanding on how the rational design of structural heterogeneity can improve this reaction to achieve longer cycle life and high capacity batteries. The ultimate objective of this study is to guide the nanoengineering of CTAMs to target high capacity Li-ion batteries with excellent cycling and rate performance.

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Cap_01

Supramolecular assembly of nanostructured conducting polymer hydrogels by hydrotropic agents for energy storage applications

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Recently, nanostructured conducting polymer hydrogels (CPHs) demonstrated competitive advantages over their bulk and nano-powder counterparts for energy storage applications. One of the main reasons for the enhanced performance is related to their straightforward processing and three-dimensional architecture that provides hierarchical pores[1]. This feature affords a continuous conjugated network to facilitate electron transport, short ion diffusion paths and the ability to accommodate the detrimental volume expansion of conducting polymers (CPs) during the charge-discharge process. Up to now, only a few strategies have been developed to synthesize pure CPHs, a recent survey identified only three strategies to physically crosslink the CPs[2]. In spite of the progress, it is necessary to find new crosslinkers and techniques to produce pure CPHs with higher conductivity[3]. In the present work, we propose and explore the formation of CPHs by using a supramolecular approach. The molecular assemblies consist on hydrotropes (Hts) that provoke self-aggregation in the presence of molecules with scarce water solubility as in the case of pyrrole (Py). Particularly, we focus on two Hts, p-Toluene sulfonic acid (PTsa) and camphor sulfonic acid (CPsa), the last also acting as doping agents. The CPHs were characterized by scanning electron microscopy, Raman spectroscopy and electrochemical techniques. In order to gain insight on the effects of the synthesis conditions on the CPH physical chemical properties, we evaluate the effect of monomer-dopant ratio. Our results demonstrated that the highest conductivity and mechanical stability was achieved by the dopant to monomer ratio of 0.75 PTsa/Py ratio for the PTsa-PPy CPH whose electronic conductivity was 2.3 $S.cm^{-1}$. Due to its high electronic conductivity and electrochemical properties, we assembled a semi solid state flexible supercapacitor with the PTsa-PPy CPH whose capacity delivered a value of 160 F.g at a current density of 1 A. g^{-1}.

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Cap_02

Thin-film YSZ electrolyte on all solid state Nanosupercapacitor based on Symmetric Ru electrodes for mild temperatures

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We report on the performance of a symmetric nanosupercapacitor by using atomic layer deposition (ALD) for yttria-stabilized zirconia (YSZ) as the electrolyte and sputtering for ruthenium as the electrode. 70nm of ruthenium and 100 nm of YSZ were used for this device. The thin-film symmetric nanosupercapacitor exhibit excellent thermal stability and high capacitance for mild temperatures up to 210 °C. Galvanostatic measurements indicate that the capacitance obtained can be regulated by modifying the measuring temperature yielding 1.6 μF cm^{-2} (87.87643 nWh cm^{-2}) at 210 ºC (Fig. 1). Coulombic efficiency obtained can be explained by activation energy change detected by impedance spectroscopy (Fig.2).

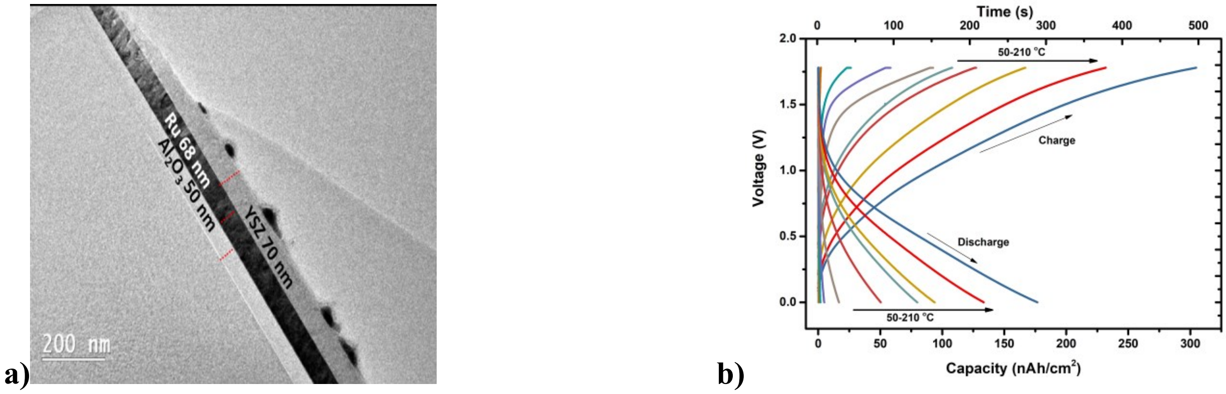

Fig. 1: a) Representative cross-section TEM micrograph of bottom structure Ru-YSZ deposited on a mechanical support of 50 nm of Al_2O_3 film with Si substrate. b) Galvanostatic charge/discharge curves under increasing temperatures from 50 to 210 °C at constant current density of 2.20 μA cm^{-2}.

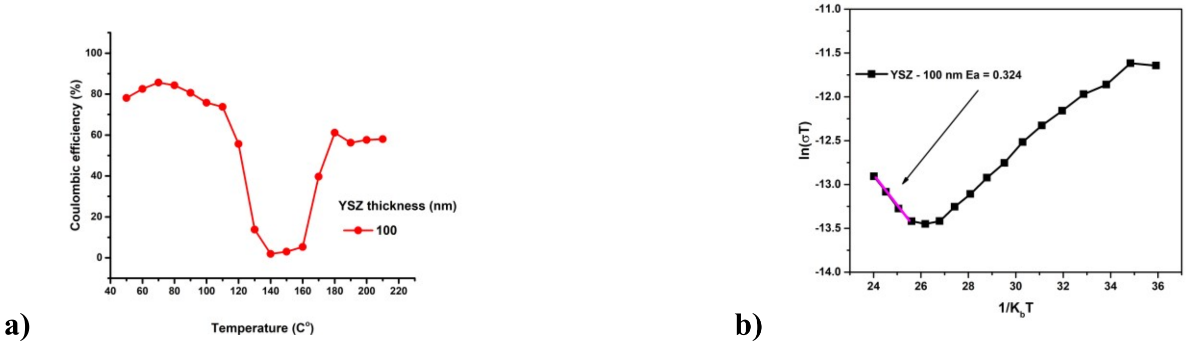

Fig. 2: a) Coulombic efficiency as a function of temperature, and b) Activation energy change obtained by impedance spectroscopy at 20 Hz

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Cap_03

Chemical vapor deposition few layer graphene films for microsupercapacitors

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The fabrication in the last years of miniaturized electrochemical energy storage systems has increased because its demand in smaller electronic devices. The understanding of the behavior of the components in a microsupercapacitors has led to try different materials.

Graphene has been used in microsupercapacitors for its electrical, and thermal conductivity, also for its specific surface area and elasticity. Theoretically, graphene has a specific capacitance of ~21 µF cm-2 [1] and it's been reported a specific capacitance of ~6 µF cm-2 obtain from few layer graphene (FLG) microsupercapacitors..

Nevertheless, chemical vapor deposition (CVD) has the advantage of scalability, high production efficiency, large areas of synthesized graphene and its versatility of determining different conditions to get a specific number of layers of graphene [2], therefore, it is considered a good candidate to increase the electrical conductivity in the current collector to be used in microdevices

In this work, FLG was obtained by a CVD, where it was considered an atmospheric pressure system, also different ratios of concentration of catalytic and precursor gas flow (0.5:1, 2.5:1, 5:1 H_2:CH_4) in an argon system, and reaction times (20, 10, and 5 min). FLG was grown on 25 µm thick copper at a temperature of 1000 ˚C, with a cooling rate of 5.3 ˚C/min (Fig.1 a). The FLG were transferred and buckled on PMMA substrate for a 1x1 cm electrode that had shown a specific capacitance range of 6.41 - 8.60 µF cm^{-2}; in a KOH 6 M and two electrode system (Fig. 1 b).

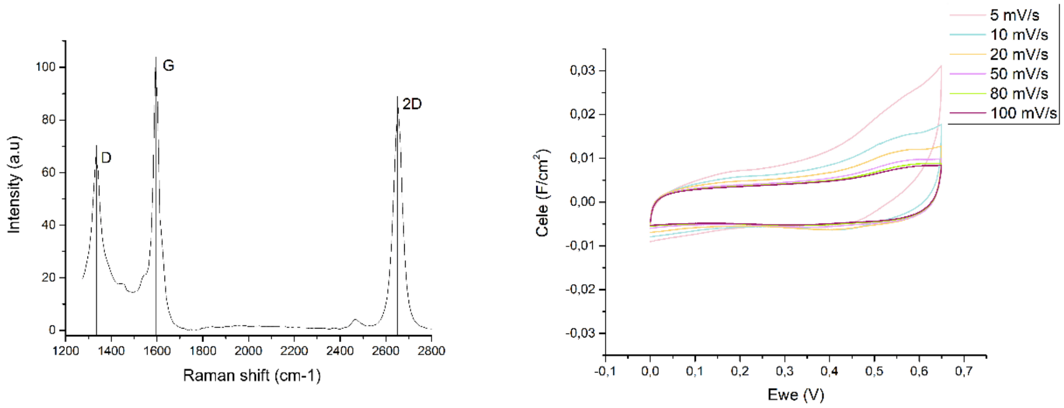

Fig. 1: FLG obtained by AP-CVD a) Raman, b) Cyclic voltammetry.

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Cap_04

Performance as a supercapacitor under potentiostatic floating tests of carbon electrodes prepared from avocado stones

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Electrochemical capacitors based on activated carbon store energy by forming the electrochemical double layer at the electrode-electrolyte interface [1]. Carbons were prepared by a pyrolysis process, the first charring of avocado stones powders was at 400 °C for an hour , then the char was activated with KOH in a ratio 1:4 at 700 °C. The carbon prepared had a surface area greater than 1800 m^2g^{-1} and a mean pore size between 1-5 nm. The electrochemical performance of the carbon electrodes was evaluated in coin cell fixtures, the electrochemical conditions were typical of an accelerated ageing electrochemical tests (potentiostatic floating tests at one selected maximum voltage intercalated with charging- discharging cycles) [2]. To perform the ageing tests, the device was charged at 1.5V for periods of 2, 5 and 10 h. A specific capacitance higher than 220 Fg^{-1} was obtained in Li_2SO_4 1M as aqueous electrolyte, the large capacitance can be attributed to the easy access of the electrolyte ions to the pores of the material. Results show that degradation of the system is more severe when the device was under short times of applied voltage, then all the floating tests were carried out for 2 h before the charge-discharging cycles (Fig. 1). The stability study of the supercapacitor devices shows that up to 100 hours the device operates with an specific capacitance loss under 20% (Fig. 2) of the initial one and that there is room for great improvement of carbon electrodes prepared form avocado stones.

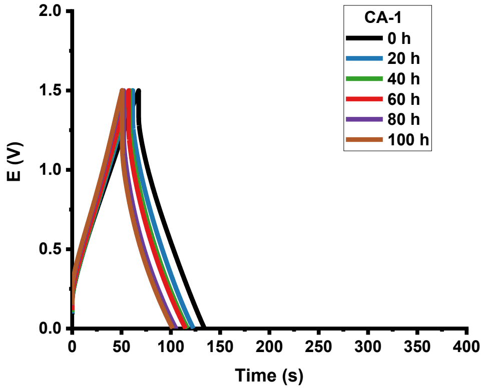

Fig. 1: Charge and discharge cycles at 1.5 V every 20 h.

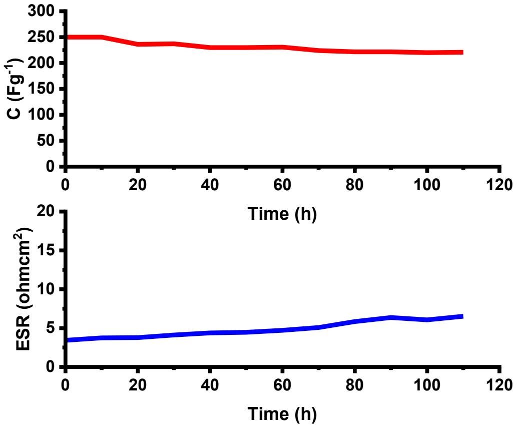

Fig. 2: C and ESR performance.

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Cap_05

Bimodal mesoporous carbons - PMo_{12} composites for supercapacitor

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Bimodal mesoporous carbons were synthesized by use of double pore forming method and resorcinol-formaldehyde resin as a precursor. Poly-diallyldimethylammonium chloride (pDADMAC) and commercial silica (Sipernat® 50) were used as structuring agent and hard template, respectively [1-2]. Through the proposed procedure carbon powder with bimodal mesoporous size distribution (around 4-5 nm and 20-40 nm) and different pore volume ratios can be obtained, by changing the ratio pDADMAC/silica used in the synthesis. Pore volumes between 0.70 and 2.10 $cm^3 \cdot g^{-1}$, and specific surface areas between 662 to 998 $m^2 \cdot g^{-1}$ were obtained.

The incorporation of PMo_{12} into the carbon matrix was carried out by a very simple method. The relationship between PMo_{12} adsorption and carbon structure was analyzed. Carbon with a higher amount of mesoporous < 10 nm showed the highest PMo_{12} loading, reaching a pseudocapacitance of 326 $F \cdot g^{-1}$, 120% larger than the pristine material, as seen in figure 1. Finally, all materials showed great stability up to 3,000 galvanostatic charge-discharge cycles.

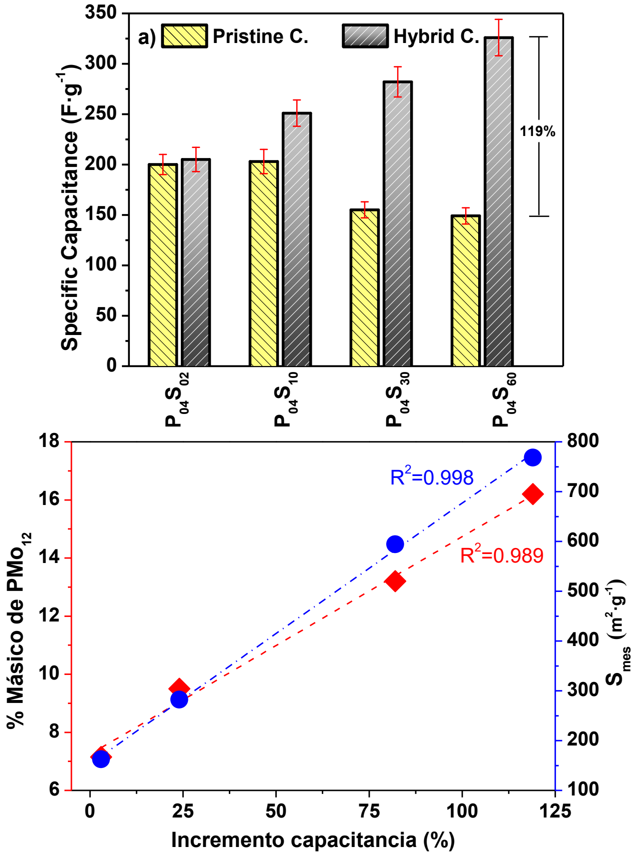

Fig. 1: a) Capacities obtained from pristine and hybrid materials. b) Increase of capacitance *vs* mass percentage of PMo_{12} (♦) and mesoporous area < 10 nm (●) for hybrid materials.

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Cap_07

Nanostructured $VOPO_4$ for Electrochemical Capacitors

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The energy demand is increasing everyday due to depletion of fossil fuels, the increment of modern portable electronic devices and electric vehicles. This has motivated the interest in energy storage devices such as electrochemical capacitors [1-3]. Their power density and charge-discharge cycle stability are higher than batteries. However, their energy density is lower than modern batteries [2,3]. The aim in the field of electrochemical capacitors is to increase the energy density without sacrifice the power density and cycle stability [2]. Thus, it is necessary to prepare new materials to increase the energy density of electrochemical capacitors. In this work, we report nanostructured vanadium phosphate as electrode materials for electrochemical capacitors. The effect of crystalline structure, morphology and surface area on the specific capacitance was evaluated. Figure 1 shows the electrochemical window (1.0 V) of nanostructured $VOPO_4{\cdot}2H_2O$, C-$VOPO_4$ and K-$VOPO_4$ in 3M LiOH. The volammograms show an ideal capacitive behavior that remains at high scan rates up to 100 mVs^{-1}. The specific capacitance are 75, 25.17 and 10.36 Fg^{-1}. There is insertion of Li ions into the two dimensional tunnels of the crystalline structure for the case of $VOPO_4{\cdot}2H_2O$. In the case of C-$VOPO_4$ and K-$VOPO_4$ the two dimensional tunnels are hindered by ions or molecules, avoiding the insertion of Li ions into the crystalline structure, thus the specific capacitance is lower than in the case of $VOPO_4{\cdot}2H_2O$ with a free path for Li ions into its tunnels.

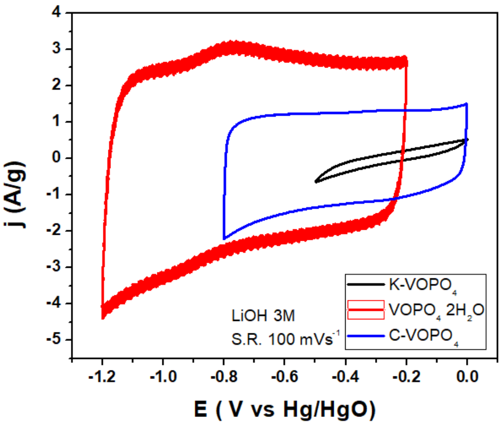

Fig. 1: Electrochemical windows for $VOPO_4$•$2H_2O$, C-$VOPO_4$ and K-$VOPO_4$ electrodes in LiOH at 100 mVs^{-1}

References

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Cap_08

$Mn_3(PO_4)_2\cdot 7H_2O$ as Electrode Material for Electrochemical Capacitors

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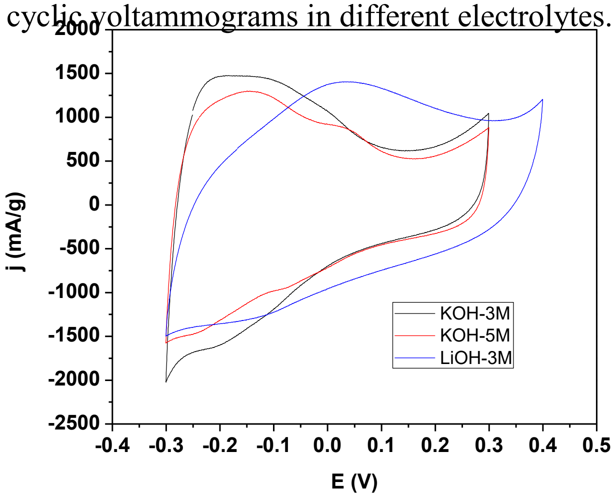
Electrochemical capacitors are energy storage devices with higher power density and charge-discharge cycle stability than batteries [1,2]. However, transition metal oxides, nitrides, carbon based materials, redox polymers and composites that have been used as electrode materials for electrochemical capacitors typically show lower energy densities than batteries [3]. In order to improve the energy density without sacrifice the power density and cycle stability of the electrode materials, it is necessary to prepare new materials and to understand their charge storage process. In this work, we report the electrochemical properties of $Mn_3(PO4)_2\cdot 7H_2O$ as electrode materials for electrochemical capacitors. The electrodes were tested in aqueous neutral, acid and alkaline electrolytes. Figure 1 shows the cyclic voltammograms in different electrolytes.



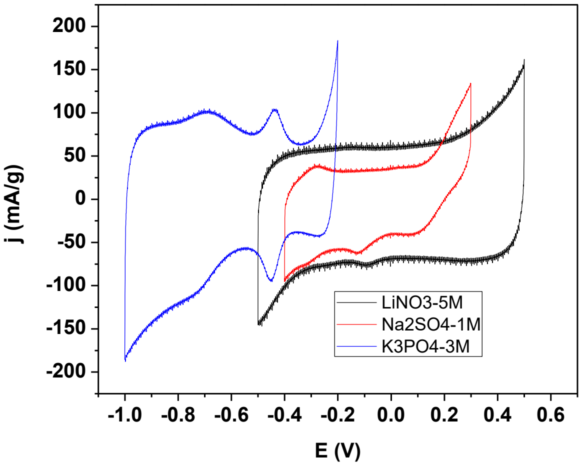


Fig.1: Cyclic voltammograms of $Mn_3(PO_4)_2 \cdot 7H_2O$ in different electrolytes.

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Cap_09

$MnHPO_4$ as Electrode Material for Electrochemical Capacitors

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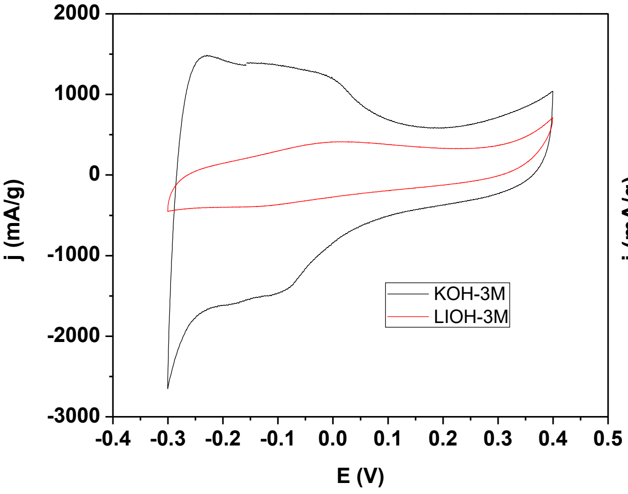
Electrochemical capacitors are a new alternative to store the energy for different electronic devices or electric vehicles [1-3]. This originated by their higher power density and charge-discharge cycle stability than batteries. However, the aim in the field of electrochemical capacitors is to increase the energy density without sacrifice the power density and cycle stability [2]. Transition metal oxides and metal nitrides have been used as electrodes in electrochemical capacitors, but their energy density is not as high as the energy density of batteries [2,3]. Recently, transition metal phosphates has been proposed as electrode materials for electrochemical capacitors with a high energy density [2]. In this work, we report the $MnHPO_4$ electrode, material for elecrochemical capacitor. The manganese phosphate was characterized by XRD, SEM, BET and FTIR. The electrochemical characterization was performed in acid, neutral and alkaline electrolytes and evaluated by cyclic voltammetry, chronopotentiometry, electrochemical impedance spectroscopy and charge-discharge cycles. Figure 1 shows the cyclic vomtammograms of $MnPO_4$ in different electrolytes.



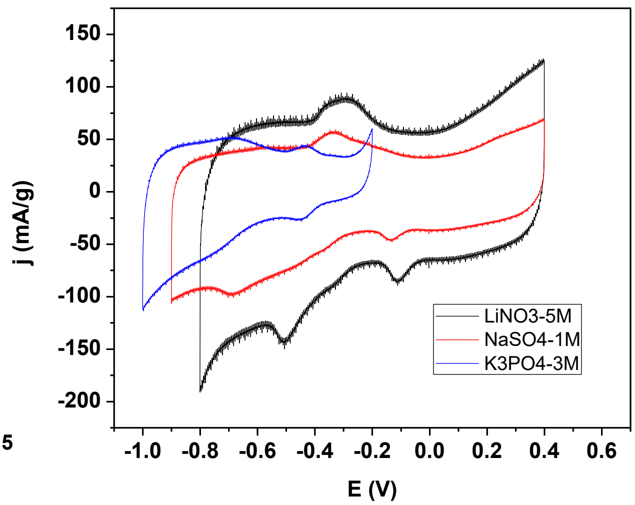


Fig.1: Cyclic voltammograms of $MnHPO_4$ in different electrolytes.

References

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Cap_10

Green supercapacitors assembled with activated carbons obtained from Agave residues by solar pyrolysis

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Due to its properties, such as high surface and electrochemical stability, activated carbon (AC) is a widely employed material in energy storage field [1]. In this work, we produced AC from lignocellulosic residues of agave angustifolia (a waste from mezcal industry), by using as sustainable process a solar pyrolysis at temperatures between the range of 450°C-900°C, being solar energy the heat source and K_2CO_3 the friendly environmental activating agent. Biomass was previously characterized by TGA, XRD, SEM, EDS and CHONS. Obtained ACs were characterized by XRD, nitrogen physisorption, Raman spectroscopy, SEM, EDS, CHONS and cyclic voltammetry in 3-electrode cells. The ACs with the best electrochemical performance (Fig. 1) were selected to be tested as supercapacitor electrodes in asymmetric assembles. In order to assemble green supercapacitors, we used a neutral solution (1M Na_2SO_4) instead of an organic or an acidic electrolyte. Results showed that devices assembled with these activated carbons can deliver similar specific power and energy than carbon/carbon supercapacitors assembled with commercial ACs. In conclusion, solar pyrolysis of lignocellulosic residues in combination with K_2CO_3 as activating agent, have demonstrated to be a sustainable alternative to the traditional pyrolysis to obtain ACs for energy storage purposes.

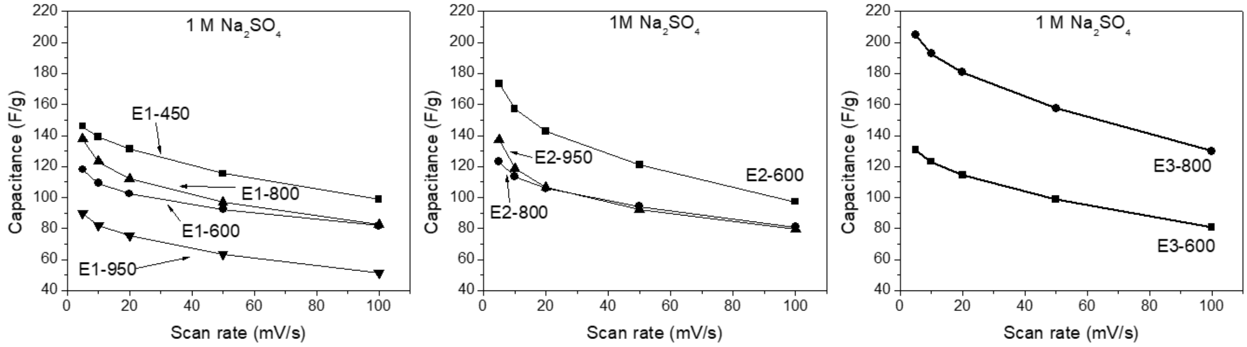

Fig. 1: Specific capacitances of activated carbons, obtained from solar pyrolysis of agave leaf, in 3-electrode cells. Low biomass-activating agent ratio (left), average ratio (center) and high ratio (right).

References

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Sim_02

Ab initio calculation of the effect of M-N (M= Fe, Ni, Co) on the stability and catalytic activity for the Oxygen Reduction Reaction in Metal-Air batteries.

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Metal air batteries have driven research efforts in the past years due to promising electrochemical performance and high energy density, which could go beyond Li-ion batteries, with a wide variety of applications such as electric vehicles. However, the kinetics of the electrochemical reactions (such as the ORR) are slow and the volatility and stability of the electrolytes make the practical application of metal-air batteries a challenge. Carbon-based materials, such as graphene, have been explored as cathodes for metal-air batteries due to their excellent electrical conductivity and high porosity[1,2]. MN modified graphene materials are one of the most promising materials as catalysts, they combine the conducting properties of graphene with the presence of catalytic sites well attached to the material. Although it has been previously proved that the presence of a Metal has a drastic effect on the catalytic activity for the Oxygen Reduction, the specific metal, coordination mode and number of Nitrogen atoms that lead to the maximum catalytic activity is unknown. Thus, in this work we have performed Density Functional Theory (DFT) simulations of the effect of substituting carbon atoms by M (Ni, Fe, Co) in four different situations. The preliminary results indicated that when the nitrogen is already present within the structure, the introduction of the metal is easier, except for the M-3N coordination. Moreover the presence of M-4N allows the formation of a positive charge accumulation in the neighboring carbon atoms. Further analysis of the interaction with O_2 will be presented during the event.

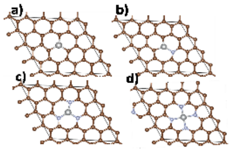

Fig. 1: DFT optimized structures of Metal substituted N doped graphene, a) M doped, b) M-N doped, c) M-3N doped and d) M-4N structure.

This work was supported by project SECITI/080/2017. The authors acknowledge the supercomputing facilities provided by LSCVP at UAM and supercomputer Yoltla.

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Sim_04

Hydrogen storage on Mg and Ca-functionalized siligene: A DFT study

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Since metal-decorated single monolayers have been considered one of the most promising candidates for practical hydrogen storage. In the present study we report the structural and electronic properties of the interaction between adsorbed H_2 molecules and the Mg and Ca-functionalized siligene have been thoroughly examined using density functional theory calculations with long-range van der Waals dispersion correction. A supercell consisting of 4 × 4 siligene unit cells is employed for all the calculated structures [1,2]. The binding energy between Mg and Ca atoms and siligene is greater than the cohesive energy of bulk metal so that clustering of adatom will not occur once it is bonded with siligene. The adsorption of H_2 on Mg and Ca decorated siligene is a weak physisorption. In particular for Ca-decoreated siligene, the van der Waals corrected H_2 adsorption energies fall within the range of 0.15–0.32 eV, suitable for practical H_2 storage applications. Siligene with Mg, and Ca have a capacity to seven hydrogen molecules storage capacity (see Figure 1) for each alkaline earth atom with desirable adsorption energy, indicating that the metal-decorated siligene can serve as a high capacity hydrogen storage medium. These results revealed that Ca-functionalized siligene could be a potential candidate for hydrogen storage.

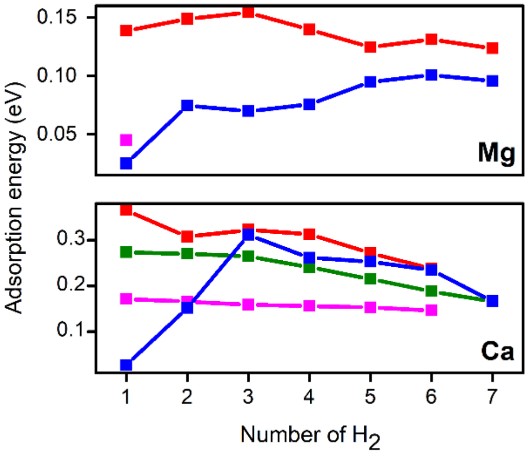

Fig. 1: Calculated adsorption energy (eV/H_2) as a function of the number of adsorbed H_2 molecules for Mg and Ca-decorated siligene.

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Oth_01

The potential of energy storage in the national electricity system and its potential contribution to the decarbonization of the electricity sector.

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This work presents some advances in the evaluation of the potential that energy storage systems could have within the national electricity system in Mexico, focusing the assessment on the possible contribution to the mitigation of greenhouse gas emissions in the power generation sector.

Energy Storage Systems (ESS´s) could potentially contribute in several ways to a low carbon development in the Mexican power generation sector; e.g. ESS´s could provide the required flexibility of renewable energy sources (RES) and thereby contribute to increase their efficient integration into the energy system, by facilitating the matching of generation with demand; the ESS´s could also provide several ancillary services to the national electricity system minimizing the use of fossil fuels. Furthermore, ESS's could provide further services that could range from energy management (e.g. time shifting or capacity firming) or even deferral of investments.

The National Institute of Ecology and Climate Change (INECC) carries out the study ***"Technology Roadmap and Mitigation Potential of Utility-scale Electricity Storage in Mexico"*** with support from the Mexican-Danish Partnership Program for Climate and Energy In Mexico, this study seeks among other things: the identification of energy storage technologies that are feasible in the Mexican context, including their possible costs and benefits and the identification of barriers and enablers of storage technologies in the technical and economic context. It also seeks to carry out five case studies of interest in Mexico to assess the storage potential of feasible technologies for the country and evaluate their potential to reduce emissions of greenhouse gases and compounds through a life cycle analysis, focused on the operation phase of the technologies, and thus on the potential displacement of fossil fuels through the efficient integration of higher shares of RES.

To estimate the storage potential on a regional basis, a methodology has been proposed that seeks to identify the local characteristics, such as transmission and distribution capacity, conventional and renewable generation capacity, and the needs and the problems related to the generation and distribution of energy. This allows undertaking an assessment of the benefits of storage at local level both for the current market regulation scenario and for an enhanced market regulation scenario for ESS's and ancillary services. For this, an estimation of the congestion and losses in the region based on node prices will be carry out as well as among other criteria to estimate a potential for storage at local or regional level.

As part of the study a catalogue of storage technologies with technical and economic data are included, and a regulatory framework for storage is reviewed. The goal is to suggest realistic scenarios of ESS deployment under economically viable conditions within the electrical system.

Oth_02

Magnesium alloys for hydrogen storage

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In the search for alternative fuels, hydrogen is the ideal candidate as a carrier of clean energy. There are different ways to store it, making it through metal hydrides seems to be a promising way. Magnesium hydride is considered a promising hydrogen storage candidate owing to its high hydrogen storage capacity (7.6 wt.%), good reversibility and low cost [1]. However, the hydrogenation and dehydrogenation processes of the Mg/MgH_2 system normally require temperatures higher than 300° C. In addition, it is known that nanostructured powders and nanoparticles display improved hydriding and dehydriding kinetics [2]. However, the performance of nanostructured MgH_2 may degrade rapidly because of unwanted reactions with water vapor, oxygen and carbon dioxide, particularly when the material is used as a fine powder. In the present work, the powders of Mg, Ni and Nb_2O_5 are mixed by ball milling, with a nominal composition of Mg-5% by weight of Ni-2% by weight of Nb_2O_5, and after that, this mixture is used for produce bulk nanostructured materials (BNM), in this way the reactivity of fine powders is avoided. These BNMs are manufactured by high pressure torsion (HPT). The material has been subjected to 10 or 20 turns in an HPT system to produce consolidated disks. Hydrogenation experiments were performed on these NMBs to explore the kinetics of hydrogen capture at different temperatures.

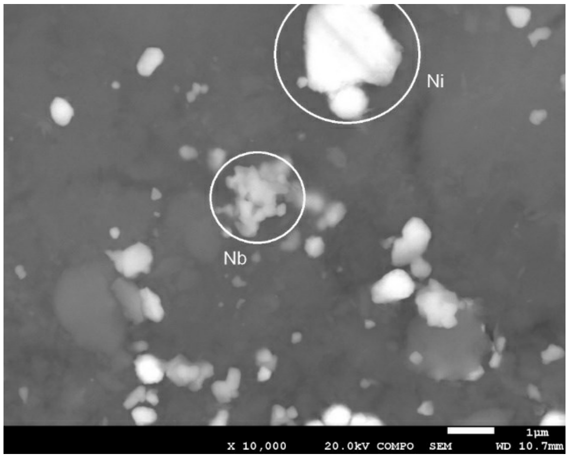

Fig. 1: SEM micrograph (BSE signal) of the Mg-5Ni-2Nb_2O_5 mixture after 1 h of milling.

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Oth_03

Synthesis of vanadium oxide as phase change material for mitigate energy use in buildings

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Today, latent heat storage using phase change materials (PCM) has become attractive for heating and cooling in buildings. The main advantage of latent heat storage is the higher storage density in small temperature intervals compared to other heat storage techniques. The PCM has the ability to absorb or release heat as a function of its phase change temperature. For building application, the most studied PCMs are organic paraffins presenting a solid-liquid phase change. However, some disadvantages such as low thermal conductivity, flammability, as well as runoff in the buildings have been limited their application [1][2][3]. An attractive alternative is to use PCM's with a solid-solid phase change. Among them, vanadium oxide (VO_2) undergoes a reversible and fast structural phase transition of monoclinic to rutile at 68°C. It had been widely used as thermochromic material in smart windows [4][5], but, it has not been evaluated as a PCM in the building's envelopes. In this project, VO_2 was synthesized by and hydrothermal method and the effect of thermal treatment in its thermal properties (transition temperature, specific heat and thermal energy storage density) were evaluated. The material was characterized by X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM) and Differential Scanning Calorimetry (DSC). Results showed that VO_2 was obtained as a monoclinic single phase after thermal treatment whit a reversible phase transition at 57.87 ºC. According to the results obtained the VO_2 presented less temperature of phase transition, probably due to the reduction of size. Based on the literature and results, the VO_2 could be a material viable to be used as PCMs for keeping a comfortable environment in the buildings and because its way to mitigate the c ergy

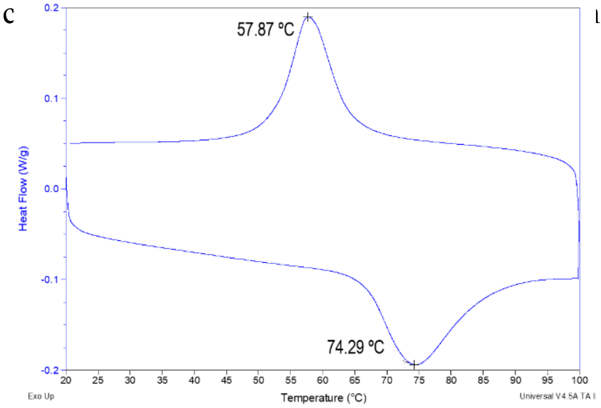

Figure 1. DSC of VO_2

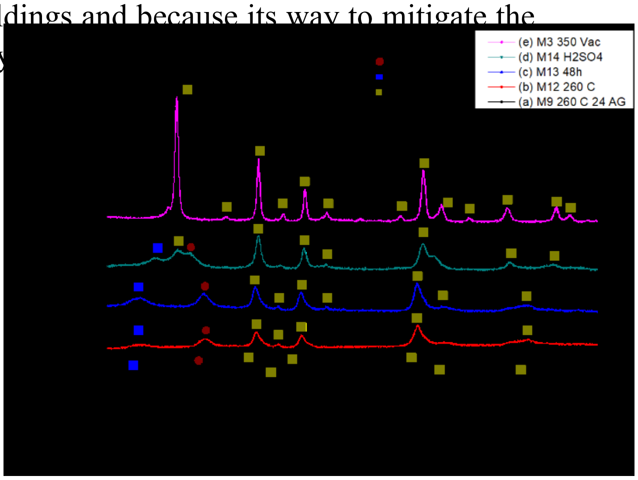

Figure 2. DRX of VO_2

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Oth_04

Synthesis of nanohybrid aerogels based on GO-TiO_2/PVDF for energy storage applications

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Hybrid materials for energy storage have become one of the main topics in research due to the rapid development of economy worldwide, environmental pollution and energy crisis of modern society. In recent years, reduced graphene oxide (rGO)-TiO_2 hybrids have attract the attention as potential candidates for energy storage system applications. While graphene offers electrical conductivity properties, TiO_2 can promote electrochemical activity and stability. On the other hand, 3D nanostructured carbon aerogels can promote large internal reactive areas and improve kinetics [1].

Herein, we report the construction of hybrid aerogels based on GO-TiO_2/polivinylidene fluoride (PVDF) ternary system in two steps. First, the synthesis of GO-TiO_2 nanohybrids was carried out through microwave-assisted method using $TiCl_4$ and titanium (IV) isopropoxide as titanium sources. **Figure 1** shows a TEM image of needle-like TiO_2 nanostructures supported on rGO. Then, GO-TiO_2/PVDF aerogels were prepared via hydrothermal and subsequent freeze-drying technique. The morphology of the ternary aerogel system was analyzed by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). X-ray diffraction (XRD) and Raman spectroscopy confirm the presence of TiO_2 rutile phase. The synthetic route represents a useful tool for the design of new 3D hybrid materials for energy storage applications.

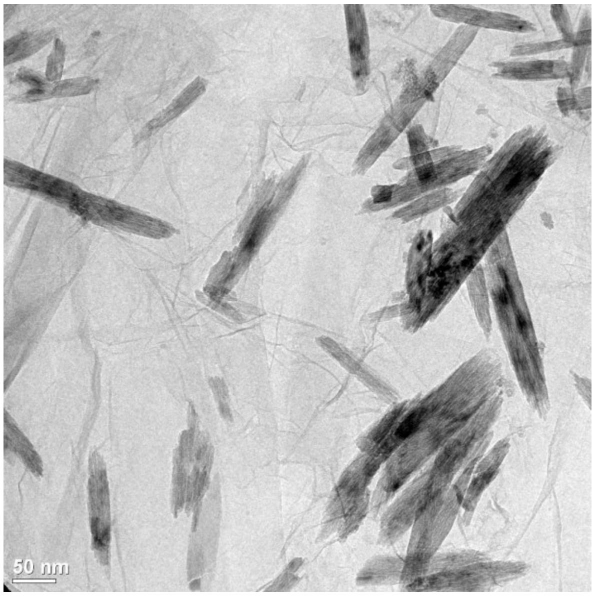

Fig. 1: TEM micrograph of TiO_2 needle-like nanostructures supported on a graphene oxide monolayer.

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Oth_05

Effect of dispersion on the average intercalation voltage in Prussian Blue Analogues

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Nowadays the production of electricity from renewable sources is an alternative to diminish the fossil fuel consumption. However, these types of sources are intermittent so new materials are under development to further improve the efficiency of energy storage. Among these, the Prussian Blue Analogues are promising cathodic materials in sodium-ion and potassium-ion batteries.

In the present work, a comparative study of different Prussian Blue Analogues was carried out by calculating their electronic structure within the framework of Density Functional Theory with periodic conditions using the VASP code. Our computational predictions are compared with experimental results obtained in our group.

The intercalation process was analyzed to compute average intercalation voltages relative to the corresponding metal electrodes, using the method proposed by Aydinol et al. [1], according to the general reaction $A_yM[Fe^{II}(CN)_6] \rightarrow yA^0 + M[Fe^{III}(CN)_6]$ where M = Bi, In and A = Li, Na, K. In a previous work [2] it was shown that considering the inclusion of dispersion effects in these types of systems is important to obtain voltages in agreement with their corresponding experimental values, so in this work, van der Waals interactions with two different schemes were included: the Tkatchenko-Sheffler method [3] with iterative Hirshfeld partition [4] and with the optB86b-vdW functional [5].

Acknowledgements

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Oth_06

Synthesis of $LiMn_{1.5}Ni_{0.5}O_4$ (LMNO) high voltage spinel cathode

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The improvement of materials for energy storage technologies, like lithium-ion batteries, is crucial for the proper implementation and operation of variable renewable energies, mainly for off-grid power systems. High voltage cathode materials such as $LiMn_{1.5}Ni_{0.5}O_4$ (LMNO), where the redox process is attributed to $Ni^{2+/4+}$ are quite promising for residential and mobile applications due to their high energy density and efficiency [1,2].

In this work, the LMNO solid-state synthesis parameters are evaluated thoroughly, among them temperature and time as well as Li, Mn and Ni precursors, are taken into consideration. Crystalline phase purity is evaluated through X-ray diffraction while electrochemical properties were performed through cyclic voltammetry and charge-discharge analyses. The preliminary results indicate that a two-steps synthesis allows to obtain high purity LMNO. In this synthesis process $Ni_{0.67}Mn_2O_{4-\delta}$ spinel is initially obtained as intermediate (first stage) by using the corresponding Mn and Ni acetate precursors. After that, Li_2CO_3 is incorporated to the material through a thermal process (second stage). Moreover, it was further identified that prolonged synthesis times (> 24h) affect the morphology and particle size of this material.

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Oth_07

Study of gases generation in Li_2CuO_2 cathode through Differential Electrochemical Mass Spectrometry in situ (DEMS-in situ)

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In situ techniques for electrochemical batteries analyses are important for a better understanding of the different processes occurring during the operation of the cell. Differential Electrochemical Mass Spectrometry (DEMS) for *in situ* battery analysis has been relevant due to the possibility of a directly comparing the electrochemical performance with the formation of different gaseous and volatile species. The analysis of gases is of fundamental importance for materials suffering irreversible changes during oxidation. Li_2CuO_2 has caught the eye of researchers due to its high theoretical capacity; however, during the first charge cycle, irreversible phase changes occur at higher potentials (starting near 4.0 V) which results in oxygen evolution and therefore, low coulombic efficiency, low specific capacities and poor cyclability [1-2]. To inhibit the evolution of oxygen and increase the overall stability of the material, fluorine ions are introduced in the solid-state synthesis in the form of CuF_2 in different molar equivalents to substitute oxygen in the crystalline structure of Li_2CuO_2. In this work, we report the initial steps needed to implement the DEMS technique including the adaptation of an El-Cell DEMS® and El-Cell std® to DEMS, controlling different factors affecting the obtention of reliable measurements, such as pipe thickness and length, as well as the type of control in the opening valve between the cell and the DEMS. The electrochemical characterization of fluoride doped systems have shown a significant decrease in capacity fade and better cyclability in comparison with Li_2CuO_2. These improvements could be attributed to the inhibition of gas evolution. *In-operando* DEMS is used to quantify the amount of oxygen produced during the oxidation of the active phase (Fig. 1). While the oxygen evolution increases at more positive potentials (Fig.1 a) for the unmodified material, the inclusion of 5.0% mol of fluorine diminishes meaningfully the oxygen production (Fig. 1b); however beyond 20% there is no longer any significant improvements in the electrochemical behavior or inhibition of gas evolution.

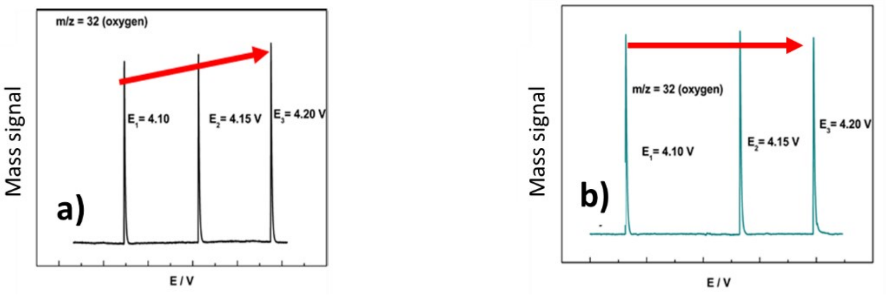

Fig. 1: Oxygen detected by *in-operando* DEMS (m/z= 32) during the cell operation at different potentials indicated in the figure. Comparing two active materials as cathodes: a)

Li_2CuO_2 and b) 5.0% F doped Li_2CuO_2. The red arrow shows the trend of the signal vs potential.

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Oth_08

Fungi-derived hierarchically porous carbon for energy storage application

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Electrochemical capacitors are good alternative as energy storage system for today's portable device [1], among its advantages are ultrahigh power density, fast charge-discharge rate and long cycling stability [2]. In the present investigation, the pyrolysis of the biomass of *Pleurotus djamor* fungus is reported (Figure 1a), evaluating entire fruiting body to obtain hierarchically porous carbon; fungi of basidiomycota division have hydroxyl groups on the cell wall, which prevent agglomeration during heat treatments and maintain their intrinsically porous structure [3]. In elementary analysis, values of 47% carbon were obtained, comparing it with other biomass used to obtain biocarbon, this fungus is suitable for this purpose.

Fungi were activated with KOH pyrolized at 600, 800 and 1000 °C in argon atmosphere; figure 1b shows the morphology of carbon obtained at 600 °C (PD600), in the morphology of the biomass and carbon, a certain amorphous similarity of the pores can be found on the surface of both materials, with which the porous base matrix of fungus was maintained once biomass was pyrolized, in addition to Raman spectrum it was possible to denote that the carbon obtained is disordered, for example, PD8000 has an ID/IG ratio of 1.35. This material was characterized by CV and charge-discharge cycles for evaluate their electrochemical performance.

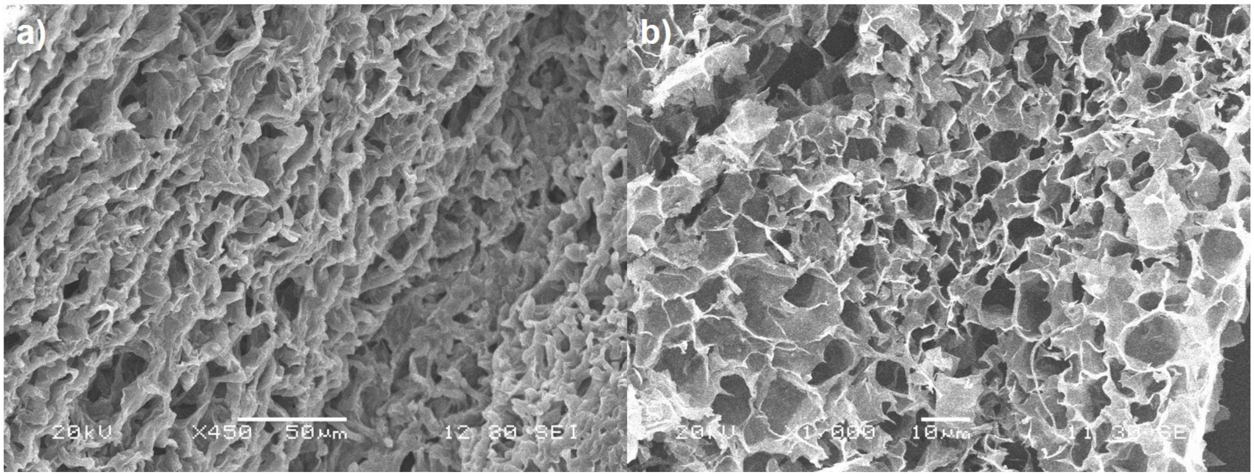

Fig. 1: SEM image of a) *Pleurotus djamor* and b) PD600 carbon.

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Oth_09

Cerium oxide thin films as electrolyte in SOFC.

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Nowadays, electricity production is one of the humanity greatest concern. Current energy production depends almost entirely on fossil fuels. However, it is very difficult to justify the use of these fuels due to their rapid depletion and the irreparable damage to the planet that they producing. Then, the implementation of clean and renewable energies is a necessity. In general, energy generation using renewable sources depends on different factors (light intensity, wind power, etc.), which requires the development of energy storage devices. Within the energy storage, hydrogen is of a great interest. The devices for obtaining electrical energy from hydrogen are called fuel cells, and among these cells are the so-called solid oxide (SOFC).

This work proposes the application of thin films of cerium oxide as electrolyte in solid oxide fuel cells, since it has been reported that they have excellent properties of ionic conductivity and low operating temperatures [1]. To obtain the thin films, the Ultrasonic Pyrolytic Spray technique is used, as it is an accessible and easily scalable method, in addition to which it allows obtaining dense and homogeneous films [2]. The films were optimized varying the flow rate, the substrate temperature and the Gd concentration [3]. Films were characterized by X-ray diffraction, UV-vis spectroscopy, ellipsometry, scanning electron microscopy. Variations in temperature and flow rates modified the morphology, grain size and the texture of films. The nanometric grain size increase the conductivity of these materials, which allows the reductions of operating temperature in SOFC.

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Oth_10

Cerium oxide films for photoelectrocatalytic applications

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Conventional electrolysis is one of the ways to produce hydrogen as a clean fuel, however, is a low efficient method for the industrial production.[1] One way to improve efficiency and reduce costs is the development of catalysts, which decrease time and the energy consumption of the reaction[2]. In this work, nanostructured ceria thin films have been prepared on FTO substrates by ultrasonic spray pyrolysis using cerium acetylacetonate as metallo-organic precursor dissolved in anhydrous methanol. The temperature of the heating plate (Ts) was fixed at 450 ºC, the deposition time (td) was 30 min, and the carrier and director gas flow rates, air in both cases, were fixed at 1.0 L/min and 1.5 L/min respectively. The morphology, structure, optical and electrical properties were studied using scanning electron microscopy, X-ray diffraction (XRD), Raman spectroscopy, UV-Vis and electrochemical impedance spectroscopy (IS). The influence of thermal annealing at 500 ºC on the structural properties of films was studied. Thermal annealing do not modified the morphology and texture of films, but reduce the oxygen vacancies concentration. The band gap was 3.23 eV for as grown samples and 2.98 eV for treated films. Photoelectrochemical measurements indicate variations in the Voc higher than 0.1 eV when 360 nm UV-LEDs light is turn on. The flat-band potential was calculated from the Mott-Schotky relation with values of -0.36 V in dark and -0.47 V for the illuminated sample. Using the cerium oxide film as electrode, an increase in the evolution of the reaction is observed.

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Oth_11

Transition metal pentacyanoferrates: a new family of materials for energy storage in aqueous solutions.

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The present work describes the use of transition metal cyanomethalates as active materials to be used in electrochemical energy storage devices in aqueous media. This family of materials has appropriate characteristics that may allow its use in hybrid electrochemical storage devices of Li^+, Na^+, K^+, Mg^{2+} and Zn^{2+} ions in aqueous solutions. The formation of the materials and their composition was verified by FTIR, Raman and ICP. The performance of materials in energy storage was evaluated by electrochemical techniques such as cyclic voltammetry, chronopotentiometry and electrochemical impedance spectroscopy. The reduction / oxidation processes, as well as the energy storage capacity, were modulated by the transition metal used for the precipitation of the compound, as verified by IR-in situ measurements. The excellent performance of the materials is related to the modification in the coordination of the binders to the Fe within the structure, which allows the formation of solids with greater internal porosity, facilitating the transport of the cations within the solid.

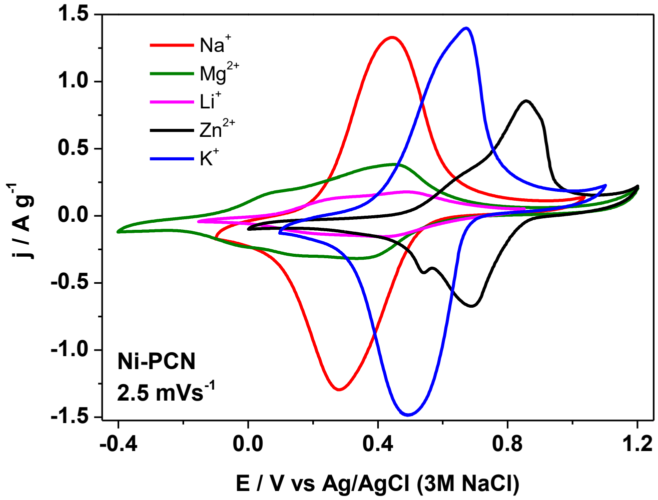

Figure 1. Cyclic voltammetry of the material Ni-PCA en 0.5 M $M_{(2/n+)}SO_4$ *(M =* Na^+, Mg^{2+}, Li^+, Zn^{2+}, K^+*).*

Oth_12

Mathematical modeling for the adjustment of parameters of a battery

Title of the abstract

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Nowadays due to a high penetration of intermittent renewable energies wind and sun, as well as in a short future where electric vehicles can buy and sell energy to the grid, it is necessary to have mathematical models that faithfully reflect the dynamics of the variables of battery storage systems, such as the state of charge and voltage in terminals, depending on the current of charge and discharge that it has. There is also a great diversity of technologies, where each of them has its characteristics. In this work, a metaheuristic method is applied to determine the parameter values of an electrical model, which can reflect the transient dynamics of different types of batteries, such as lead-acid, lithium-ion, AGM, gel, and Ni-Cd. In such a way that from the data provided by the manufacturers through the characteristic curves depending on the type of battery, the algorithm finds those values of resistances and internal capacitances, to predict the electrical behavior of the battery. The methodology was tested experimentally with a lead-acid battery on a test bench, and from obtaining its curves through different charge and discharge cycles with pulsating currents of different values, the algorithm was developed to search for the electrical parameters that best fit the theoretical curves with the experimental ones, obtaining satisfactory results. The state of charge of the battery depends in turn on the manufacturer and the type of battery chosen, so by adjusting the model we can be able to do a better characterization of different models and types, which will allow us to make improvements to the design of batteries through computationally simulation, this as a previous step in the design of a new battery. This model seeks to find the necessary constant values for the battery parameters, based on experimental data obtained previously. The experimentation was carried out by the charge and discharge of the battery with currents of 1, 2 and 3 amps during the period of 10 minutes, taking 6 samples per minute, taking a blocking voltage of 9.5 volts. Where it can be noted that when discharging it to 2.3A it is not enough to take all the samples because it reaches the discharge limit faster, so it was established that the experimental discharge current would be 1 A.

This experimentation is the one that is programmed in the mathematical modeling, which allows to evaluate the difference between the theoretically calculated and the obtained in an experimental way so that every time the programmed routine is carried out this difference (error) is smaller.

Oth_13

From gasifier residue to useful material for energy storage

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Biochars from solid residues have been very successful in many applications due to their high surface area, porosity properties, and surface chemistry. Biomass gasification process generates large amounts of solids. In this work, a biochar obtained as residue from corn cob gasification (GAS) is used as electrode material of supercapacitor (SC). An activated biochar (LAB) obtained from pyrolysis of acid treated corn cob wastes at 800 °C has been also evaluated in SC application for comparison. From physical characterization was observed that both biochars are amorphous carbons, which have well-developed microporous surface of different features related with a pretreatment of corn cob and production of biochars. GAS and LAB were electrochemically evaluated by cyclic voltammetry in 0.5M H_2SO_4 electrolyte using a three-electrode system, obtaining capacitances at 5 mVs^{-1} of 150 Fg^{-1}. Finally, asymmetric carbon-carbon SC cells were assembled showing excellent performance compared to commercial activated carbons, with capacitances around 27 Fg^{-1} at 0.5 Ag^{-1} with only about 10% of capacitance loss after 5000 cycles, for both biochars. However, GAS performance in SC was higher than activated biochar and activated commercial carbons (Fig. 1). This study provides a novel useful application to use gasifier residues from agricultural biomass waste for energy storage devices.

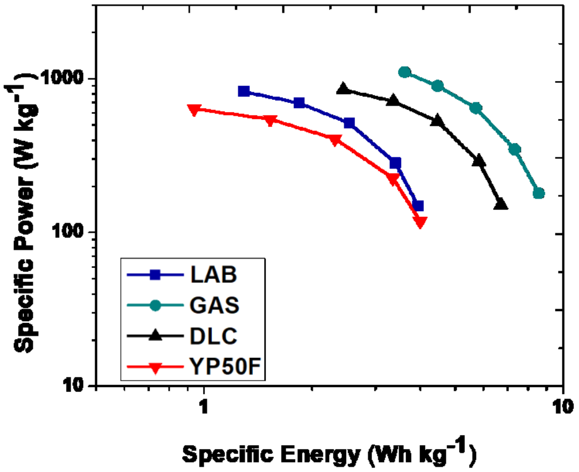

Fig. 1: Ragone plot for SCs using corn cob waste-derived biochars as electrodes. Commercial activated carbons Norit® DLC Supra 50, and Kuraray YP50F are included for comparison.

Oth_14

Immobilization of POMs on carbon nanotubes for the development of Negative electrodes for hybrid energy storage devices.

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Polyoxometalates (POMs) are large clusters of metal oxides with applications in energy storage due to their multielectron redox reactions. A theoretical study related with nanocomposite materials based on SiW12 Keggin polyoxometalate anchored through functional groups to a carbon nanotube was performed, suggesting that carboxylic groups form a covalent bond with SiW12 [1] This study was the inspiration for our experimental work, where SiW12 was proposed for the development of a negative electrode due to the negative potentials of their redox reactions. We synthetized nanocomposite materials based on functionalized multiwall carbon nanotubes with carboxylic acid to study the anchoring of SiW12 nanoparticles, expecting a different electrochemical behavior.

Each material was characterized by XRD, FTIR, Raman spectroscopy, TGA, TEM and cyclic voltammetry (VC) in 3-electrode cells. The interaction between the POM and the functional group appears to help in charge transfer that may be determinant at the charge/discharge cycling performed in energy storage devices. This result suggests that a selective bond exist between the POM and carboxylic acid functional group (Fig. 1). The VC presents the characteristic rectangular profile of the electrochemical double layer from carbon nanotubes, aside from several redox processes: one redox pair at 0.13 V/0.19 V (*) related with the functional group, and two redox processes related with the SiW12 at negative potentials (I/I' and II/II') (Fig. 1). Usually between potential -0.2 V and -0.55 V the process of the polyanion are presented, but in the hybrid materials these two processes appear to overlap creating a wide peak with a more pseudocapacitive character.

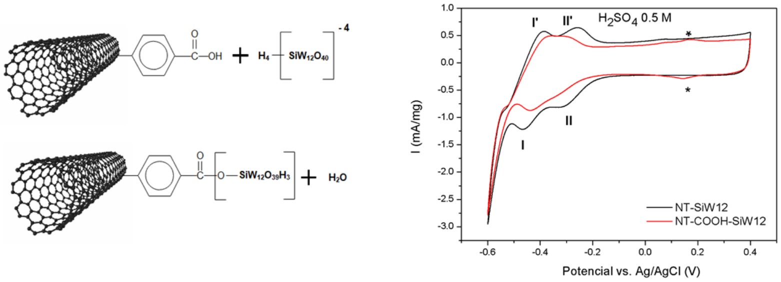

Fig. 1: Representation of chemical reaction of the hybrid composites (left), Comparation of the VC of nanocomposite materials (right).

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Oth_15

Sb/Sb_2O_3/carbon nanocomposites for Li-ion storage: Effect of the carbon matrix dimensionality

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As one of the promising material for anode in Lithium-ion batteries (LIB), antimony-based materials with high specific capacities are attracted great attention to substitute the common graphite anode. Herein, we report a one-step hydrothermal route for the synthesis of Sb/Sb_2O_3 nanoparticles anchored on different carbon matrices as an anode material for Li-ion batteries (LIB). The effectively integration of a 3D carbon matrix composed of 1D carbon nanotubes (CNT) and 2D graphene nanoribbons (GNR) along with Sb/Sb_2O_3 nanoparticles (Sb/Sb_2O_3/CNT/GNR nanocomposites) improves the Li-storage performance and chemical stability of the nanocomposite. When used as an electrode for LIB, Sb/Sb_2O_3/CNT/GNR nanocomposites exhibits a reversible specific capacity as high as 399 mAh g^{-1} after 50 cycles at 50 mA g^{-1} and excellent cycling performance. Meanwhile, the cycling performance of Sb/Sb_2O_3 nanoparticles anchored on GNR and CNT only obtains specific capacity of 288 and 191 mAh g^{-1} after 50 cycles at 50 mA g^{-1}. The obtained results indicate the beneficial effect of the 3D carbon matrix providing an effective strategy for the synthesis of high capacity anodes based on Sb-materials for LIB.

Oth_17

Improving the Electrochemical Behavior of Layered Cobaltous Terephtalate by Co-Co Interaction Through Pyrazine Linker

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Metal–organic frameworks (MOFs) are a new kind of porous material with porosities, and they have been widely used in many felds including gas separation and storage, catalysis, sensing and drug delivery [1]. Very recently, investigations into the direct use of MOFs as supercapacitor electrode materials have expanded.

This contribution evaluates the energy storage capacity and mechanism, in alkaline medium, of laminar MOF (Metal Organic Framework) of cobalt coordinated with therephtalate, using water (Co-H_2O) and pyrazine (Co-Pyz) as a linker pillar.In this study, Co- MOF were synthesized through a hydrothermal method and the structures of materials were characterized by X-ray diffraction (XRD), Raman, FT-IR and UV-Vis espectroscopy. The supercapacitive performance was evaluated by cyclic voltammetry (CV), galvanostatic charge/discharge and electrochemical impedance spectroscopy (EIS) measurements. Co-Pyz exhibit specific capacity values of 66, 75, 80, 79 and 71 Cg^{-1} at 0.5, 1, 2, 4 and 8 Ag^{-1} respectively, which are considerably higher than Co-H_2O (47, 49, 50, 51 and 50 at 0.5, 1, 2, 4 and 8 Ag^{-1}, respectively). In-situ spectroscopy techniques (XANES and FTIR) suggest that in the second process Co^{2+}/Co^{3+} redox couple take place, accompanied by the insertion and extraction of OH^- ions to stabilize the structure.

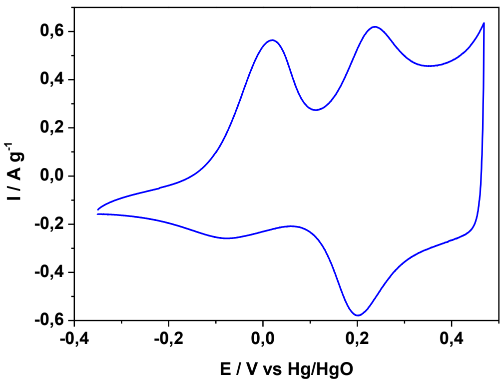

Fig. 1: Cyclic voltammetry curves of a Co-MOF at 5 mVs^{-1} in 1M NaOH

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Oth_18

Protocol for evaluation of the ionic conductivity in alkaline anion exchange membranes

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The ionic conductivity is a key performance property of polymer electrolyte membranes (PEM, AAEM, etc.). Low conductivity values normally gives poor performance in the fuel cell due to the high resistance in the membrane electrode-assembly (MEA). Today, there isn´t a clear understanding of ex situ technics to measure ionic conductivity of the sole membrane. Usually, the procedure consists of measuring the membrane ohmic resistance by Electrochemical Impedance Spectroscopy (EIS) to indirectly calculate the ionic conductivity[1, 2]. Currently, there are two methods reported to measure the EIS of the membranes, on-plane (longitudinal or transverse directions) and through-plane (through the thickness of the membrane). The through- plane measurement was used for our study. This document describes the in-house manufacture of a PTFE-made conducitivity cell to evaluate the EIS of three different alkaline anion exchange membranes (AAEM), the test stand, and testing protocol design are reported here, and results from the ionic conductivity are discussed for the AAEMs with the further interest to integrate MEAs for Alkaline Anion Exchange Membrane Fuel Cells.

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Oth_19

New generation GDLs´performance characterization for fuel cell technology

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Nowadays there is state-of-the-art Gas Diffusor Layers (GDLs) with improved mass transport proprieties that are being considered to outperform known polymer electrolyte membrane fuel cell technology. It is known that the Membrane Electrode-Assembly (MEA) is the core component of the fuel cell. A typical MEA is composed of a Polymer Electrolyte Membrane, two catalyst layers, and two Gas Diffusion Layers (GDLs). A MEA with this configuration is known as a 5-layer MEA. In Proton Exchange Membrane Fuel Cells, the standard commercial materials used are: Nafion® membrane and Pt/C as catalyst. In this work, four different state-of-the-art- GDLs were used (29BC, 38BC, 39BC, and 29BA) in the 5-layer MEA configuration to compare performance in a single cell hardware. Toray paper (90 PTFE w%) was also used for comparison. The MEAs were fabricated with an active area of 9 cm^2 and 0.5 mgPt/cm^2, and electrochemically characterized to compare the effect of the GDLs and Toray paper on the fuel cell performance. Thechnical specifications of the GDLs can be found in [1]. The results (Figure 1) show the polarization curve for each MEA material. In this work, the correlation between GDL properties and effects in the overpotential zones of the I-V curves are discussed in the scope of identifying the most promising GDLs for next fuel cells to be developed in INEEL.

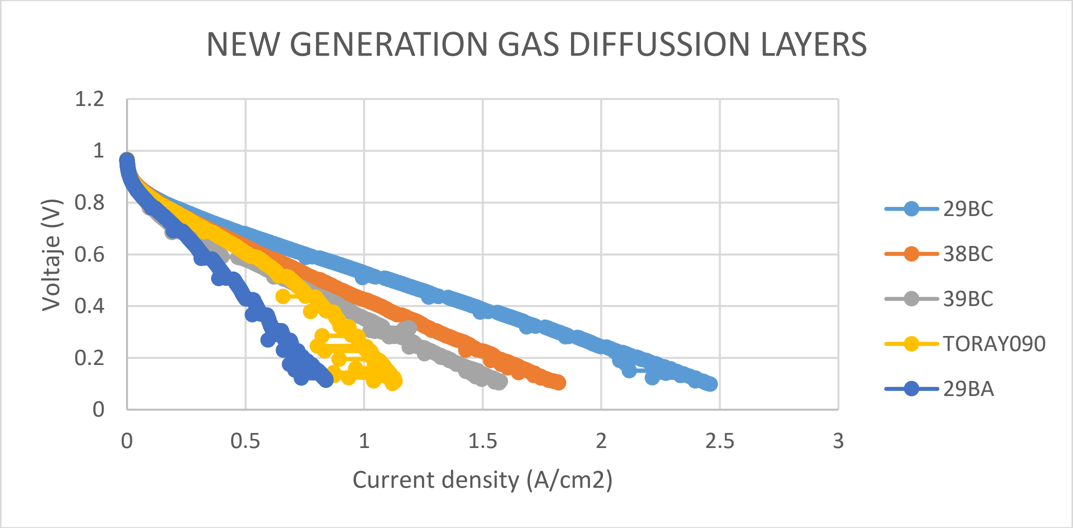

Figure 1. Polarization curves (I-V) comparing MEAs fabricated with different GDLs. The single fuel cell was operated at 60 °C with H_2 and O_2 at 10 psi.

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Oth_20

ADSORBED METHANE MOLECULES IN A HETEROESTRUCTURED SYSTEM

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The use of new porous materials, such as organic metal frameworks (MOFs) and carbonaceous nanostructures (CNT), have been explored as a matrix for methane storage [1] in order to combine exceptional high surface areas and wide non-polar pore distribution [2]. The present work makes use of the structural characteristics of both lattices, obtaining an heterostructure. The structural versatility of this type of system opened the possibility of expanding storage surface area and surface properties, such as its pore geometry, pore dimensions and channel structure. Inside this system, the study of the interaction with methane [3] provides critical information in applications of storage or separation processes. The new heteroestructured system consists of functionalized single walled carbon nanotubes (SWCNT) and Zn-methylimidazolate framework (ZIF-8). The new pore system mimics the isothermal SWCNT curve, with a notable increase in the amount of adsorbed N_2 (see Fig. 1). Methane storage capacity at 248 K and up to 9.5 bar was evaluated: no maximal storage capacity was reached at 9.5 bar. Moreover, recorded adsorption isotherm of CH_4 showed hysteresis. Data until this point rise the question: What is inside this new heteroestructured system able to retain methane molecules even at low pressures?

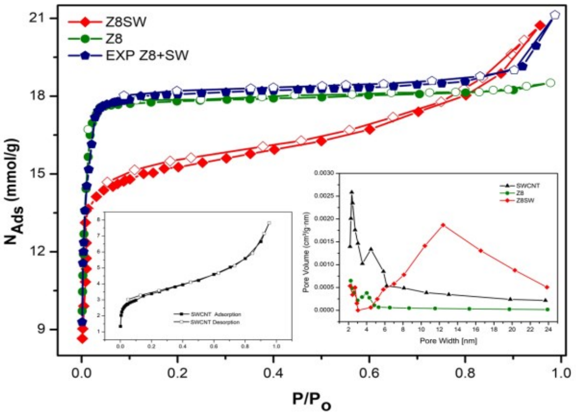

Fig. 1: Adsorption – Desorption N_2 isotherms at 75 k for Z8, Z8SW and EXP Z8+SW Inset: a) ads-desorption N_2 in SWCNT and b)Pore size distribution for studied structures.

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