ENERGY STORAGE DISCUSSIONS 2023

MONTERREY, MEXICO

16 - 17 November 2023

BENEMÉRITA UNIVERSIDAD AUTÓNOMA DE PUEBLA · 1578 ·

CONCYTEP
Consejo de Ciencia
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"Energy Storage Discussions" is a forum of analysis of different aspects of energy storage, born in 2014. In the era of renewable energies and mobile electronics, the need of better energy storage devices is every time more evident. The areas of materials science, electrochemistry, power electronics and control systems, and combined areas like nanotechnology are all merged when discussing about energy storage. The 2014, 2016, 2017 and 2019 editions of the conference have been very successful with the participation of over 100 experts. This conference is the flagship event of the Mexican Energy Storage Network. The present 2023 edition of the event promises rewarding discussions.

Conference Chair:

Dr. Enrique Quiroga-González (IFUAP-BUAP)

Scientific commitee:

Dr. Ana Karina Cuentas-Gallegos (CNyN-UNAM).

Dr. Eduardo M. Sánchez-Cervantes (UANL).

Dr. Daniella E. Pacheco-Catalán (CICY).

Dr. Raúl Lucio-Porto (UANL).

Thursday, November 16th	
Time	
08:45	Registration to the conference
09:10	Opening ceremony
09:20	Keynote talk "**Operando monitoring of interfacial processes in capacitive energy storage systems**" By Dr. Krzysztof Fic
10:20	Oral Session 1
11:00	Poster session with coffee break
13:30	Lunch break
15:30	Oral Session 2
16:10	Coffee break
16:30	Oral Session 3
17:30	Concluding remarks of day 1

Friday, November 17th	
Time	
09:20	Keynote talk "**Unveiling Lithium-Solid Electrolyte Interface Evolution in All-Solid-State Batteries through Operando Characterizations**" by Dr. Yan Yao
10:20	Oral session 4
11:00	Coffee break
11:20	Oral session 5
12:00	Round Table: "**Present and prospectives of Energy Storage**"
13:00	Lunch break
15:00	Keynote talk "**Effects of Fast Charging on Battery Electrode Materials**" by Dr. Molleigh Preefer
16:00	Coffee break
16:20	Oral session 6
17:20	Closing ceremony

Oral session 1

Thursday, November 16th, 10:20-11:00 Chairman: Dr. Raúl Lucio Porto (UANL)

ID	Name of the work	Authors	Institutions
ESD2023_6	Influence of structural and chemical composition of lignocellulosic precursors for porous carbon production useful in Supercapacitors	Ana Karina Cuentas-Gallegos	Centro de Nanociencias y Nanotecnología, UNAM
ESD2023_67	Tuning Prusian Blue Analogs properties for assembling hybrid supercapacitors in aqueous electrolytes	Próspero Acevedo-Peña	CICATA, IPN

Oral session 2

Thursday, November 16th, 15:30-16:10 Chairman: Dr. Próspero Acevedo Peña (IPN)

ID	Name of the work	Authors	Institutions
ESD2023_9	Hybrid Energy Storage: Relevance, Features and Applications	M. G. Reveles-Miranda and D.E. Pacheco-Catalán	Centro de Investigación Científica de Yucatán (CICY)
ESD2023_15	Exploring the Alkali Metal Intercalation Mechanism in δ-MnO_2 Structure: A First-Principle Study	Christian A. Celaya, Jesús Muñiz, Jonathan Guerrero-Sánchez and Ana Karina Cuentas Gallegos	Centro de Nanociencias y Nanotecnología, UNAM

Oral session 3

Thursday, November 16th, 16:30-17:30 Chairman: Dr. Daniella Pacheco Catalán (CICY)

ID	Name of the work	Authors	Institutions
ESD2023_3	Modeling, Simulation and Optimization of a Commercial Lithium-Ion Battery with Charge Cycle Predictions	Camas-Náfate Mónica; Coronado-Mendoza Alberto; Vega-Gómez Carlos; Espinosa-Moreno Francisco	Centro Universitario de Tonalá, Universidad de Guadalajara
ESD2023_24	Advanced spectral analysis of electrical cycling signals for early failure detection in lithium ion batteries	M. Carbonó, J. Gómez and R. Nava	Instituto de Energías Renovables, UNAM
	Energy storage for industry in Mexico	Alejandro Fajer	Quartux

Oral session 4

Friday, November 17th, 10:20-11:00 Chairman: Dr. Eduardo M. Sánchez Cervantes (UANL)

ID	Name of the work	Authors	Institutions
ESD2023_44	Direct, Multimodal Visualization of Zinc Metal Plating and Stripping via Transmission X-ray Microscopy	David N. Agyeman-Budu, Yechuan (Leo) Chen, Molleigh B. Preefer and Johanna Nelson Weker	Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory
ESD2023_27	Electrospun coaxial carbon nanofibers with high performance as anodes of sodium ion batteries	L.A. Rodríguez-Guadarrama, I.L. Alonso-Lemus and J. Escorcia-García	CINVESTAV, Unidad Saltillo

Oral session 5

Friday, November 17th, 11:20-12:00 Chairman: Dr. Ivonne Liliana Alonso Lemus (CINVESTAV)

ID	Name of the work	Authors	Institutions
ESD2023_38	Advances on the evaluation of exfoliated $ZnS(en)_x$ nanolayers as electrodes in rechargeable lithium-ion batteries	E. Gonzalez, A. Hernandez-Gordillo, Y. Gonzalez, N.A. García and E. Sanchez	Facultad de Ciencias Químicas, UANL
ESD2023_19	Ion transport mechanism of LLZO-PEO composite solid electrolyte and its all-solid-state lithium-sulfur batteries	P.M. Gonzalez Puente, Fei Chen and Yiluo Zhang	Departamento de Química, UAM

Oral session 6

Friday, November 17th, 16:20-17:20 Chairman: Dr. Ana Karina Cuentas Gallegos (UNAM)

ID	Name of the work	Authors	Institutions
ESD2023_54	Synchrotron radiation insights into $LiNiO_2$ and Mn, Co-doped cathodes at different states of charge via TXM and XANES analysis	E. Espinosa-Villatoro, M.B. Preefer, Z. Cui, A. Manthiram and J. Nelson Weker	Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory
ESD2023_28	Hierarchical implementation of electrochemical techniques to provide a reliable diagnosis of commercial lithium-ion pouch cells under selected operational conditions	R. Suarez, G. Ramos and I. Gonzalez	UAM, Consejo Nacional de Humanidades, Ciencia y Tecnología CONAHCYT
ESD2023_62	FFT impedance spectroscopy for real time analysis of phenomena in energy storage devices operando	M.A. San-Pablo-Juárez, A. Arroyo-Balseca, L. Valverde-Serrano and E. Quiroga-González	Instituto de Física, BUAP

Poster session

Thursday, November 16th, 11:00 - 13:30

ID	Name of the work	Authors	Institutions
ESD2023_2	Synthesis of δ-MnO_2 by electro-oxidation of Mn_3O_4 in Na_2SO_4 electrolyte	P. J. Pérez-Diaz, J.M. Bass López, Y. Esqueda-Barrón, A.K. Cuentas-Gallegos, D.E. Pacheco-Catalán	Centro de Investigación Científica de Yucatán
ESD2023_4	A DFT investigation : Hydrogen storage in metal-decorated doped germanene	Akari Narayama Sosa, Álvaro Miranda, Luis Antonio Pérez, Gregorio Hernández Cocoletzi, Miguel Cruz-Irisson	IPN-ESIME and Instituto de Física, BUAP
ESD2023_5	Synthesis and characterization of lithium complex oxide powders for application in Li-Ion batteries	Sael Beltran Torres, Rafael García Gutiérrez	Departamento de Investigación en Física, Universidad de Sonora
ESD2023_7	High-performance supercapacitors using biocarbon:bismuth oxide composites as active materials	S. Mena Picón, J.A. Díaz-Guillén, I.L. Alonso-Lemus, F.J. Rodríguez Valera	Tecnológico Nacional de México, Instituto Tecnológico de Saltillo
ESD2023_8	High-performance supercapacitors based on sewage sludge-derived biocarbon	S. Ravichandram, I.L. Alonso-Lemus, B. Escobar-Morales, F.J Rodríguez Varela	Nanociencias y Nanotecnología, CINVESTAV Satillo
ESD2023_10	Determination of structural, electronic and optical properties of β-$NaFeO_2$ ferrites doped with Ni and Cu: a joint experimental and theoretical study	Nayeli Gómez-Garduño, Daniel G. Araiza, Christian A. Celaya, Jesús Muñiz and Heriberto Pfeiffer	Insituto de Ciencias Aplicadas y Tecnología, UNAM
ESD2023_11	Evaluation of Fe/Co nitrogen-doped subbituminous coal from Coahuila as electrodes of supercapacitors	C.D. Manuel-Ramírez, I.L. Alonso-Lemus, J.C. Martínez-Loyola, M.Z. Figueroa Torres, F.J. Rodríguez-Valera, M.E. Sánchez Castro	Sustentabilidad de los Recursos Naturales y Energía, CINVESTAV Saltillo
ESD2023_12	$ZnCo_2O_4$/SSB (sewage sludge-derived biocarbon) composite as electrode material for supercapacitors applications	M.O. Fuentez-Torrres, B. Escobar-Morales, I.L. Alonso-Lemus, F.J. Rodríguez-Varela	Nanociencias y Nanotecnología, CINVESTAV Satillo
ESD2023_13	Understanding the mechanism of alkali ion intercalation into δ-MnO_2 structure: A combined experimental and theoretical study	Jorge Alejandro Manzo Mendoza, Christian A. Celaya, Yasmín Esqueda-Barron and Ana Karina Cuentas Gallegos	Centro de Nanociencias y Nanotecnología, UNAM
ESD2023_14	Electrochemical performance influenced by size dispersion of Fe_3O_4 synthesized via thermal decomposition	M. Molina, J. López and K. Cuentas	Centro de Investigación Científica y de Educación Superior de Ensenada (CICESE).
ESD2023_16	Carbon black-surfactant dispersion for negative electrodes	V. García, V. Garza, P. Cárdenas, D. Hernandez and S. Martinez	Clarios México

ESD2023_17	Theoretical modelling of porous silicon decorated with metal atoms for hydrogen storage	I. González, F. de Santiago, L.G. Arellano, A. Miranda, A. Trejo, F. Salazar and M. Cruz-Irisson	Instituto de Energías Renovables, UNAM
ESD2023_18	Sodium effects on the electronic and structural properties of porous silicon for energy storage	I. González, J. Pilo, A. Trejo, A. Miranda, F. Salazar, R. Nava and M. Cruz-Irisson	Instituto de Energías Renovables, UNAM
ESD2023_20	Functionalization of Single-Wall Carbon Nanotubes via Diazonium Chemistry: Insights from DFT Calculations and physicochemical characterizations	Elizabeth Fernandez-García, Christian Celaya-López, Yasmín Esqueda-Barrón, José M. Romo-Herrera, Jesus Muñiz, Ana Karina Cuentas-Gallegos	Centro de Investigación Científica y de Educación Superior de Ensenada (CICESE).
ESD2023_21	MnO_2 thin film deposited in conductor substrate for energy storage applications	Y. Esqueda-Barrón and A.K. Cuentas-Gallegos	Centro de Nanociencias y Nanotecnología, UNAM
ESD2023_22	Carbon electrodes obtained of lignocellulosic and biomass compounds by selective laser pyrolysis	Y. Esqueda-Barrón, I. Valdez, E. Aguilar, A.K. Cuentas-Gallegos	Centro de Nanociencias y Nanotecnología, UNAM
ESD2023_23	Producción de combustible solar a partir de un proceso termoquímico en un reactor Auger	N.A. Cisneros-Cárdenas, C.A. Estrada-Gasca and C.A. Pérez-Rábago	Instituto de Energías Renovables, UNAM
ESD2023_25	Effect of the carbonization temperature of N/O-codoped electrospun carbon nanofibers on the performance anodes of sodium ion batteries	M.G. Ayala-Sánchez, L.A. Rodríguez-Guadarrama, I.L. Alonso-Lemus and J. Escorcia-García	CINVESTAV del IPN, Unidad Saltillo
ESD2023_26	Tuning the Supercapacitance of PEDOT:PSS with the Molecular Weight of the Macromolecular Dopant PSS	R. Mirón-Velázquez, C.St. Thomas, J.G. Ramos-Sanchez, J.J. Alcaraz-Espinoza and I. Gonzalez	Centro de Investigación en Química Aplicada, Departamento de Procesos de Polimerización. UAM
ESD2023_29	N-doped subbituminous coal from Coahuila as anode of sodium-ion rechargeable batteries	C.A. Hernández-Siller, I.L. Alonso-Lemus and M.Z. Figueroa-Torres	Sustentabilidad de los Recursos Naturales y Energía, CINVESTAV Saltillo
ESD2023_30	A Cationic Poly (Ionic Liquid) as multifunctional binder for Lithium-Sulfur Batteries	A. Hernández-Sánchez, José Jarib Alcaraz-Espinoza, G. Ramos Sánchez, C St Thomas, I. González	Departamento de Química, UAM
ESD2023_31	Evaluation of lithium manganese oxide cathodes doped with aluminum and niobium for lithium-ion batteries	Luis Antonio Solís-Balderas, Salomé Maribel de la Parra-Arciniega, Jesús Guzmán-Torres, Luis Carlos Torres-González, Eduardo M. Sánchez-Cervantes	Facultad de Ciencias Químicas, UANL

ESD2023_32	Study of lithium cuprate modified with metal ions as an alternative cathode for lithium-ion batteries	A. García-Carrillo, M.A. Martínez-Cruz, G. Ramos-Sánchez and I. González	Departamento de Química, UAM
ESD2023_33	Supramolecular chitosan binder for lithium sulphur batteries	A. Mayrén, I. Gónzalez and G. Ramos	Departamento de Química, UAM
ESD2023_34	Electron withdrawal and structural design key to ionic conductivity enhancement in polymers based on tetra-coordinated boron atoms	P. E. Pedro-Cruz, G. Ramos-Sánchez, I. González and G. Guzmán-González	Departamento de Química, UAM
ESD2023_35	Pulse electrodeposition of crystalline structures of MnO_2 for electrochemical capacitors	Roxana Berlanga Pérez, Johanna García Montemayor, Javier Osvaldo Terán Carlín, Emilio Antonio García Montes, Jorge Zúñiga Martínez and Raúl Lucio Porto	Facultad de Ingeniería Mecánica y Eléctrica, UANL
ESD2023_36	Investigating the Role of Oxygen Vacancies in Manganese Oxide Thin Films for Enhanced Energy Storage	C. Bohórquez, Y. Esqueda and A.K. Cuentas	Centro de Nanociencias y Nanotecnología, UNAM
ESD2023_37	The effect of adding MgO nanostructures to a magnesium polymer electrolyte	Y. Gonzalez, E. Gonzalez, A.J. Guzman, M. Estrada-Villegas, A. Espinoza-Roa and E. Sanchez	Facultad de Ciencias Químicas, UANL
ESD2023_39	Raman Characterization of thin-layer FexOx by AP-CVD for energy storage applications	V. Parra-Elizondo, Abril Álvarez, Erick Hipolito, D. Pacheco-Catálan	Centro de Investigación Científica de Yucatán
ESD2023_40	Synthesis of LISICON-like lithium copper (I) phosphate and its evaluation as cathode for LIBs	Sergio Alfonso Garcia-Mata, Salomé Maribel de la Parra-Arciniega, Jesús Guzmán-Torres and Eduardo Maximiano Sánchez-Cervantes	Facultad de Ciencias Químicas, UANL
ESD2023_41	Nanoporous carbon fibers obtained by incomplete combustion of cotton fabric waste	I.L. Alonso-Lemus, F.J. Rodríguez-Varela, C.R. García and M.A. Garcia-Lobato	Sustentabilidad de los Recursos Naturales y Energía, CINVESTAV Saltillo
ESD2023_42	The first principal study focuses on the interface between perovskite materials and various carbon allotropes for potential applications in photosupercapacitors	J. Muñiz-Soria and A. Gómez-Coronel	Instituto de Energías Renovables, UNAM
ESD2023_43	Single lithium-ion conducting binders for high voltage LNMO electrodes studied through X-ray photoelectron spectroscopy (XPS)	J. Olmedo-González, L. Lartundo-Rojas, R. de G. González-Huerta and G. Ramos-Sánchez	IPN-ESIQIE and UAM

ESD2023_45	Sustainable batteries with carbonaceous materials obtained from biomass, in-situ spectroscopic study of intercalation processes	G. Rojas, J. Mendoza and G. Ramos	Departamento de Electroquímica, UAM
ESD2023_46	Charge transfer of Li, Na, K, and S ions in the electrolyte using Fe_3O_4 and MnO_2 surfaces as electrodes in a supercapacitor: A DFT study	Cornelio Delesma, Orlando Castro-Ocampo, Christian A. Celaya and Jesús Muñiz	Instituto de Energías Renovables, UNAM
ESD2023_47	Electronic properties of Magnetite (Fe_3O_4) and transfer Mechanisms of ions at its surface	O. Castro-Ocampo, Jesús Muñiz, Cornelio Delesma and Christian A. Celaya	Instituto de Energías Renovables, UNAM
ESD2023_48	Understanding Li interaction in TiO_2/graphene composites for high performance Li-ion battery anodes: A first principles study	Abdel Ghafour El Hachimi, Jesús. A. Jiménez-Juárez, Christian A. Celaya, Dage Sundholm, Pekka Pyykko and Jesús Muñiz Soria	Instituto de Energías Renovables, UNAM
ESD2023_49	First principles study of the energy storage properties of the α-MnO_2/functionalized-graphene interface	Jesús A. Jiménez-Juárez, Christian A. Celaya and Jesús Muñiz Soria	Instituto de Energías Renovables, UNAM
ESD2023_50	Enhancing the performance of pyrolusite MnO_2 in supercapacitors by solid state incorporation of potassium cathions	E. López, K. Chávez and E. Quiroga-Gonzalez	Facultad Ciencias de la Electrónica, BUAP
ESD2023_51	Sulfur and Nitrogen-Doped Multiwalled Carbon Nanotubes and Graphene for Supercapacitors	Yoxkin Estévez-Martínez, Enrique Quiroga-González, Erick Cuevas-Yañez and Víctor Castaño-Meneses	Instituto Tecnológico Superior de Acatlán de Osorio, TecNM
ESD2023_52	Energy production from biomass	Carolina Pano-Azucena, Javier A. Arcibar-Orozco, Liliana E. Arrvizu-Rodriguez and Oscar E. Valdivia-Moreno	CIATEC
ESD2023_55	Operando Raman spectroscopy of supercapacitors of carbon-coated Fe_3O_4 films	K. Chávez, B. Capilla and E. Quiroga-González	Instituto de Física, BUAP
ESD2023_56	Tuning the electrochemical performance of manganese oxides used as the active material of Li-ion batteries by thermal treatments: phase changes	M. L. Barrios-Reyna and E. Quiroga-González	Instituto de Física, BUAP
ESD2023_57	Metallurgical grade silicon as electrode material of lithium-ion batteries	J. Rojas and E. Quiroga-González	Facultad Ciencias de la Electrónica, BUAP
ESD2023_58	Aqueous supercapacitors with extended operation voltage range through polyelectrolyte coating	X. León, César Márquez-Beltrán and E. Quiroga-González	Insituto de Física, BUAP

ESD2023_59	Novel MgC_2O_4 cathode material for its application in Mg_2+/Li+ hybrid ion batteries: Synthesis and electrochemical performance	J. Guzmán-Torres, E. González-Juárez, L.L. Garza-Tovar and E.M. Sánchez-Cervantes	Facultad de Ciencias Químicas, UANL
ESD2023_60	Implicit solvent effect on the binding energy of the functional groups with impact in Li-S batteries	A. Ochoa-Calle, G. Ramos-Sanchez and I. Gonzalez	UAM
ESD2023_61	Unveiling the Charging/Discharging Mechanisms of Calcium carbonate and calcium hydroxide as High Performing Electrodes of Sustainable Lithium-Ion Batteries	E. Tecpa-Flores and E. Quiroga-González	Instituto de Física, BUAP
ESD2023_63	Solar reactor for the concentration of lithium carbonate	B. Falcón-Varela, C. Pérez-Rábago, R. Pérez-Enciso and P. Zavala-Rivera	Instituto de Energías Renovables, UNAM
ESD2023_64	Electrochemical and recycling protocols to guarantee the second life of lithium-ion batteries and the obtention of "Black mass"	D. Alba, S. Rodriguez, R. Pérez, H. Ávila, R. Suárez and G. Ramos	Departamento de Química, UAM
ESD2023_65	Nail Perforation Tests for the Pretreatment of Spent Lithium-Ion Batteries	O. Sánchez-Dena, A.E. Grado-Zubiate and R. Farías	Consejo Nacional de Humanidades, Ciencias y Tecnologías CONAHCYT, Instituto de Ingeniería y Tecnología, Universidad Autónoma de Ciudad Juárez
ESD2023_66	Bi_2O_3/coal-based composites as supercapacitor electrodes	S. O Mena-Picón, J. A. Díaz-Guillen, F.J. Rodríguez-Varela and I.L. Alonso-Lemus	Tecnológico Nacional de México, Instituto Tecnológico de Saltillo
ESD2023_68	Development of graphene nanobuds for energy storage: lithium-ion batteries and supercapacitors	I. Zeferino Gonzalez, A. M. Valenzuela Muñiz and R. Gauvin Y. Verde Gómez	Tecnológico Nacional de México, campus Cancún
ESD2023_69	β-FeOOH and α-Fe_2O_3 as ELECTROACTIVE MATERIALS FOR BIOSUPERCAPACITORS	Eva Paola Zamora Gutiérrez, Roxana Berlanga Pérez, Francisco Javier Mendoza Martínez, Emilio Antonio García Montes, Johanna García Montemayor, Javier Osvaldo Terán Carlín, Jorge Alexis Zuñiga Martínez	Univesidad Autónoma de Nuevo León, Facultad de Ingeniería Mecánica y Eléctrica
ESD2023_70	Layered vanadium phosphate with Cu ions in the interlayer space: Inducing faradaic behavior	Jorge Alexis Zuñiga Martinez, Raúl Lucio Porto, Domingo Ixcoalt García Gutiérrez, Thierry Brousse	Univesidad Autónoma de Nuevo León, Facultad de Ingeniería Mecánica y Eléctrica

ORAL PRESENTATIONS

Influence of structural and chemical composition of lignocellulosic precursors for porous carbon production useful in Supercapacitors

Ana Karina Cuentas-Gallegos[1*]

[1] *Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, , Km 107 Carretera Tijuana-Ensenada, Ensenada, B.C. C.P. 22800, Mexico*

**e-mail akcg@ens.cnyn.unam.mx*

Carbon materials play a crucial role across a wide spectrum of applications, notably in energy storage. Their appeal arises from their diverse physicochemical attributes, including high-surface area, chemical stability, and the presence of heteroatoms on their surfaces, among others. These characteristics, however, exhibit considerable variability depending on the choice of carbon precursor employed. Currently, there is no definitive approach for predicting the precise properties of carbon materials based on their lignocellulosic precursor and carbonization parameters. This research addresses this knowledge gap by conducting a thorough analysis of the diverse properties and characteristics of various lignocellulosic precursors. Our goal is to uncover the optimal carbon materials for supercapacitors. The investigation incorporates a range of physicochemical parameters, including ash content, cellulose, hemicellulose, lignin content, and macromolecular ordering (phenotype). The resulting activated carbons underwent thorough characterization through SEM, EDAX, Raman spectroscopy, physisorption, and CHONS analysis. Furthermore, these materials underwent rigorous electrochemical testing to assess their suitability for energy storage applications in diverse aqueous electrolytes. This assessment utilized 3-electrode cells and employed cyclic voltammetry and galvanostatic cycling as key electrochemical techniques. The outcome of this study revealed the carbon materials with the highest performance, which subsequently underwent testing in 2-electrode supercapacitor cells. These materials demonstrated exceptional stability and yielded significant specific energy storage capabilities, showcasing their potential for practical application."

Tuning Prussian Blue Analogs Properties for Assembling Hybrid Supercapacitors in Aqueous Electrolytes

Próspero Acevedo-Peña[1*], and Edilso Reguera[2]

[1] *CONAHCYT- Instituto Politécnico Nacional, Laboratorio Nacional de Conversión y Almacenamiento de Energía, CICATA-Legaria, Calzada Legaria 694, Col. Irrigación, 11500 CDMX, Mexico.*

[2] *Instituto Politécnico Nacional, Laboratorio Nacional de Conversión y Almacenamiento de Energía, CICATA-Legaria, Calzada Legaria 694, Col. Irrigación, 11500 CDMX, Mexico.*

* *prosperoster@gmail.com*

Hybrid supercapacitors provide the opportunity to increase the energy of conventional supercapacitors by incorporating a faradaic electrode, preserving the traditional high power of supercapacitors by maintaining a double-layer electrode. However, faradaic electrodes experience structural stress during extended galvanostatic charging-discharging cycles, limiting the stability of the devices. Prussian Blue Analogs represent a family of materials with well-recognized electrochemical activity capable of hosting various cations in their interstices [1], which makes them suitable for energy storage applications. Moreover, these materials can be easily obtained under mild conditions through chemical precipitation at room temperature and offer the opportunity to incorporate abundant transition metal cations in their lattice [2, 3].

During this talk, our recent results in tuning the properties of Nickel cyanoferrates for stabilizing the redox processes of iron in the coordination polymer and assembling fast and stable hybrid supercapacitors in neutral and acidic electrolytes using activated carbon as negative electrodes will be discussed.

References

[1] Y. Ávila, P. Acevedo-Peña, L. Reguera, E. Reguera, *Coord. Chem. Rev.*, 453 (2022) 214274

[2] D.R. Lobato-Peralta, J. Vazquez-Samperio, O. Pérez, P. Acevedo-Peña, E. Reguera, A.K. Cuentas-Gallegos, *J. Energy Storage*, 31 (2020) 101667.

[3] D.I. Villalva-Mejorada, P. Acevedo-Peña, C. Leyva-Porras, J. Rodríguez-Hernández, E. Reguera, *Int. J. Energy Research*, 46 (2022) 23310.

Hybrid Energy Storage: Relevance, Features and Applications

M.G. Reveles-Miranda[1] and D.E. Pacheco-Catalán[1]*

[1] *Centro de Investigación Científica de Yucatán (CICY), PCTY, Sierra Papacal, Mérida 97205, México.*
** Correspondence: dpacheco@cicy.mx; Tel.: +52-999-930-0760 (ext. 1210).*

The complementary characteristics of the supercapacitors (SC) and the batteries allow their hybridization into hybrid energy storage systems (HESS). Hybridization enhances specific power and energy characteristics, reduces storage dimension requirements, and optimizes the overall device's operational efficiency [1]. Fig. 1 shows the normalized main features of SC and batteries to confirm their hybridization potential. The HESS integrates characteristics of energy-based and power-based storage. The battery is the primary source for low-frequency energy requirements, and the SC is the support source for frequent high-power demands with rapid response capabilities [2]. The HESS allows energy management of the battery charge cycles, protecting it from thermal stress and improving the operating conditions [3]. Besides, it is an option for a secure, stable, and uninterruptible energy supply capable of providing ancillary services (i.e., power smoothing, auxiliary systems, or energy arbitrage). This work performs a specific classification that includes power-oriented and energy-oriented storage characteristics for a novel classification for HESS based on power quality support, power systems protection, and energy management services; additionally, a sub-classification of the HESS applications and their ancillary benefits it establishes shows in Fig. 2. Maximizing operational efficiency and providing additional services that increase its value while considering future storage needs is crucial in advancing HESS technologies.

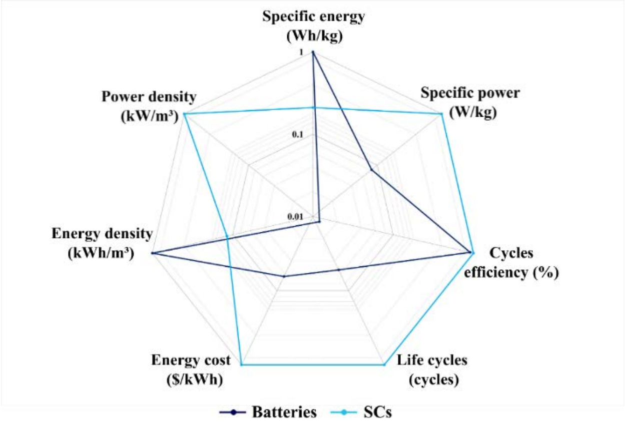

Fig. 1: Normalized technical parameters of hybridized devices.

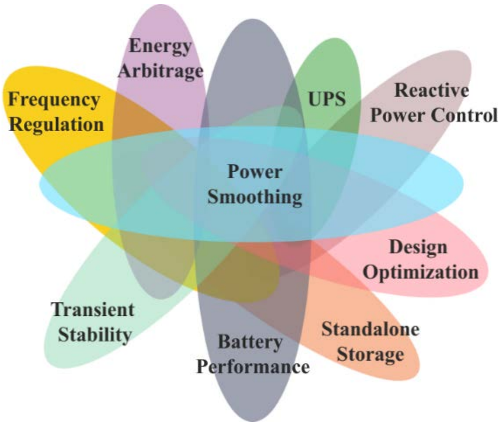

Fig. 2: Graphical analysis of the HESS ancillary services.

References

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Exploring the Alkali Metal Intercalation Mechanism in δ-MnO_2 Structure: A First-Principle Study

Christian A. Celaya[1*], Jesús Muñiz[2], Jonathan Guerrero-Sánchez[1], and Ana Karina Cuentas Gallegos[1]

[1]*Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, KM 107 Carretera Tijuana-Ensenada, Ensenada BC., C.P. 22800, México.*

[2]*Instituto de Energías Renovables, Universidad Nacional Autónoma de México, Priv. Xochicalco*

s/n, Col. Centro, Temixco, Morelos. CP 62580, México.
**acelaya@ens.cnyn.unam.mx*

Supercapacitors have emerged as a promising alternative to address power density limitations observed in conventional batteries. Supercapacitors show very attractive features such as high-power density, long cycle life, and tunable specific capacitance.[1] Nowadays, the progress in these energy storage devices employing transition metal oxides, specifically in pseudocapacitors, hinges on factors such as chemical composition, crystalline structure, morphology, theoretical capacitance, and oxidation states.[2] In this sense, manganese oxide (MnO_2) has been considered as one of the active pseudocapacitors non-precious metal electrodes.[3] Unfortunately, the poor electrical conductivity ordinarily results in low electron transfer, which limits the experimental capacitance of the obtained materials. However, due to its characteristic structure, it is possible to enhance its storage properties via intercalation of alkaline ions. With the aid of density functional theory (DFT) calculations, we study the stability, electrical properties, quantum capacitance, and surface charge storage for δ-MnO_2 structure when introducing alkaline ions (M= Li, Na, K) in its interface. This research contributes to a better understanding of MnO_2 material for its use in supercapacitor applications.

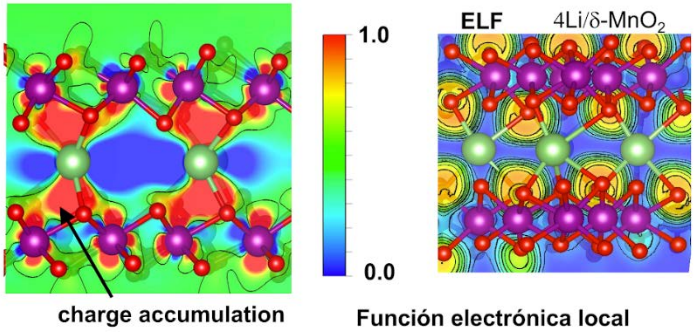

Fig. 1. Charge electronic difference slice and electron localization function (ELF) for Li atom intercalates on δ-MnO_2 (4Li/ δ-MnO_2).

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Modeling, Simulation and Optimization of a Commercial Lithium-Ion Battery with Charge Cycle Predictions

Camas-Náfate Mónica[1]; Coronado-Mendoza Alberto[1]; Vega-Gómez Carlos [2]; Espinosa-Moreno Francisco[3].

[1]*Centro Universitario de Tonalá, Universidad de Guadalajara, Avenida Nuevo Periférico 555, Ejido San José Tatepozco, Tonalá 45425, México*
[2] *Centro Universitario de CuTlajomulco, Universidad de Guadalajara, Tlajomulco de Zuñiga 45670, México*
[3]*Dirección de Investigación y Posgrado, Universidad Tecnológica de Tlaxcala, Carretera a El Carmen, Xalpatlahuaya, Huamantla 90500, México*

Modeling and simulation of lithium-ion batteries has become an important research topic in recent years due to the increasing demand for reliable and efficient energy storage systems.

Accurate predictions of charge cycles are essential for optimizing the performance and lifetime of lithium-ion batteries, and this requires the development of robust and reliable models that can capture the complex electrochemical and thermal behaviours of these systems.

Optimization algorithms are crucial tools for fine-tuning the parameters to increase model accuracy and performance of the battery.

For this work, optimization has been carried out using the PSO algorithm in the context of reducing the error between the proposed model, the experimental results with the optimized model, focused on commercial lithium-ion batteries, including predictions and forecasts of charge cycles. and download. The bio-inspired algorithm seeks to correct certain battery parameters, by correcting the root mean square error (RMSE) in the battery current.

A model was developed that integrates electrochemical parameters into an electrical circuit to estimate the behaviour of the battery under different conditions, including temperature changes and charge/discharge cycles. The model was implemented, and simulations were run using MATLAB/Simulink, and the results of the optimization were evaluated based on the reduction of the RMSE, algorithm convergence and computation time as well as the battery electrical parameters estimated by the algorithm.

The analysis of the behaviour of lithium-ion batteries has gained considerable interest in recent years. There are different alternatives for the analysis of this behaviour; however, depending on the type of Modeling, there are application and optimization restrictions. In this work, a hybrid model has been made that is capable of predicting the characteristics of a lithium-ion battery. As a novelty, the simplification, at the same time, facilitates the sampling of parameters for their prompt selection for optimization. A new model open to the user is proposed, which has proven to be efficient in simulation time. For example, one hour simulates it in 5 min, providing information detailing how these parameters, State of Health (SOH), Open Circuit Voltage (VOC), State of charge (SOC), and Number of charge and discharge cycles, in the face of temperature variations and charge and discharge cycles.

Advanced spectral analysis of electrical cycling signals for early failure detection in lithium ion batteries

M. Carbonó[1], J. Gómez[1] and R. Nava[1*]

[1] *Instituto de Energías Renovables, Universidad Nacional Autónoma de México, Privada Xochicalco S/N, 62580 Temixco, Morelos, México.*

**e-mail* rnava@unam.mx

The increasing demand of energy density and charging rate of lithium ion batteries rises concerns about safety hazard. Critical battery failures as thermal run away can evolve in explosions and be a serious safety risks for users. In this work, we developed a novel method for early fault detection in lithium ion batteries based on the spectral analysis of the cycling test signals. We analyzed voltage and current of cycling tests in lithium-ion batteries with silicon base anodes. The spectral analysis is performed by the Fourier and wavelet transforms (continuous, cross and coherence). Results show that in advance to an irregular event or critical failure occurs, new frequencies superimpose to the main cycling one, that are related to the beginning of degradation or a failure in the battery. In addition, the estimation of a standardized power index, in combination with other parameters (e.g., temperature, remaining useful life), contributes to stablish risk levels. We conclude that the spectral analysis together with the power index of the cycling signal allows early failure detection in the batteries. This method could be implemented in battery management systems to reduce the risk of critical failures

Direct, Multimodal Visualization of Zinc Metal Plating and Stripping via Transmission X-ray Microscopy

David N. Agyeman-Budu*, Yechuan (Leo) Chen, Molleigh B. Preefer, and Johanna Nelson Weker

Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA 94025

**agyeman@slac.stanford.edu*

It is undeniable that the realistic path to a clean energy future requires substantial effort in developing alternative battery technologies beyond Li-based battery chemistry. Aqueous zinc metal (and by extension zinc ion) batteries are regarded as an alternative to Li-ion. Namely, zinc is low cost and relatively abundant. It is also environmental benign, has a high volumetric capacity (5854 mAh cm^{-3}), and safe. These attributes make rechargeable zinc batteries attractive particularly for grid-scale, battery energy storage systems (BESS). However, attaining long-lifespan cycling of zinc metal batteries is still a challenging feat due to dendrite formation during plating and stripping, which forms separator piercing dendrites [1,2]. Therefore, understanding the early-stage nucleation and growth of zinc and characterizing the dendrite morphology is crucial. Herein, we have developed a model cell for 2D in-situ transmission X-ray microscopy (TXM) to visualize and quantitatively study the formation and dissolution of the dendrites. The Zn||Zn symmetric cell has a lithographically fabricated working gold electrode allowing the flexibility to track zinc deposits from early-stage nucleation and growth, to coalescing. The implication of this work is in part of the broader effort to explore the prospects of multivalent metal anode batteries (Ca, Zn, Mg) to replace current lithium-ion graphite hosts as a highly desirable alternative for cheaper, high-capacity energy storage [3].

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Electrospun coaxial carbon nanofibers with high performance as anodes of sodium ion batteries.

L.A. Rodríguez-Guadarrama[1*], I.L. Alonso-Lemus[2], J. Escorcia-García[3]

[1]*CINVESTAV del IPN, Unidad Saltillo, Av. Industria metalúrgica 1062, Parque Industrial Saltillo-Ramos Arizpe, Ramos Arizpe 25900, Coahuila, México.*
[2]*CONAHCyT-CINVESTAV Saltillo, Sustentabilidad de los Recursos Naturales y Energia. Av. Industria metalúrgica 1062, Parque Industrial Saltillo-Ramos Arizpe, Ramos Arizpe 25900, Coahuila, México.*
[3]*CONAHCyT-CINVESTAV, Unidad Saltillo, Av. Industria metalúrgica 1062, Parque Industrial Saltillo-Ramos Arizpe, Ramos Arizpe 25900, Coahuila, México.*

* *Corresponding author : alberto.rodriguez@cinvestav.edu.mx*

ABSTRACT

Currently, green energy storage plays a key role for to achieve a low-carbon economy. It is estimated that in the coming years lithium-ion batteries (LIBs) will be widely used in electric vehicles and energy backup of renewable energy systems (e.g., wind and solar). However, world lithium reserves will not be enough to supply market demand. In this regard, next generation batteries such as sodium-ion batteries (SIBs) have emerged as a promising alternative for energy storage. Despite the high theoretical power densities of SIBs (450 kWh $^{-1}$), the development of anodes materials is one of the biggest challenges, mainly due to volumetric expansion issues causing low cyclability and poor performance.

In this work, we develop and easy and eco-friendly method to synthesize coaxial carbon nanofibers ($CxNF_c$) by coaxial electrospinning. XRD, TEM and RAMAN analyses show coaxial amorphous carbon nanofibers with diameters of between 177 and 287 nm, with a well-defined core and shell by using two immiscible solvents (methanol and N, N-dimethylformamide). X-ray photoelectron spectroscopy, EDS and IF-IR analyzes show the presence of nitrogen and oxygen in the $CxNF_c$. The evaluation of $CxNF_c$ as anode of SIBs have showed a discharge capacity from 201 to 246 mA h g^{-1} with a columbic efficiency of ~ 80% after 10 cycles. Finally, CxNFc has great potential to be used as anode material for SIBs.

Keywords: coaxial electrospinning, coaxial nanofibers, anodic material, sodium ion battery.

ESD2023_38

Advances on the evaluation of exfoliated ZnS(en)$_x$ nanolayers as electrodes in rechargeable lithium-ion batteries.

E. Gonzalez[1], A. Hernandez-Gordillo[2], Y. Gonzalez[1] , N.A. García[1] and E. Sanchez[1*]

[1] *Facultad de Ciencias Químicas, Universidad Autónoma de Nuevo León*

[2] *Instituto de Investigaciones de Materiales, Universidad Nacional Autónoma de México*

**eduardo.sanchezcv@uanl.edu.mx*

Lithium-ion (Li-ion) batteries have revolutionized the portable energy and electric mobility industry due to their high energy density and long lifespan. In this context, zinc sulfide (ZnS) emerges as a promising candidate for improving lithium-ion batteries due to its crystalline structure and economic availability. To enhance the electrochemical properties of ZnS as an electrode, research is focused on generating interlayers separated by ethylenediamine (EDA), which could prevent electrode degradation [1] and improve battery stability [2]. Additionally, the exfoliation of ZnS interlayers is considered to increase the exposure of active surfaces and facilitate the diffusion of lithium ions. This work is aimed at characterizing and evaluating the potential of exfoliated ZnS(en)$_x$ nanosheets as electrodes in rechargeable lithium-ion batteries. The objectives include characterizing the nanosheets, assessing their structure, composition, and optical properties, and analyzing their lithium storage capacity as an electrode.

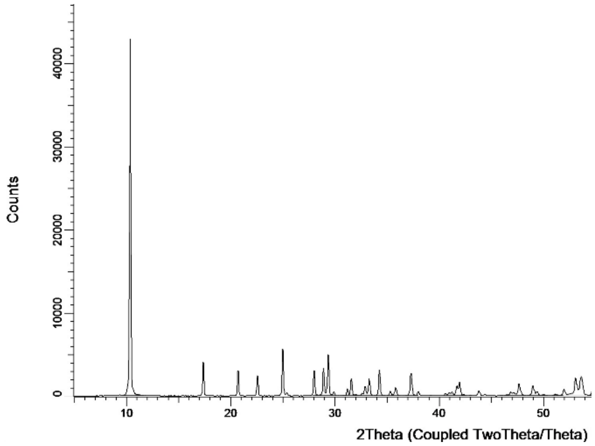

Fig. 1 XRD of ZnS(en)$_x$.

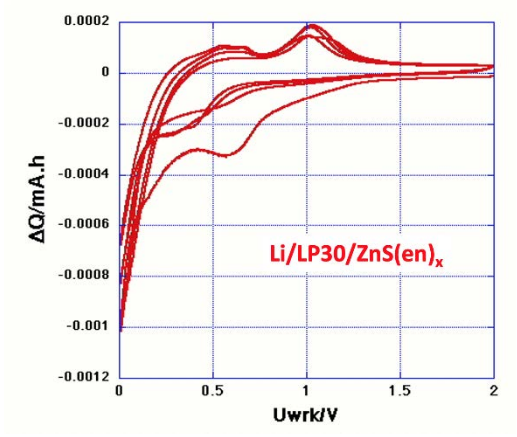

Fig. 2 Cyclic Voltammetry of Li/LP30/ZnS(en)$_x$ cell.

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Ion transport mechanism of LLZO-PEO composite solid electrolyteand its all-solid-state lithium-sulfur batteries

P.M. Gonzalez Puente[1*], Fei Chen[2] and Yiluo Zhang[2]

[1] *Departamento de Química, Universidad Autónoma Metropolitana – Iztapalapa, 09340, Iztapalapa, CDMX, Mexico*

[2] *State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, Wuhan University of Technology, 430070, Wuhan, China*

**e-mail: paulina.glezpuente@gmail.com*

The garnet type solid electrolyte $Li_7La_3Zr_2O_{12}$ (LLZO) has demonstrated excellent overall performance good environmental stability, high lithium ion conductivity (10^{-4}-10^{-3} S cm^{-1}), wide electrochemical window (6 V) [1]. Therefore, it is very likely to be used in all solid -state batteries.

In this work LGLZO with different ionic conductivity (**Fig. 1**) will be obtained by varying the amount of Ga doped, and then added into PEO polymer matrix to prepare composite solid electrolyte (CSE). The electrochemical performance and lithium ion transport mechanism of low and high (7.5 wt% and 60 wt%, respectively) content LGLZO on CSE were studied. Then, 7.5 wt% $Li_{6.4}Ga_{0.2}La_3Zr_2O_{12}$ CSE was chosen due to their best electrochemical performance. We built a composite cathode electrode with amorphous S/rGo material and test the performance of all solid-state lithium sulfur batteries (ASSLSBs). The ASSLSBs can operate reliably at temperatures as high as 60 °C with current densities of 0.2C, 0.5C, 1.0C and 2.0C. It can run for 100 cycles at 0.2 C, with a capacity retention of 820mAh g^{-1} and a capacity retention rate of 81%, showing excellent electrochemical cycling [2]. The synergistic effect between the CSE and the amorphous S/rGO composite cathode electrode brings insights further improvements in the cycling performance of ASSLSBs.

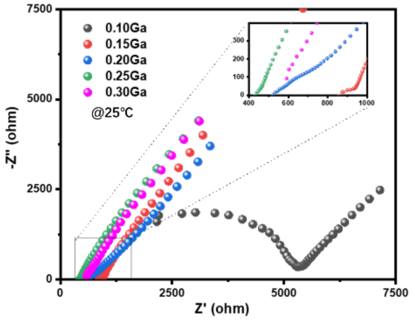

Fig. 1: Impedance plots for the LGLZO samples at room temperature.

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ESD2023_54

Synchrotron radiation insights into $LiNiO_2$ and Mn, Co-doped cathodes at different states of charge *via* TXM and XANES analysis

E. Espinosa-Villatoro[1*], M. B. Preefer[1], Z. Cui[2], A. Manthiram[2], and J. Nelson Weker[1*]

[1]*Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, California 94025, United States of America.*

[2]*Materials Science and Engineering Program & Texas Materials Institute, The University of Texas at Austin, Austin, Texas 78712, United States of America.*

* erickleo@slac.stanford.edu, jlnelson@slac.stanford.edu

Based on the research conducted by Z. Cui, et al. [1], the rational design of composition plays a crucial role in exploiting the potential of $LiNiO_2$-based cathodes [2], where the nickel content exceeds 90%, presenting them as promising candidates as cathode material for the next generation of energy storage devices. Nevertheless, the complex interaction of key elements such as cobalt and manganese in these high-nickel cathodes poses significant challenges, mainly due to the absence of a fundamental understanding of their intrinsic roles. In this comprehensive study, we delve into the influence of dopants in $LiNiO_2$-based cathodes, specifically $LiNi_{0.95}Co_{0.05}O_2$ and $LiNi_{0.95}Mn_{0.05}O_2$, each doped with a single-element dopant of 5%. Undoped $LiNiO_2$ (LNO) is used as the reference point [1,3,4]. Our research systematically covers electrochemical properties by controlling the cut-off charge energy density, and by means of TXM measurements (see Fig. 1) and XANES analysis based on synchrotron radiation, we investigate the chemical and morphological features of $LiNiO_2$, $LiNi_{0.95}Co_{0.05}O_2$ and $LiNi_{0.95}Mn_{0.05}O_2$ cathodes at different states of charge. The present work yields valuable information on the compositional design of high-energy, high-nickel cathodes and contributes to our understanding of the challenges regarding cobalt removal in these systems.

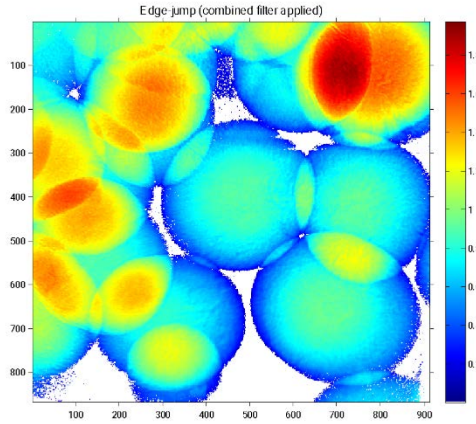

Fig. 1: Ni thickness map of $LiNi_{0.95}Co_{0.05}O_2$ pristine cathode.

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Hierarchical implementation of electrochemical techniques to provide a reliable diagnosis of commercial lithium-ion pouch cells under selected operational conditions

R. Suarez[1,2*], G. Ramos[1] and I. Gonzalez[1]

[1]*Universidad Autónoma Metropolitana-Iztapalapa, Av. San Rafael Atlixco No. 186, 09340 México City, México, Departamento de Química.*

[2]*Consejo Nacional de Humanidades, Ciencias y Tecnologías CONAHCYT, Av. Insurgentes Sur 1582, Col. Crédito Constructor,*

Benito Juárez, 03940, Ciudad de México.

**ruben.suarez@conahcyt.mx*

Understanding the performance of commercial Lithium-Ion batteries (LIBs) under various operational conditions is a paramount concern for ensuring their long-term stability. While numerous methodologies exist from a materials perspective to enhance comprehension of fundamental phenomena, electrochemical engineers often rely only on charge/discharge curves. Although these curves provide valuable insights, their information can be enriched through the systematic implementation of electrochemical protocols. This approach offers more nuanced data that can facilitate swift diagnostics of LIBs conditions and enable in-depth analysis of underlying physicochemical processes. In this study, we propose a comprehensive methodology for assessing the reversibility, stability, dominant processes, and degradation effects of LIBs. This involves combining charge/discharge curves with complementary electrochemical techniques and specific methodologies to extract maximum information from the data. We sequentially applied Galvanostatic Cycling with Potential Limitation (GCPL), Galvanostatic Electrochemical Impedance Spectroscopy (GEIS), Distribution of Relaxation Time protocols (DRT) [1], and Differential Capacitance (DC) [2] analysis to a range of commercial pouch cell LIBs under diverse conditions. By correlating the results obtained through these techniques, we established meaningful interpretations of battery performance under various operational case scenarios where we executed specialized protocols based on DRT and DC analysis: the effect of temperature, C-rate, and extended cycling. These protocols yielded crucial electrochemical parameters and relevant characteristics, enabling advanced diagnostics. The proposed framework serves as a guide for methodologically analyzing commercial batteries, it underscores that traditional characterization techniques can be augmented with additional analyses to comprehensively grasp the performance of commercial LIBs.

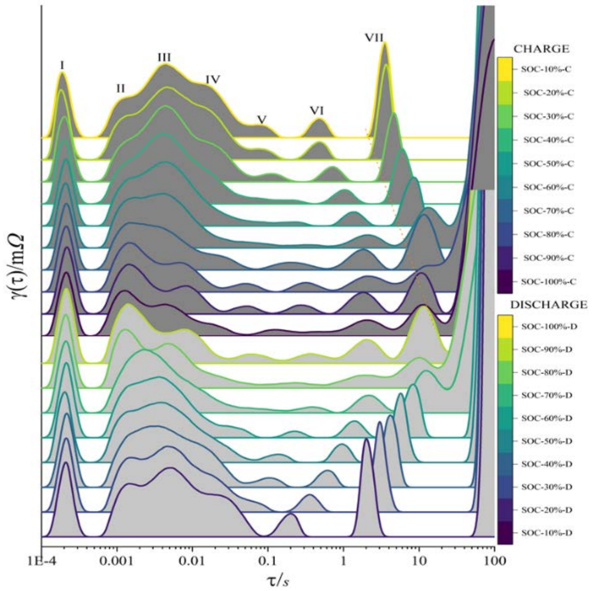

Fig. 1. Distribution of relaxation times (DRT) of the PL-605060-2C pouch cell battery during the charge for 10% to 100% SOC, the measurements were obtained at 25°C, over the charge/discharge profile of the battery. [1]

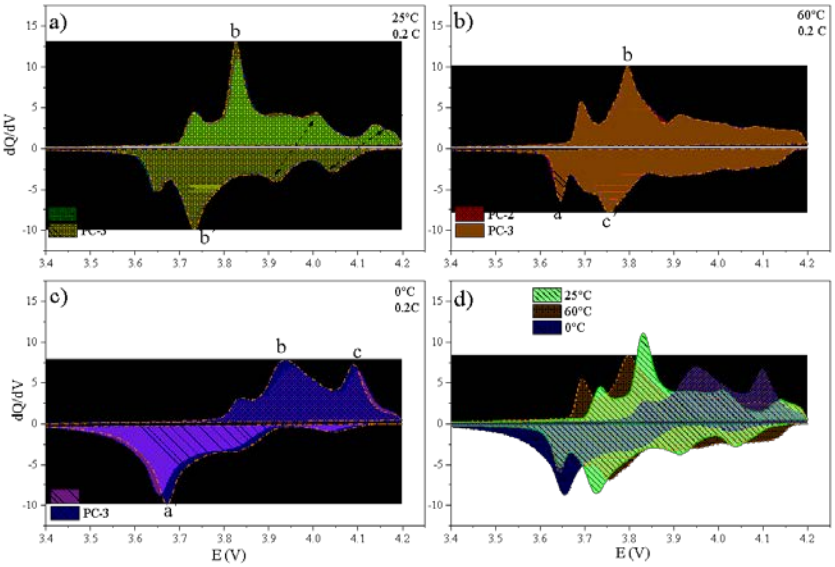

Fig 2. The differential capacity as a function of voltage (dQ/dV vs V) for two pouch cell batteries PL-605060-2C. The capacity was obtained at 0.2 C between 3-4.2 V and different temperatures, 0, 25 and 60 °C. indicated in the figure. [2]

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FFT impedance spectroscopy for real time analysis of phenomena in energy storage devices operando

M.A. San-Pablo-Juárez[1], A. Arroyo-Balseca[2], L. Valverde-Serrano[2] and E. Quiroga-González[1*]

[1] *Institute of Physics, Benemérita Universidad Autónoma de Puebla, 72570 Puebla, Mexico*

[2] *Faculty of Electronic Sciences, Benemérita Universidad Autónoma de Puebla, 72570 Puebla,*

**equiroga@ieee.org*

Impedance spectroscopy is a powerful electrical technique to determine phenomena of different characteristic times in diferent systems, like microelectronic devices, solar cells, batteries and supercapacitors. The spectra can be modeled with electrical elements, which represent physical parts of the system, or charactristic times of phenomena taking place. However, as it is common that the recording of the spectra is performed varying the frequency of the probing signal one frequency at the time, it is not suitable for measuring systems evolving in time, as is the case of electrochemical systems. In this case, the measurements are just performed when the system is in a stationary state, which is commonly observed at open circuit potential. The limitations of the impedance spectroscopy technique could be overcome with its variation called FFT impedance spectroscopy. With this technique, it is possible to work in a quasi-stationary state. The technique is based on the principle that a dynamical system looks like stationary if the measurement is performed much faster than the velocity of change. A probing signal with a range of frequency components is applied to the measured system, instead of a signal with a single frequency component [1]. To obtain a spectrum, FFT is applied.

In the Energy Laboratory of BUAP, and impedance spectroscope has been built with commercial off-the-shelf low-cost devices (oscilloscope, signal generator and voltage source). The main feature of the spectroscope is that it allows impedance measurements sampling with 46 frequencies in 600 ms. This represents a a big step towards real-time measurements.

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POSTER PRESENTATIONS

Synthesis of δ-MnO_2 by electro-oxidation of Mn_3O_4 in Na_2SO_4 electrolyte

P. J. Pérez-Diaz[1], J.M. Bass López[1], Y. Esqueda-Barrón[2], A.K. Cuentas-Gallegos[2], D.E. Pacheco-Catalán[1]

[1] *Centro de Investigación Científica de Yucatán A. C. Carretera Sierra Papacal-Chuburná Puerto, km 5. Sierra Papacal, Mérida, Yucatán. C.P. 97302, México.*

[2] *Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, Km 107 Carretera Tijuana-Ensenada, Ensenada, B.C., C.P. 22800, México.*

Energy storage is among the most important topics for the planet's decarbonization transition, aiming to reduce the contamination caused by fossil fuels. Numerous methods exist for energy storage, including chemical, electrochemical, mechanical, and thermal approaches. This work is focused on electrochemical energy storage (EES), specifically on electrode materials for supercapacitors. A particular type of supercapacitor has the ability to store energy through a phenomenon known as pseudocapacitance. This involves storing energy through a combination of electrostatic (capacitive process) and electrochemical reactions (faradaic process) that are localized on the surface. [1]. To facilitate this mechanism, the presence of a pseudocapacitive material is essential, with manganese oxide being a great example. Manganese dioxide (MnO_2) is an attractive option due to its abundance in the Earth's crust, its non-toxic nature, and its high specific capacitance. MnO_2 is found in diverse crystallographic arrangements [2], among which δ-MnO_2, distinguished by its layered structure and more open channels, has demonstrated the optimum energy storage properties for supercapacitors. The present study is centered around synthesizing this crystallographic structure of MnO_2, using an electro-oxidation process via cyclic voltammetry (CV) employing 1M Na_2SO_4 as the electrolyte. The precursor for this process involves Mn_3O_4 thin films synthesized through an atmospheric pressure chemical vapor deposition (AP-CVD) setup. The resulting material was characterized using scanning electron microscopy (SEM), Raman spectroscopy, and X-ray photoelectron spectroscopy (XPS).

CV profiles showed an increase in current with the number of cycles, along with the emergence of a redox pair. This points to the manganese oxide phase transition and the intercalation/deintercalation of Na^+ within the structure. SEM images showed differences on the thin film's surface after electro-oxidation, forming prominent flat bars across the film. Raman findings exhibit a phase change in the manganese oxide, transitioning from Mn_3O_4 to δ-MnO_2, as evidenced by the distinctive Raman spectra of each phase. Lastly, XPS revealed the presence of Na 1S, indicative of Na^+ ion intercalation within the structure. This observation is in good agreement with the layered crystalline arrangement of δ-MnO_2. Finally, this δ-MnO_2 as a thin film electrode on a supercapacitor, synthesized by AP-CVD, can allow the study of the pseudocapacitive phenomenon for energy storage.

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ESD2023_4

A DFT investigation : Hydrogen storage in metal-decorated doped germanene

Akari Narayama Sosa[1,2*], Álvaro Miranda[1]*, Luis Antonio Pérez[3], Gregorio Hernández Cocoletzi[2], and Miguel Cruz-Irisson[1]

[1] *Instituto Politécnico Nacional, ESIME-Culhuacán, Av. Santa Ana 1000,*
C.P. 04440, Ciudad de México, México

[2] *Benemérita Universidad Autónoma de Puebla, Instituto de Física, Avenida San Claudio y Boulevard 18 sur,*
Colonia San Manuel, Ciudad Universitaria, Puebla 72570, México
[3] *Instituto de Física, Universidad Nacional Autónoma de México, C.P. 04510, Ciudad de México, México*

**asosa@ifuap.buap.mx*

Germanene is a two-dimensional nanomaterial that has been successfully synthesized and has promising applications in sensing and energy storage. Recent research has focused on exploring the potential of M-decorated (M = K, Ca, and Sc) X-doped (X = B, Al, and Ga) germanene for hydrogen storage. In this theoretical work, a strong binding between K, Ca, and Sc metal atoms and doped germanene is revealed, suggesting that metal atoms adsorbed on doped germanene are energetically stable. Among the systems studied, Sc-decorated boron-doped germanene has a gravimetric hydrogen storage capacity of 5.32 wt%, close to the technical targets of the Department of Energy of the United States. Moreover, a three-atom Sc cluster on boron-doped germanene can adsorb up to 11 hydrogen molecules, with an average adsorption energy of 0.35 eV, desorption temperatures between 285-363 K and pressures between 5 and 100 bar. Sc-decorated Al(Ga)-doped germanene systems could also be suitable for hydrogen storage at slightly increased temperatures or pressures.

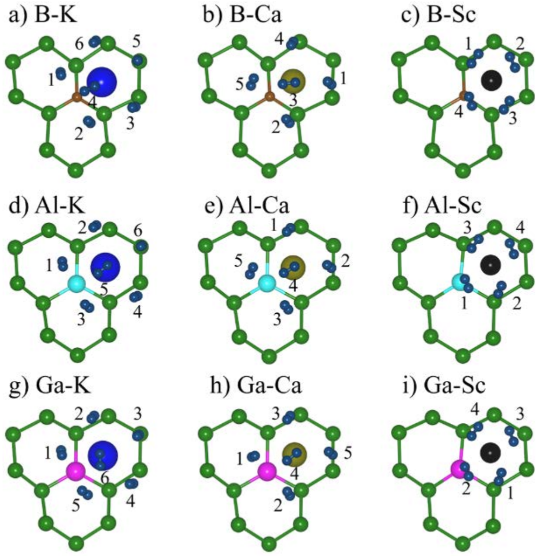

Fig. 1: Optimized structures of metal-decorated doped germanene supercells with the maximum number of hydrogen molecules per adsorption site.

ESD2023_5

Synthesis and characterization of lithium complex oxide powders for application in Li-Ion batteries

Sael Beltran Torres[1*], Rafael García Gutiérrez[1]

[1] *Departamento de Investigación en Física, Universidad de Sonora, Blvd. Luis Encinas y Rosales, Col. Centro, Hermosillo, Sonora, 83000, México, (662)-289-37-92*

**a213205710@unison.com*

Lithium-ion batteries have an unmatched combination of high energy and power density, making them the technology of choice for portable electronics, power tools, and hybrid/all-electric vehicles. The high energy efficiency of these batteries may enable their use in various power grid applications, including improving the intermittency of power collected from wind, solar, geothermal, and other renewable sources. [1]

Lithium cobaltate (LCO or LiCoO2) and lithium manganate (LMO or LiMn2O4) powders were synthesized using the solution combustion synthesis method, these powders were created to be applied as positive electrodes of lithium-ion batteries. To create LCO: lithium nitrate (LiNO3), cobalt nitrate (Co(NO3)2), carbohydrazide (CH6N4O), and deionized water were placed in a beaker until dilute. The solution was then placed in a muffle furnace at 480 °C, until it burned in approximately 3 minutes. Finally, the resulting powders were ground in a mortar. The same procedure was followed to create LMO, replacing cobalt nitrate with manganese nitrate (Mn(NO3)2). [2][3] The properties of the powders were studied using XRD, SEM and EDS characterization techniques. The diffractograms show that $LiCoO_2$ powders have a hexagonal crystal structure. $LiMn_2O_4$ powders have a cubic crystal structure. The SEM images show that both powders are homogeneous and have nanometer-sized grains. (Fig. 1).

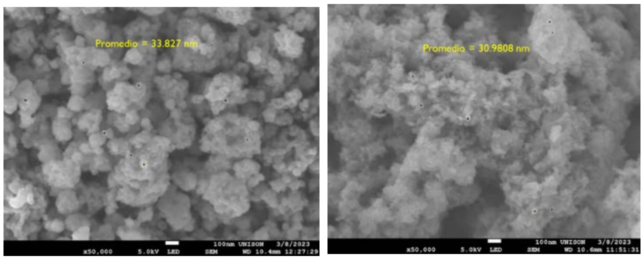

Fig. 1: $LiCoO_2$ (left) and LiMn2O4 (right) SEM images, amplified by x5000.

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ESD2023_7

High-performance supercapacitors using biocarbon:bismuth oxide composites as active materials

S. Mena-Picón[1,*], J. A. Díaz-Guillén[1] I. L. Alonso-Lemus[2], F.J. Rodríguez-Varela[3]

[1] Tecnológico Nacional de México, Instituto Tecnológico de Saltillo, 25280, Saltillo, Coahuila, México.
[2] CONAHCyT-Cinvestav Saltillo. Sustentabilidad de los Recursos Naturales y Energía. Av. Industria Metalúrgica 1062, Parque Industrial Ramos Arizpe. Ramos Arizpe, Coahuila, C.P 25900, México.
[3] Sustentabilidad de los Recursos naturales y Energía, Cinvestav Unidad Saltillo, Parque Industrial Saltillo-Ramos Arizpe, Ramos Arizpe, Coahuila, 25900, México
**e-mail: smena0708@gmail.com*

Energy storage devices have gained relevance over the past two decades because of the need of always having available energy to satisfy the current world demand. Supercapacitors are among the most studied electrochemical devices due to their fast charge and discharge capacity, long useful life, and low manufacturing costs [1]. Indeed, the implementation of low-cost active materials for supercapacitors has been a topic of discussion. On this issue, cheap carbon and metal oxides-based electrodes have been proposed for this application because of their high pseudocapacitive behavior [2]. In this work, a biocarbon has been obtained from sewage sludge from the water treatment plant in Saltillo and labeled as SSB. Bismuth oxide (Bi) has been acquired commercially. SSB:Bi composites having 3:1, 2:1, 1:1, 1:1, 1:2, and 1:3 wt. ratios are evaluated as active materials for supercapacitors. Figure 1 shows their cyclic voltammograms (CVs). The composite having a 1:1 wt. ratio shows the highest current density and thus specific capacitance (150.2 F g^{-1}), improving that of SSB alone (30.3 F g^{-1}).

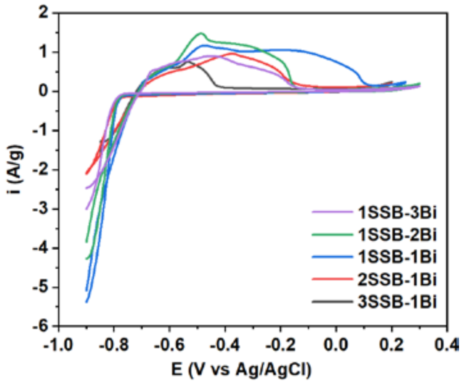

Figure 1. CVs of composites in 6 M KOH. Scan rate: 2 mV s^{-1}.

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ESD2023_8

High-performance supercapacitors based on a sewage sludge-derived biocarbon

S. Ravichandran[1,*], I.L. Alonso-Lemus[2], B. Escobar-Morales[3], F.J. Rodríguez-Varela[1,4]

[1]Nanociencias y Nanotecnología, Cinvestav Unidad Saltillo, Av. Industria Metalúrgica 1062, C.P. 25900, Ramos Arizpe, Coahuila, México.
[2]CONAHCyT-Cinvestav Saltillo. Sustentabilidad de los Recursos Naturales y Energía. Av. Industria Metalúrgica 1062, Parque Industrial Ramos Arizpe. Ramos Arizpe, Coahuila, C.P 25900, México.
[3]CONAHCyT, Centro de Investigación Científica de Yucatán, Unidad de Energía Renovable, Calle 43, No. 130 Col. Chuburná de Hidalgo, C. P. 97200, Mérida, Yucatán, México.
[4]Sustentabilidad de los Recursos Naturales y Energía, Cinvestav Unidad Saltillo, México.
**Corresponding author:* ravichandran@cinvestav.mx

Abstract

In this research, a Sewage Sludge-based Biocarbon (SSB) was produced using biomass from the water treatment plant in Saltillo, Coahuila. It was found that activation of the biomass with $ZnCl_2$ reduces the oxygen content of SSB, which may increase its electrical conductivity. SSB showed a specific surface area of 202.9 $m^2\ g^{-1}$ and a pore diameter of 5.5 nm. Evaluation in a two-electrodes symmetrical supercapacitor of the SSB||SSB type showed a high-rate performance of SSB even when the scan rate was increased, maintaining a relatively rectangular shape without any obvious distortion. Such feature indicated that the symmetric supercapacitor possesses high-rate capability as well as favorable electrochemical capacitive behavior, with rapid diffusion of electrolyte ions to the interface of the electrodes [1]. Fig. 1 a) depicts cyclic voltammograms (CVs) of the supercapacitor in 6 M KOH at scan rates ranging from 1 to 100 mV s^{-1}. Even at the high scan rate of 100 mV s^{-1}, the CVs maintain a quasi-rectangular shape, indicating its good rate capability. Fig. 1 b) depicts the galvanostatic charge-discharge (GCD) plots of the supercapacitor performed using a range of current densities. It shows straight lines with distinct triangular forms and a modest iR drop, indicating high reversibility and high coulombic efficiency. The SSB||SSB supercapacitor has a specific capacitance of 144.80 F g^{-1} at 1 mV s^{-1}. The study provides a method for efficiently manufacturing high-performance electrodes for supercapacitors from earth-abundant biomass.

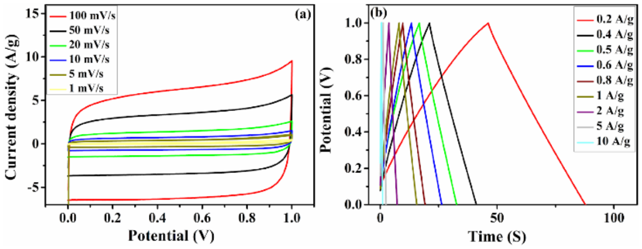

Fig. 1. (a) CVs of the symmetric two-electrode supercapacitor at different scan rates and (b) GCD plots of the supercapacitor at different current densities. Electrolyte: 6 M KOH.

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ESD2023_10

Determination of structural, electronic and optical properties of β-$NaFeO_2$ ferrites doped with Ni and Cu: a joint experimental and theoretical study

Nayeli Gómez-Garduño[1], Daniel G. Araiza[2]*, Christian A. Celaya[3], Jesús Muñiz[4], and Heriberto Pfeiffer[1]

[1] *Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México*

[2] *Instituto de Ciencias Aplicadas y Tecnología, Universidad Nacional Autónoma de México*

[3] *Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México*

[4] *Instituto de Energías Renovables, Universidad Nacional Autónoma de México*

**daniel.araiza@icat.unam.mx*

M-doped b-$NaFeO_2$ samples (where M = Cu or Ni) were synthesized through the nitrate-pyrolysis method. For the first time, these doped ferrites were studied with a combined experimental and theoretical approach, to unveil the modifications in the structural, electronic, and optical properties. Several experimental techniques were employed to perform an in-depth characterization (XRD, XPS, SEM and N_2-ads–des, as well as Raman, FTIR-ATR, and UV-vis spectroscopies), while the stable structure configurations of pristine β-$NaFeO_2$ and different doped ferrites were calculated through density functional theory (DFT) at the DFT + U level. Besides, ab initio molecular dynamics (AIMD) simulations were performed to analyze the temperature effect on the Na-ion diffusion, within the ferrite's crystal structure. Results showed that effective doping was achieved with less than 5 mol% of metal, while the efficiency was higher in the nickel-containing samples, as these systems showed the generation of oxygen vacancies with the insertion of divalent Ni^{2+} cations into the ferrite structure. On the other hand, time-dependent DFT (TD-DFT) calculations showed significant changes in the structural, electronic, and optical properties of both doped systems, which corroborate the characterization performed for the synthesized materials, Fig. 1. In addition, AIMD simulations evidence a Na-ion mobility increment based on the obtained diffusion coefficients, due to thermal effects.

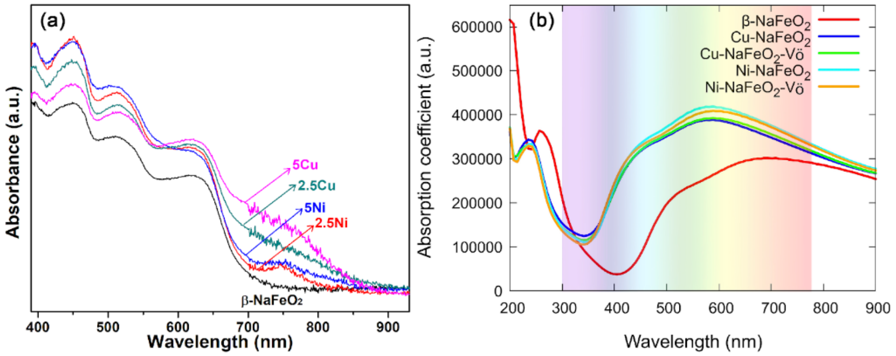

Fig. 1. (a) Experimental UV-Vis spectra of *X*Ni-$NaFeO_2$ and *X*Cu-$NaFeO_2$ samples doped at 2.5 and 5.0 mol%. (b)Theoretical UV-Vis spectra for pristine β-$NaFeO_2$, Ni-$NaFeO_2$, Ni-$NaFeO_2$-Vö, Cu-$NaFeO_2$ and Cu-$NaFeO_2$-Vö simulated structures.

Evaluation of Fe/Co nitrogen-doped subbituminous coal from Coahuila as electrodes of supercapacitors.

C.D. Manuel-Ramírez[1], I.L. Alonso-Lemus[2*], J.C. Martínez-Loyola[3], M.Z. Figueroa Torres[4], F.J. Rodríguez-Varela[1], M.E. Sánchez Castro[1]
[1]*Sustentabilidad de los Recursos Naturales y Energía, Cinvestav Unidad Saltillo, Av. Industria Metalúrgica 1062, C.P. 25900, Ramos Arizpe, Coahuila, México.*
[2]*CONAHCyT-Cinvesta Saltillo, Sustentabilidad de los Recursos Naturales y Energía, Av. Industria Metalúrgica 1062, Parque Industrial Ramos Arizpe. Ramos Arizpe, Coahuila, C.P 25900, México.*
[3]*Escuela de Ingeniería y Ciencias, Tecnológico de Monterrey, Eugenio Garza Sada 2501, Monterrey 64849, NL, México.*
[4]*Facultad de Ingeniería Civil, Universidad Autónoma de Nuevo León, Avenida Universidad S/n, Niños Héroes, Ciudad Universitaria, 66450 San Nicolás de los Garza, N.L.*
**ivonne.alonso@cinvestav.edu.mx*

Supercapacitores are storage energy devices which are ideal in applications where fast power delivery is required such as consumer electronics, clean energy storage and electric vehicles [1]. In this work, sub-bituminous carbon (SC) from Coahuila, northeast of Mexico, was modified and evaluated as electrode for supercapacitors. The two-step process for the preparation of the electrodes consists in i) mechanical milling for particle size reduction and ii) chemical activation for increase the porosity.

The electrodes were doped with nitrogen using urea as nitrogen precursor, and $FeCl_2$ and $CoCl_2$ as transition metal precursors of Fe and Co, respectively. The electrodes were labelled as N-SC, Fe-N-SC, and Co-N-SC. The structural properties of the electrodes were analyzed by X-ray diffraction (XRD), functional groups were determined by Fourier transform infrared spectroscopy (FTIR), the pore size distribution and specific area were determined by BET and BJH methods, respectively. The morphology and chemical composition were characterized by scanning electron microscopy coupled to energy dispersive X-ray spectroscopy (SEM-EDS).

The results showed that Fe (5.0 wt. %) and Co (6.2 wt. %) were incorporated successful into the carbon lattice forming M^{2+} and M^{3+} species. High specific surface area was achieved up to 2011 m^2g^{-1} and 1.8 nm pore size for Co-N-SC. In addition, Co-N-SC had a specific capacitance of 217 F g^{-1}. This work shows the subbituminous carbon from Coahuila treated in two steps can be a good alternative as electrode for supercapacitor.

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ESD2023_12

ZnCo$_2$O$_4$/SSB (sewage sludge-derived biocarbon) composite as electrode material for supercapacitors applications

M.O. Fuentez-Torres[1,*]; B. Escobar-Morales[2]; I.L. Alonso-Lemus[3]; F.J. Rodríguez-Varela[1,4]
[1]Nanociencias y Nanotecnología, Cinvestav Unidad Saltillo, Av. Industria Metalúrgica 1062, C.P. 25900, Ramos Arizpe, Coahuila, México.
[2]CONAHCyT, Centro de Investigación Científica de Yucatán, Unidad de Energía Renovable, Calle 43, No. 130 Col. Chuburná de Hidalgo, C. P. 97200, Mérida, Yucatán, México.
[3]CONAHCyT-Cinvestav Saltillo. Sustentabilidad de los Recursos Naturales y Energía. Av. Industria Metalúrgica 1062, Parque Industrial Ramos Arizpe. Ramos Arizpe, Coahuila, C.P 25900, México.
[4]Sustentabilidad de los Recursos Naturales y Energía, Cinvestav Unidad Saltillo, México.
* octavio.fuentez@cinvestav.mx

This study investigated a ZnCo$_2$O$_4$/ sewage sludge-derived biocarbon (SSB) composite material for its application in supercapacitors. The composite material was produced through a two-step process involving a hydrothermal reaction and subsequent annealing [1]. Materials, such as ZnCo$_2$O$_4$, SSB, and the ZnCo$_2$O$_4$/SSB composite were subjected to FTIR, Raman, XRD, and SEM-EDS characterization. Their electrochemical characterization was carried out in a three-electrode cell using 6 M KOH as electrolyte. Figure 1 a) depicts the CVs of the materials at 2 mV s^{-1}. The behavior of SSB was indicative of a double layer charge storage phenomenon. The CVs of ZnCo$_2$O$_4$ and ZnCo$_2$O$_4$/SSB revealed redox peaks between 0 to 0.35 V and -0.2 to 0.35 V, respectively, indicating processes predominantly governed by faradaic reactions. Notably, ZnCo$_2$O$_4$/SSB delivered a significantly higher current density, implying a higher specific capacitance. The specific capacitance values of SSB, ZnCo$_2$O$_4$, and ZnCo$_2$O$_4$/SSB at 2 mV s^{-1} were 48.48, 44.80, and 88.32 F g^{-1}, respectively (Figure 1 b). Such result demonstrated an improved performance of the ZnCo$_2$O$_4$/SSB composite material. The charge transfer resistance (R_{ct}) of SSB, ZnCo$_2$O$_4$, and ZnCo$_2$O$_4$/SSB was determined to be 4.35, 0.56, and 1.27 Ω (Figure 1c), respectively. In contrast, their diffusion resistance (R_d) was 75.72, 154.0, and 12.46 Ω, respectively. Therefore, a synergistic effect between SSB and ZnCo$_2$O$_4$ enhances the behavior of the composite as active material for supercapacitors applications.

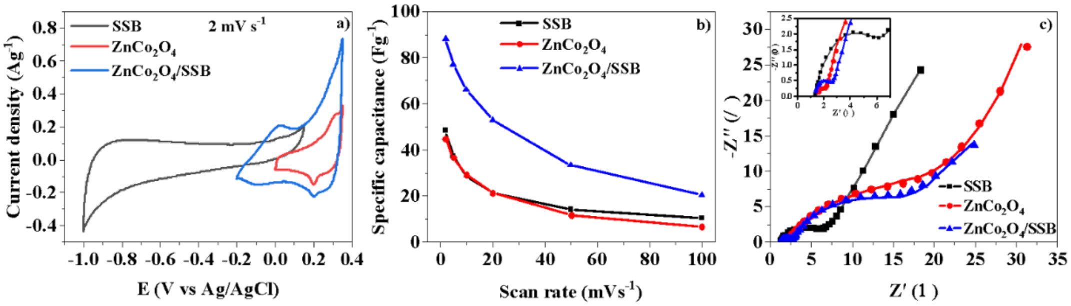

Fig. 1: a) CVs curves at 2 mV s^{-1}, b) specific capacitance vs scan rate plot, and c) Nyquist plot of the SSB, ZnCo$_2$O$_4$, and ZnCo$_2$O$_4$/SSB material. Electrolyte: 6 M KOH.

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Understanding the mechanism of alkali ion intercalation into δ-MnO_2 structure: A combined experimental and theoretical study

Jorge Alejandro Manzo Mendoza[1], Christian A. Celaya[1], Yasmín Esqueda-Barron[1], and Ana Karina Cuentas Gallegos[1*]

[1]*Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, KM 107 Carretera Tijuana-Ensenada, Ensenada BC.,C.P. 22800, México.*

**akcg@ens.cnyn.unam.mx*

Enhancing research efforts in the field of energy storage materials is essential for the improvement of several crucial characteristics. These involve energy density, power density, efficiency, cycle stability, potential window, capacitance, safety, cost-effectiveness, and environmental impact. Among these materials, manganese dioxide (MnO_2) stands out as a good candidate for energy storage applications due to its high specific capacitance and the occurrence of pseudocapacitance, which increases its charge storage capacity. In addition, its cost-effectiveness, eco- friendly attributes, and the versatility of available synthetic approaches all emphasize its status as a convincing and viable alternative. In the quest to improve conventional material properties in energy storage, the exploration of MnO_2 through computational simulation using Density Functional Theory (DFT) is an interesting research topic, which promises to help understand its characteristics at atomic level (Fig. 1). Herein, we explored intercalation of different alkaline ions at the interface of δ-MnO_2 structure, evaluated by DFT calculations. The effect of the ionic radius in the intercalation process plays an important role in the transfer of electronic charge density . This behavior is strongly linked to the processes observed in cyclic voltammetry profiles. In this work, we used MnO deposits of 100 nm synthesized by Atomic Layer Deposition (ALD) over stainless steel substrates. These deposits were electro-oxidized by using different alkaline cations in the electrolyte, and δ-MnO_2 thin films were obtained. These films were characterized by Raman spectroscopy to identify structural and chemical properties. These results seek to understand the role played by the various alkaline ions at the δ-MnO_2 structure.

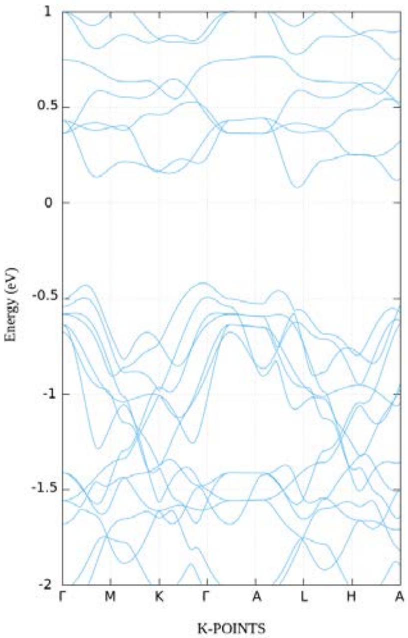

Fig. 1: Band diagram of bulk δ-MnO_2 (space group P3m1)

Electrochemical performance influenced by size dispersion of Fe_3O_4 synthesized via thermal decomposition

M. Molina[1], J. López[2] and K. Cuentas[3*]

[1] *Centro de Investigación Científica y Educación Superior de Ensenada-CICESE. Ensenada, 22860, México.*

[2] *CONACYT – Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México. Km 107 Carretera Tijuana-Ensenada s/n. B.C., C.P. 22800, México.*

[3] *Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, Km 107 Carretera Tijuana-Ensenada s/n, Ensenada, B.C., C.P. 22800, México.*

**akcg@ens.cnyn.unam.mx*

This study centers on the electrochemical characterization (cyclic voltammetry) of spherical Fe_3O_4 nanoparticles (NPs) embedded in a carbon framework (Fe_3O_4@C). This nanocomposite material is being explored for its potential use as supercapacitor electrode. Fe_3O_4 NPs were synthetized by thermal decomposition method of iron oleate in 1-octadecene as solvent, with oleic acid as surfactant [1]. A pyrolysis process (at 500 °C) was carried out to carbonize the surfactant, resulting in a porous carbon shell for Fe_3O_4 NPs. This carbon shell allowed a suitable electrochemical performance of the NPs in an aqueous electrolyte, such as Na_2SO_3. This particular electrolyte enables the exploration of the iron redox process, further improving the material´s electrochemical performance [2]. The NPs were characterized by X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, transmission electron microscopy (TEM) and cyclic voltammetry (CV) in a three-electrode cell system within 1M Na_2SO_3. XRD and Raman confirmed the presence of Fe_3O_4 phase, and the amorphous carbon formation from oleic acid carbonization. On the other hand, XPS results suggested a possible oxidation of Fe^{+2} to Fe^{+3}. According to TEM images, a slow hexane evaporation prior to the pyrolysis process decreases agglomeration of NPs during oleic acid carbonization. This evaporation condition, combined with a low heating rate (2 °C min^{-1}) and long dwell time in the carbonization process, resulted in an improved electrochemical performance.

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ESD2023_16

CARBON BLACK-SURFACTANT DISPERSION FOR NEGATIVE ELECTRODES

V. García[1], V. Garza, P. Cárdenas, D. Hernandez, S. Martinez.

[1] Clarios Mexico

[2] ITESM-campus Mty

*vladimir.garcia@clarios.com

Different types of carbons (carbon black, graphites, hard carbons) are currently used for the also different types of batteries (lead, lithium, sodium, etc). They are mostly used to enhance the electrical conductivity. It is expected that for a better conductivity threshold the relationship of the carbon particle size and concentration is important. However during the processing not always the initial conditions help to properly disperse or reduce the particle size. This is a quick study on the usage of a natural surfactant in the percolation threshold to be used for lead-acid negative electrodes.

Fig. 1 carbon black in water

Fig2. Carbon black with natural surfactant

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ESD2023_17

Theoretical modelling of porous silicon decorated with metal atoms for hydrogen storage

I. González[1], F. de Santiago[2], L.G. Arellano[2], A. Miranda[2*], A. Trejo[2], F. Salazar[2], and M. Cruz-Irisson[2]

[1] *Instituto de Energías Renovables, Universidad Nacional Autónoma de México, Temixco, Morelos, Mexico*

[2] *Instituto Politécnico Nacional, ESIME-Culhuacán, Av. Santa Ana 1000, C.P. 04440, Ciudad de México, Mexico*

**amirandad.ipn@gmail.com*

Theoretical modelling of porous silicon decorated with metal atoms for hydrogen storage. There is experimental evidence suggesting that metal adatoms enhance the physisorption of hydrogen molecules in porous silicon [1]. However, theoretical reports about the physical properties for this material to be suitable for hydrogen storage are scarce. Thus, in this work we employ Density Functional Theory [2], to study the effects of decoration with metals on the hydrogen-adsorption properties on hydrogen-passivated porous silicon. The results indicate that lithium and palladium decorating atoms are strongly bonded to the porous silicon -preventing the adverse effects of clusterization- while beryllium is not. Lithium and palladium exhibit physisorption capacity up to 5 and 4 hydrogen molecules per adatom, respectively. In contrast, adsorption of hydrogen molecules in beryllium is too weak as the adatom is not chemisorbed on the surface of the pore. The hydrogen passivation of the pore surface proves to be beneficial for a strong chemisorption of the decorating atoms.

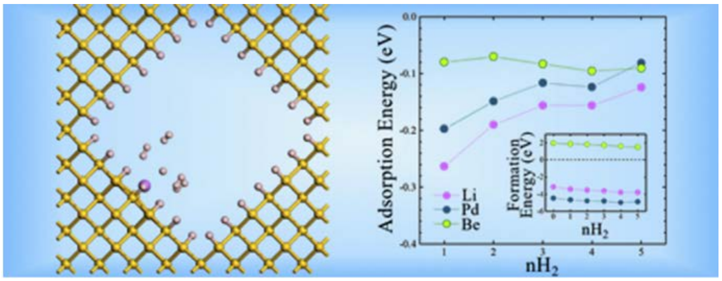

Fig. 1: Porous silicon decorated with Li atom adsorbing up to five H_2 molecules (on the left) and results of the adsorption energy and formation energy of porous silicon with surface decoration of Li, Pd and Be (on the right)

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ESD2023_18

Sodium effects on the electronic and structural properties of porous silicon for energy storage

I. González[1], J. Pilo[2], A. Trejo[2*], A. Miranda[2], F. Salazar[2], R. Nava[1] and M. Cruz-Irisson[2]

[1] *Instituto de Energías Renovables, Universidad Nacional Autónoma de México, Temixco, Morelos, Mexico*

[2] *Instituto Politécnico Nacional, ESIME-Culhuacán, Av. Santa Ana 1000, C.P. 04440, Ciudad de México, Mexico*

**alejandtb13@gmail.com*

Porous silicon is a promising anode material in Na-ion batteries [1], however, there are still no theoretical studies describing the Na storage mechanism within this material. In this work, we present a density functional theory study [2], on the effects of interstitial and substitutional Na atoms on the electronic and structural properties of hydrogen-passivated porous silicon (pSi_H). The results show that the substitutional Na reduces the band gap, while the interstitial Na induces metallic properties on the pSi_H. The diffusion analysis by the nudged elastic band scheme, reveals that the interstitial Na atoms migrate from the silicon lattice to the pore surface, while the pSi_H energy barrier decreases by 20.42% relative to the bulk silicon energy barrier value. Finally, the hydrogenated surface proves to be beneficial for both Na adsorption and diffusion. These results could be important for understanding the storage and diffusion mechanism of Na on pSi_H.

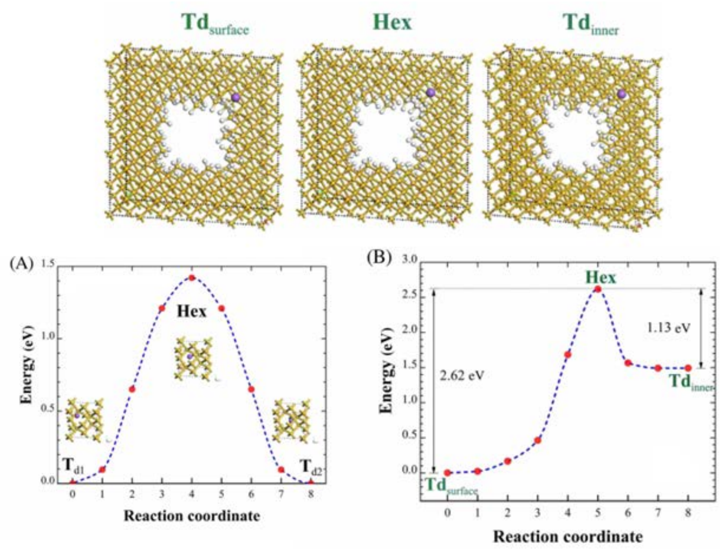

Fig. 1: NEB transition state calculation of (A) bulk crystalline silicon and (B) pSi_H

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Functionalization of Single-Wall Carbon Nanotubes via Diazonium Chemistry: Insights from DFT Calculations and physicochemical characterizations

Elizabeth Fernandez-García[1], Christian Celaya-López[2], Yasmín Esqueda-Barrón[2], José M. Romo-Herrera[2],
Jesus Muñiz[3*], Ana Karina Cuentas-Gallegos[2*]

[1] *Posgrado en Nanociencias, Centro de Investigación Científica y de Educación Superior de Ensenada,*
Apartado Postal 2732, Ensenada BC 22860, México

[2] *Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, Km 107 Carretera*
Tijuana-Ensenada, Ensenada, B.C., C.P. 22800, México

[3] *Instituto de Energías Renovables, Universidad Nacional Autónoma de México, Priv. Xochicalco s/n, Col.*
Centro, Temixco, Morelos, C.P. 62580, México

**fernandezg@cicese.edu.mx*, *ellyeh.fg@ens.cnyn.unam.unam.mx*

Supercapacitors, in conjunction with batteries, constitute prominent electrochemical energy storage devices that currently occupy a central position in energy storage research. While batteries exhibit higher specific energy, supercapacitors offer superior specific power, enabling rapid charging and discharging within seconds to minutes. Moreover, supercapacitors boast greater specific energy than conventional electrostatic capacitors. A variety of materials find application in the construction of supercapacitor electrodes. Notably, metal oxides and carbon materials are exceptionally compatible choices due to their capacity to provide high pseudocapacitance and superior electrical conductivity. This compatibility, in turn, results in heightened specific energy and power, respectively. Nevertheless, the deposition of metal oxides onto various carbon allotropes presents several challenges when it comes to harnessing the full potential of carbon's extensive specific surface area and electrical conductivity. Achieving the optimal metal oxide loading on a specific carbon allotrope surface is a key challenge. With this in mind, we are conducting an investigation into the interactions between carbon nanocomposite materials with functional groups (such as OH, COOH, NH_2). Therefore, we introduce in silico models of carbon nanostructures with the mentioned functional groups (Fig. 1). The Density of States reveals a higher charge density accumulation at the Fermi level, resulting in improved charge transfer. This enhancement is associated with an increased charge-discharge capacity in electrode materials designed for supercapacitors. This research aims to enhance the deposition of metal oxides for energy storage applications. We will specifically examine the impact of nanostructured carbon and the significance of incorporating functional groups on the carbon surface in our study.

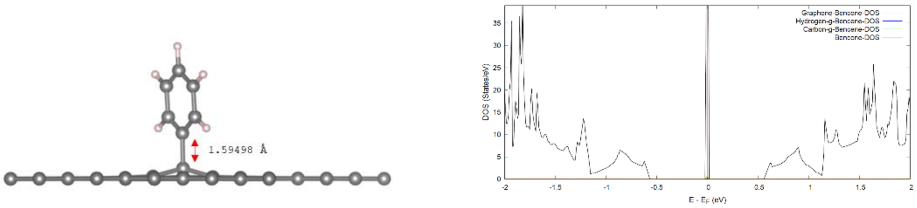

Fig. 1: Density of States and representation model of a 5x5 carbon cell and and phenyl group.

MnO_2 thin film deposited in conductor substrate for energy storage applications

Y. Esqueda Barrón[1*], A. K. Cuentas-Gallegos[1]

[1] *Universidad Nacional Autónoma de México, Centro de Nanociencias y Nanotecnología, Km. 107 carretera Tijuana-Ensenada, Apdo. postal 14, C.P.22800 Ensenada, Baja California, Mexico*

yesqueda@ens.cnyn.unam.mx, *akcg@ens.cnyn.unam.mx*

Manganese dioxide has a great variety of crystallographic phases, each showing distinct structures that can be broadly classified into two types. The first type is characterized by a tunnel structure, wherein the arrangement of lattice chains creates tunnels of varying dimensions. These tunnels occur in configurations such as 1x1 (pyrolusite β-MnO_2), 1x2 (ramsdellite R-MnO_2, and nsutite γ- MnO_2), and 2x2 (hollandite α-MnO_2), among other variations. The second type of structure is layered in nature, where some cations such as K, Na, Ca, Mg, as well as water molecules are inserted between the layers to improve structure stability. An example of this layered structure is δ-MnO_2, known as birnessite. This layered structure has particular interest for energy storage applications, specifically for supercapacitors where cations from the electrolyte intercalate within the δ-MnO_2 structure [1,2]. This study centers around the synthesis and characterization of birnessite thin films, intending to elucidate their physicochemical properties. The MnO_2 thin films were obtained through a two-step process. First, a manganosite (MnO) thin film was deposited over ITO-glass or stainless-steel substrates by Atomic Layer Deposition (ALD). Then, MnO thin films were immersed into the electrolyte in a three-electrode cell configuration, and cyclic voltammetry was used as the electrochemical oxidation process until their full transformation into MnO_2. These materials were characterized by Raman spectroscopy, SEM, and XPS to determine their properties. XRD results confirmed the MnO formation after the ALD process obtained a cubic structure, while SEM images showed a rough homogeneous surface (see Fig. 1A). Following the electrochemical oxidation process, a noticeable shift in the thin film color was observed to brown. Raman spectroscopy played an important role by detecting new bands that were absent in the MnO Raman spectrum (Fig. 1C). In addition, SEM demonstrated a large difference between the oxidized sample and its MnO-synthesized counterpart. The oxidized sample morphology showed the growth of wall-like structures or flakes, as illustrated in Fig. 1B. These differences confirmed the presence of birnessite structure on the thin film electrodes.

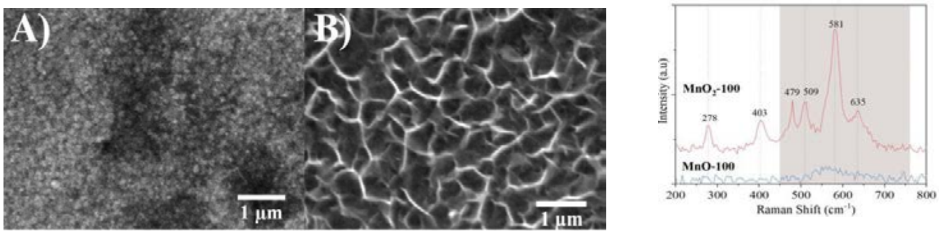

Fig 1. SEM micrographs of A) MnO thin film deposited by ALD in ITO-glass, B) MnO2 obtained by electrochemical oxidation, and C) Raman spectra of MnO and MnO2.

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Carbon electrodes obtained of lignocellulosic and biomass compounds by selective laser pyrolysis

Y. Esqueda Barrón[1*], I. Valdez[2], E. Aguilar[2], A. K. Cuentas-Gallegos[1]

[1] *Universidad Nacional Autónoma de México, Centro de Nanociencias y Nanotecnología, Km. 107 carretera Tijuana-Ensenada, Apdo. postal 14, C.P. 22800 Ensenada, Baja California, México*

[2] *Universidad Autónoma de Baja California (UABC), Facultad de Ingeniería, Arquitectura y Diseño. Km 107 Carretera Transpeninsular Ensenada-Tijuana 3917, Ensenada B.C., C.P. 22860, México*

yesqueda@ens.cnyn.unam.mx, *akcg@ens.cnyn.unam.mx*

A wide variety of biomass have been tested as raw materials to produce carbon by different thermochemical processes, for their application in supercapacitor electrodes [1,2]. Among them, solar pyrolysis has been show to be a sustainable process to obtain those carbons [3]. Nevertheless, it is not known which part of the solar radiation is responsible for the resulting carbon materials. Is it purely a thermal process induced by infrared radiation, or does UV-VIS is also participating? Due to expensive set-ups and long-lasting experiments in the solar furnace, this study introduces a novel approach: using laser pyrolysis with varying incident wavelengths to identify the changes in the resultant carbons, attributed to the interacting radiation. To understand the effects of Laser radiation on biomass conversion to carbon materials, a systematic study was carried out. This involved the use of individual biomass components (lignin, cellulose), and different wavelengths to selectively mimic solar radiation. The behavior of individual commercial lignin and cellulose was analyzed by diffuse reflectance spectroscopy, and by applying the Kubelka-Munk function their absorbance spectra were obtained. In the case of cellulose, an intense band was observed within the spectral range of 211 nm to 282 nm, which corresponds to the UV radiation region. In contrast, the absorbance spectrum of lignin, despite its lack of high purity, showed a wide absorbance band between 200 nm to 700 nm, centered around 450 nm. This spectral profile includes both the UV and visible radiation. Based on the absorbance spectra, laser-pyrolysis was performed under atmospheric air ambient conditions with different laser parameters, such as speed scan and laser power settings. Additionally, this pyrolysis methodology was extended to biomass derived from grape pruning waste. Figure 1 shows the results of the laser pyrolysis procedure, specifically using a 450 nm laser wavelength with variations in the laser power and their respective Raman spectra.

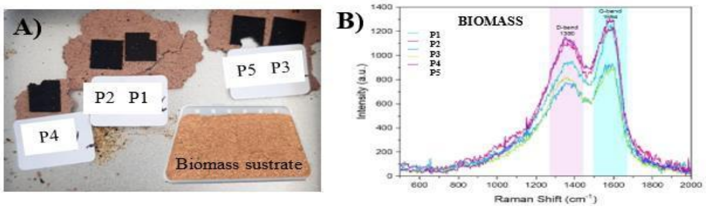

Fig. 1: A) Laser pyrolysis using a biomass substrate of grapes pruning waste. B) Raman spectra of carbons obtained with P1-2.2W, P2-2.8W, P3-2.86, P4-2.91, and P5-2.97W laser power.

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Producción de combustible solar a partir de un proceso termoquímico en un reactor Auger

N. A. Cisneros-Cárdenas[1*], C. A. Estrada-Gasca[1], C. A. Pérez-Rábago[1].

[1] *Instituto de Energias Renovables – Universidad Nacional Autonoma de Mexico.*

**ncisca@ier.unam.mx*

This work presents the proposal of a rotary reactor to produce solar fuel through the pyrolysis and gasification of organic solid waste, utilizing concentrated solar radiation as an energy source. The results of this process yield two products of interest in various fields: syngas and charcoal, valuable for chemical energy storage and soil remediation[1]. The thermochemical process takes place by exposing organic matter to temperatures between 400-700 °C in a low-oxygen atmosphere, leading to pyrolysis and the production of charcoal. Subsequently, water vapor is introduced into the reactor, promoting gasification and producing a mixture of gases, with molecular hydrogen as a significant component [2].

The conversion of solar energy into chemical energy holds the potential to address long-term energy storage and energy transportation challenges. There are several advantages by using solar energy for fuel production. Solar radiation provides high radiative fluxes, high heat rates, and, consequently, high temperatures, and it can utilize the entire solar radiation spectrum [3].

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Effect of the carbonization temperature of N/O-codoped electrospun carbon nanofibers on the performance anodes of sodium ion batteries

M.G. Ayala-Sánchez[1*], L.A. Rodrígez-Guadarrama[1], I.L. Alonso-Lemus[2], J. Escorcia-García[3]

[1]CINVESTAV del IPN, Unidad Saltillo, Av. Industria metalúrgica 1062, Parque Industrial Saltillo-Ramos Arizpe, Ramos Arizpe 25900, Coahuila, México.
[2]CONAHCyT-CINVESTAV Saltillo, Sustentabilidad de los Recursos Naturales y Energía. Av. Industria metalúrgica 1062, Parque Industrial Saltillo-Ramos Arizpe, Ramos Arizpe 25900, Coahuila, México.
[3]CONAHCyT-CINVESTAV, Unidad Saltillo, Av. Industria metalúrgica 1062, Parque Industrial Saltillo-Ramos Arizpe, Ramos Arizpe 25900, Coahuila, México.
melani.ayala@cinvestav.edu.mx

ABSTRACT

Sodium ion batteries (SIB) are a promising low-cost alternative to lithium-ion batteries (LIB), mainly due to high abundance of sodium (Na) in the earth's crust, which is higher than lithium (Li). SIBs and LIBs store energy through the same electrochemical mechanisms; however, there are some differences, the most important is that the ionic radius of Na^+ (1.02 Å) is larger than ionic radius of Li^+ (0.76 Å), which make that the development of suitable host materials for anodes of SIBs is currently a big challenge.

In this work, N/O-codoped carbon nanofiber (N-O-CNFX) were synthesized, three carbonization temperature were evaluated (X=800, 900 and 1000 °C). Morphology features shows that in this range of temperature N/O-codoped CNF were successfully obtained. It was also observed that with the increase in the carbonization temperature, the crystallinity also increased and the surface area of these decreased. The electrochemical measurements of charge and discharge showed that with the increase in the carbonization temperature the specific capacity also increased from 204.93 to 279.27 mAh g^{-1} and a coulombic efficiency of 80%.

Keywords: Sodium ion batteries, carbon nanofibers, coulombic efficiency.

Tuning the Supercapacitance of PEDOT:PSS with the Molecular Weight of the Macromolecular Dopant PSS

R. Mirón-Velázquez[1,2*], C. St. Thomas[1], J.G. Ramos -Sanchez[2], J.J. Alcaraz-Espinoza[2], and I. Gonzalez[2]

[1] *Centro de Investigación en Química Aplicada, Departamento de Procesos de Polimerización*

[2] *Universidad Autónoma Metropolitana, Grupo de Almacenamiento de Energía*

**ricardo.miron.m21@ciqa.edu.mx*

The PEDOT:PSS system exhibits a mixed ionic and electronic conduction. As a fundamental part PSS is responsible for doping PEDOT and water-dispersions. Despite being fundamental to understand PEDOT:PSS systems, most information is missed because this polymer is mainly used as commercial formulation. In a recent 2022 study, Lo *et al*. investigated the effect of average and distribution of molecular weight of PSS on mixed ion-electron conducting of PEDOT:PSS. [1] However, the relationship between molecular weight of PSS and capacitance has not been fully explored. In this work, we evaluated the influence of molecular weight of PSS on capacitance of PEDOT:PSS. The polymers were synthetized *via* RAFT polymerization to obtain well-defined molecular weights of PSSNa with well-defined molecular weights: 23 kDa (Đ=1.06), 45 kDa (Đ=1.03) and 88 kDa (Đ=1.04). Moreover, commercial PSSNa (Sigma-Aldrich) 70 kDa was also used. The abovementioned polymers were ion-exchanged from Na+ to H+. Subsequently PEDOT:PSS were obtained through EDOT polymerization in aqueous media using PSSH as dopant.

The electrochemical proprieties of synthetized PEDOT:PSS were evaluated using ~150 mg PEDOT:PSS film deposited on 1 cm^2 over graphite foil as work electrode, a second bare graphite foil as counter electrode, Ag/AgCl as reference electrode and H_2SO_4 1M as electrolyte. Cyclic voltammograms (CVs) (Fig. 1a) shown a capacitive behavior without redox peaks within a potential window between 0.64 and 0.16 V (*vs.* Ag/AgCl). Besides, the galvanostatic charge-discharge test (GCD) (Fig. 1b) showed symmetric capacitive double-layer signals. Fig 1c shows that mass specific capacitance (C_s) decreases with increasing current density. Furthermore, PEDOT:PSS with 50 kDa PSS show the lowest C_s of 46 F g^{-1} at 1 A g^{-1}, followed by 25 kDa PSS (102 F g^{-1}), 70 kDa commercial PSS (102 F g^{-1}) and 100 kDa PSS 275 F g^{-1} (Fig.1c). Finally, the PEDOT:PSS cycling charge-discharge tests were carried out at 5 A g^{-1} where 25 kDa PEDOT:PSS achieved 99% C_s retention over 2400 cycles, while over 3000cycles PEDOT:PSS with 50, 100 and 70 kDa (commercial) achieved a C_s retention of 93.4, 93.3 and 79.13%, respectively.

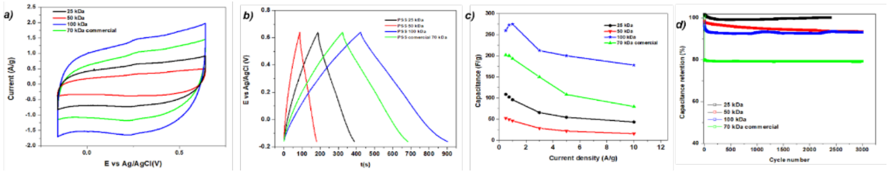

Fig. 1: PEDOT:PSS evaluation using: a) CV and b) GCD. C)Mass specific capacitance using various current densities d) cycling performance.

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N-doped subbituminous coal from Coahuila as anode of sodium-ion rechargeable batteries

C.A. Hernández-Siller[1*], I.L. Alonso-Lemus[2] and M.Z. Figueroa-Torres[3]

[1] *Sustentabilidad de los Recursos Naturales y Energía, CINVESTAV Saltillo, Av. Industria metalúrgica 1062, Parque industrial Ramos Arizpe, Ramos Arizpe, Coahuila, C.P 25900, México.*

[2] *CONAHCyT-CINVESTAV Saltillo ,Sustentabilidad de los Recursos Naturales y Energía, Av. Industria metalúrgica 1062, Parque industrial Ramos Arizpe, Ramos Arizpe, Coahuila, C.P 25900, México.*

[3] *Universidad Autónoma de Nuevo León, Facultad de Ingeniería Civil, Av. Universidad s/n, Ciudad Universitaria, San Nicolás de los Garza, Nuevo León, C.P. 66455, México*

**carlos.hdz.siller@cinvestav.mx, ivonne.alonsoonvestav.edu.mx*

Sodium-ion batteries (SIBs) present a promising prospect in the field of energy storage, offering comparable performance to lithium-ion batteries (LIBs) while avoiding the need for costly and scarce materials [1]. Despite their similarities, the larger atomic radius of Na^+ compared to Li^+ has a significant influence on the intercalation/deintercalation process, resulting in lower capacities. To address this challenge, carbon-based materials such as hard carbons have proven compatibility with the Na^+ intercalation mechanism [2]. In this study, subbituminous coal from Coahuila was evaluated as a potential anode material for SIBs. To enhance the electrochemical properties of coal, nitrogen-doped coal/graphite (N-CG) composites were synthetized using a two-step process involving mechanical milling and low-temperature heat treatment. Three different weight ratios of coal:graphite (1:3, 1:1, and 3:1) were evaluated while C/N atomic ratio was fixed at 10:1. The composite with the lowest coal loading (1:3) exhibited superior performance, yielding a specific capacity of 403 $mAhg^{-1}$ at a current of 0.1 mA. In contrast, the composites with coal-to-graphite ratios of 1:1 and 3:1 showed similar specific capacities of 374 $mAhg^{-1}$ and 342 $mAhg^{-1}$ respectively. Nevertheless, the anodes evaluated in this study exhibited a low initial Coulombic efficiency (ICE) of 5%. Therefore, despite the high initial specific capacity further research efforts are necessary to enhance ICE, to develop commercial and competitive anode materials for SIBs using this abundant natural resource. Finally, this research serves as an innovative demonstration of how a fossil fuel source can be harnessed to store clean and sustainable energy.

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A Cationic Poly (Ionic Liquid) as multifunctional binder for Lithium-Sulfur Batteries

A Hernández-Sánchez[1], *José Jarib Alcaraz-Espinoza* [1], *G Ramos Sánchez*[1 2], *C St Thomas*[3,4],
I. González[1].
[1] *Departamento de Química, Universidad Autónoma Metropolitana-Iztapalapa, CDMX, México.*
[2] *Departamento de Ingeniería de Procesos e Hidráulica, Universidad Autónoma Metropolitana-Iztapalapa, CDMX, México.*
[3] *Centro de Investigación en Química Aplicada (CIQA, Saltillo, Coahuila, 25294, México*
[4] *Conacyt-CIQA, Centro de Investigación en Química Aplicada (CIQA), Saltillo, Coahuila, 25294, México.*
**arturohdz991@gmail.com*

"Beyond lithium batteries" such as Lithium-Sulfur batteries (Li-S) are systems for the new generation of energy storage, this system possesses a high theoretical specific capacity (1675mAh·g^{-1}). Unfortunately, the concept is not commercial, due to the complex chemistry of sulfur; for instance, the solid-liquid-solid phase transition during discharge-charge implies an expansion-contraction at the cathode that compromises its structure.

There are a few ways to address and improve the performance of Li-S; in this work we propose the implementation of binders to overcome the problems mentioned above [1]. A poly (ionic liquid) (PIL) is selected as multifunctional binder, the studied PIL was synthetized by the RAFT technique which allows precise control of the polymer molecular weight based on an acrylate polymerizable [2-(Acryloyloxy) ethyl] trimethylammonium chloride (AETMAC) that possess a pendant group of quaternary ammonium. The synthesized linear PIL´s were named CFR11 and CFR12 with weights of 80kDa and 120kDa, respectively. In order to evaluate the polymers, coin cells were assembled and cycled 200 times (**Fig. 1**). The CFR12 cell exhibits a better capacity retention and efficiency after the test. If we compare the best results, CFR12 *vs* PVDF, the first one obtained 17% more capacity retention, 482mAh·g^{-1} vs 400mAh·g^{-1}, respectively.

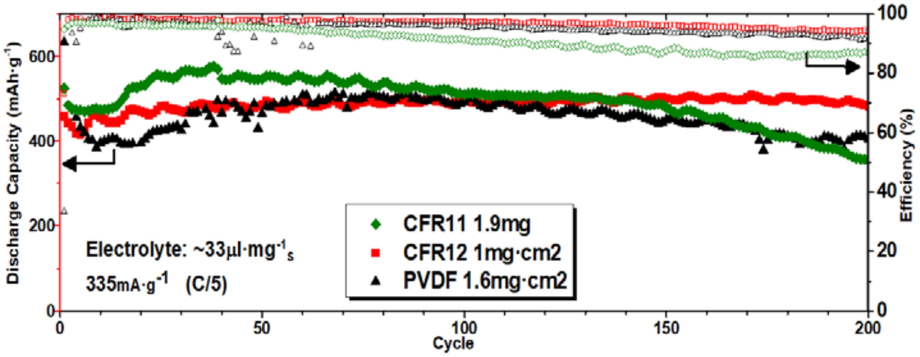

Figure 1. Ciclability of Li/LiTFSI$_{(DOL:DME1\%LiNO3)}$/Composite:CSP:binder mentioned inset.

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ESD2023_31

Evaluation of lithium manganese oxide cathodes doped with aluminum and niobium for lithium-ion batteries

Luis Antonio Solís-Balderas[1], Salomé Maribel de la Parra-Arciniega[1]*, Jesús Guzmán-Torres[1]. Luis Carlos Torres-González[1], Eduardo M. Sánchez-Cervantes[1].

[1] *Universidad Autónoma de Nuevo León, Facultad de Ciencias Químicas, Av. Universidad S/N, Ciudad Universitaria, San Nicolas de los Garza, Nuevo León, 66451, México*

E-mail: salome.delaparrarc@.edu.mx

In this work, lithium manganese oxide with dual doping of aluminum and niobium $LiAl_{(0.1-x)}Nb_xMn_{1.9}O_4$ (x ≤0.00, 0.01, 0.02) was evaluated as a cathode material for lithium-ion batteries. The materials were prepared by the modified Pechini method. Characterization was carried out by X-ray diffraction powder method and scanning electron microscopy. A cubic crystalline phase of $LiMn_2O_4$ ICDD 00-035-0782 and a trigonal phase of $LiNbO_3$ ICDD 00-020-0631 were indexed by XRD. The lattice parameters of the doped samples are lower than those of undoped spinel, which is attributed to the replacement of manganese by aluminum and niobium. The images obtained by scanning electron microscopy show a homogeneous morphology of irregular polygons. The electrode mixture used was 80:10:10 of active material, conductive carbon, and Teflon, respectively [1]. CR2032 button cells with lithium anode and LP30 electrolyte were assembled in a controlled argon atmosphere for subsequent electrochemical evaluation. In the galvanostatic charge and discharge measurements, a greater delivery of specific capacity for the $LiAl_{0.09}Nb_{0.01}Mn_{1.9}O_4$ cathode, 103.9 mAh/g, was registered than the unmodified one, which reported 101.2 mAh/g. Therefore, the modification of the lithium manganese oxide cathode with aluminum and niobium increases the performance of lithium-ion batteries.

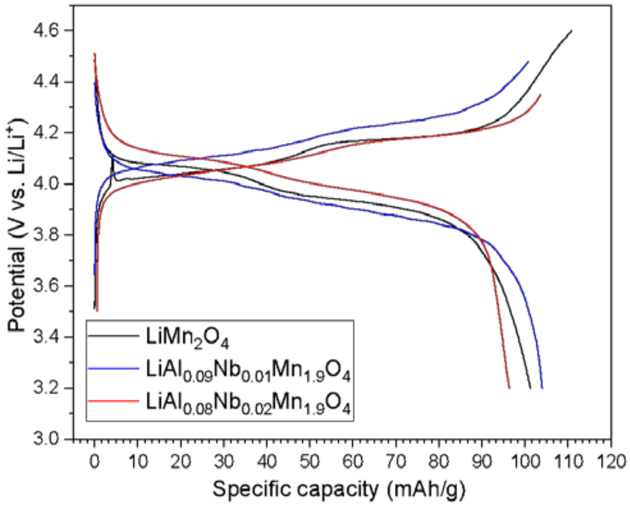

Figure 1. Galvanostatic charge/discharge profiles from 3rd charging cycle at C/10.

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Study of lithium cuprate modified with metal ions as an alternative cathode for lithium-ion batteries

A. García-Carrillo[1*], M.A. Martínez-Cruz, G. Ramos-Sánchez, and I. González

[1] *Universidad Autónoma Metropolitana-Iztapalapa, Departamento de Química, 09340 Ciudad de México, Mexico*

**bralex@live.com.mx*

Fossil fuels are increasing emissions of polluting gases, generating the need to develop new energy producing methods and devices capable of storing energy in an efficient manner, using economical materials and with minimal environmental impact.

One of the main energy storage devices is lithium-ion batteries (LIB) and they are being used in numerous applications; improving the cathode component will improve to a greater extent, battery properties such as voltage and capacity and therefore energy density. Lithium cuprate (Li_2CuO_2) is a material that has a theoretical capacity of 490 $mAhg^{-1}$ in addition to having an abundant (and, therefore, economical) transition metal (MT) in Mexico, allowing it to be considered as an alternative for cathode material. Li_2CuO_2 presents deficiencies such as the crystalline phase transition from orthorhombic to monoclinic during the extraction of a Li^+ ion and the evolution of O_2 that promotes structural instability, hindering the lithiation process and collapsing the crystalline structure after the second charge-discharge cycle. To solve these problems, previously Li_2CuO_2 has been doped with MT to improve the structural and electrochemical properties of the material, obtaining favorable results; However, the properties have not improved simultaneously, so by incorporating Ni as a doping agent, the discharge capacity increases and by incorporating Mn, greater structural stability is obtained [1].

In this work, Li_2CuO_2 was doped with different MTs using one (Co, Ni) or two (Co/Mn, Ni/Mn) doping agents. A solid-state synthesis methodology was carried out to obtain solid solutions with a molar concentration of 2.5% of the doping MTs. The structural characterization determined that the doping did not promote the formation of secondary phases, but did modify the parameters of the crystalline cell. Regarding the electrochemical characterization, a galvanostatic cycling profile was used at a potential window of 1.5 to 4.2 V to demonstrate that all materials can perform 50 charge-discharge cycles; however, Ni-doped and 2MT-doped materials did not increase the capacity of the material. On the contrary, the Co-doped material (Co-Li_2CuO_2) slightly increased the capacity of Li_2CuO_2 (Fig. 1) and improved its structural stability.

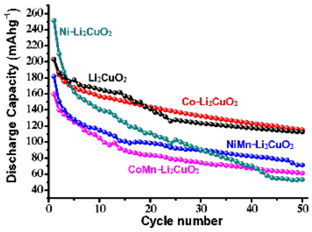

Fig. 1: Discharge capacity comparison between all doped materials and Li_2CuO_2.

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ESD2023_33

Supramolecular chitosan binder for lithium sulphur batteries

A. Mayrén[1*], I. González[1] and G. Ramos[2]

[1] *Universidad Autónoma Metropolitana. Unidad Iztapalapa. Departamento de Química. Av. San Rafael Atlixco 186, 09340, Ciudad de México, México.*

[2] *Universidad Autónoma Metropolitana. Unidad Iztapalapa. Departamento de Ingeniería de Procesos e Hidráulica. Av. San Rafael Atlixco 186, 09340, Ciudad de México, México.*

**alfonzomayren123@hotmail.com*

Among the different energy storage systems that are under development, lithium-sulphur (Li-S) batteries stand out, due to the sulphur high natural abundance and its high theoretical capacity (1675 mAh/g). However, it is still necessary to solve problems such as the dissolution of polysulphides, as well as improving the mechanical properties of the cathode to buffering the volume changes of 80 % during the charge-discharge process, phenomena that limit the useful life of the system.

As a strategy to improve the Li-S batteries performance, the design of multifunctional polymeric binders has been proposed to support the volume changes and optimize the trapping capacity of polysulphides.

Chitosan is a commercially available biopolymer, and it can be functionalized to improve its aqueous solubility, processability, mechanical and binding properties, making a multifunctional binder for Li-S batteries.

In the present work, after the addition of methanesulfonic acid (MSA) to Chitosan, it is formed a strong interaction between NH_3^+/SO_3^- groups, changing the linear structure of Chitosan, generating a different supramolecular structure between the polymer chains, improving its solubility in water and mechanical properties. Two materials with different methanesulfonic acid content were synthetized, ChMSA25 and ChMSA50 with 25 and 50 % of MSA, respectively.

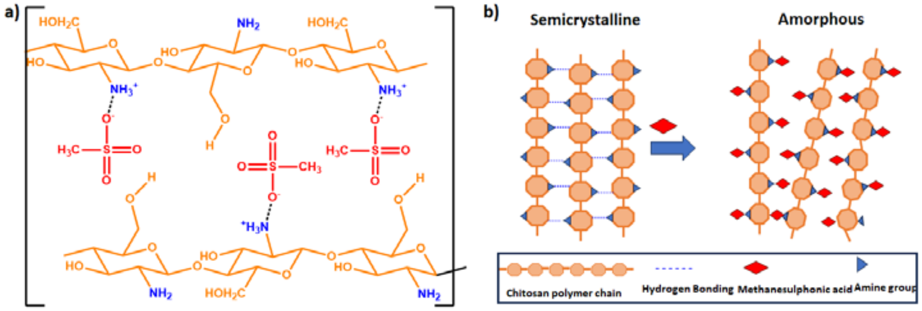

Fig. 1. a) Proposed interactions on Supramolecular Chitosan. b) Methanesulfonic acid interaction on Chitosan structure.

The performance of the materials was electrochemically tested. According to the rate capability test, even at the high current of 2 C, the cathode with ChMSA25 binder exhibit the highest capacity of 212 mAh/g and in the deep cycling, after 500 cycles at 1 C, it keeps a capacity of 223 mAh/g, showing an improvement in in the overall performance of the system.

ESD2023_34

Electron withdrawal and structural design key to ionic conductivity enhancement in polymers based on tetra-coordinated boron atoms

P. E. Pedro Cruz[1], G. Ramos-Sánchez[1], I. González[1] and G. Guzmán-González[1*]

[1] *Chemistry Departament, Autonomus Metropolitan University – Iztapalapa, Av. San Rafael Atlixco 186, 09310, Ciudad de México, México.1*

**greg@xanum.uam.mx*

INTRODUCTION Lithium-ion batteries (LIBs) are important devices in the transition to renewable energy sources. Electrolytes, are a fundamental component of batteries, among the different types solid polymeric electrolytes, composed of lithium salts and a polymer matrix, seem to be suitable candidates to face most of the associated problems. State-of-the-art single-ion conducting polymer (SLIPCE) electrolytes have a safety advantage by inhibiting the growth of dendrites in the lithium anode and improving ionic conduction in batteries [1]. However, the structural design of polymers is essential for optimal conduction properties for use in LIBs. This paper presents a series of SLICPEs based on tetracoordinated borate centers to aromatic groups that could give a high electronic offshoring and high ionic conductivity.

RESULTS Ionic conductivity of PEO/B(OPh)x mixtures (30/70 wt%) was obtained. A linear increase and thermal activation of Arrhenius-type ionic conductivity was observed, being higher for the PEO/B(OPh)2 mixtures as the temperature increased to 100 °C, well above the PEO melting temperature (~ 70 °C) [2] in which this presents greater amorficity and long-range segmental movement of the aether chains.

CONCLUSIONS The family of tetracoordinated boron-based polymeric electrolytes to phenoxide and aromatic groups whose ionic conduction properties allow them to be candidates for use in lithium batteries.

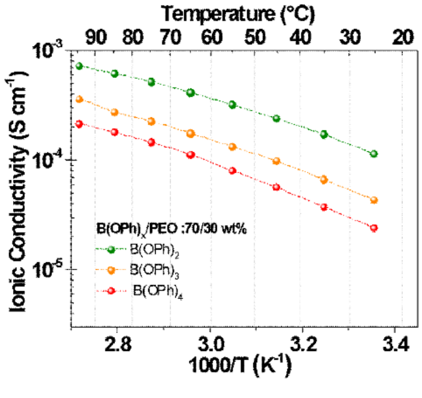

Fig. 1: Variation of ionic conductivity as a function of temperature for lithium polyphenoxyborates.

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PULSE ELECTRODEPOSITION OF CRYSTALLINE STRUCTURES OF MnO_2 FOR ELECTROCHEMICAL CAPACITORS

Roxana Berlanga Pérez[1,2], Johanna García Montemayor, Javier Osvaldo Terán Carlín,
Emilio Antonio García Montes, Jorge Zúñiga Martínez[1,2], Raúl Lucio Porto[1,2,*]

[1] *Universidad Autónoma de Nuevo León, Facultad de Ingeniería Mecánica y Eléctrica, San Nicolás de los Garza, 66455, Nuevo León, México*
[2] *Universidad Autónoma de Nuevo León, Centro de Innovación, Investigación y Desarrollo en Ingeniería y Tecnología, Apodaca, 66600, Nuevo León, México*

**raul.lucioprt@uanl.edu.mx*

Micro-supercapacitors are a new alternative to supply energy to modern miniaturized, smart, and connected devices such as implantable biomedical devices and portable electronic devices [1]. Thus, storing large amounts of energy in a reduced volume becomes a challenging task. Micro-supercapacitors are a new alternative to store energy due to a higher power and energy density and longer life cycle than micro-batteries [2, 3]. In this work, nanostructured MnO_2 thin films with 1D and 2D tunnel structure were prepared by Pulse Electrodeposition. The effect of crystalline structure, the thickness and morphology on the specific capacitance was evaluated. The charge storage process was also studied by cyclic voltammetry coupled with RAMAN spectroscopy and electrochemical impedance spectroscopy. The electrochemical study also includes the effect of several neutral electrolytes, such as Li_2SO_4, Na_2SO_4, K_2SO_4 and nitrates with different cations (Li^+, Na^+, K^+, Mg^{2+}, Ca^{2+} and Sr^{2+}). Additionally, long term cycling was performed to determine the electrode stability. δ-MnO_2 thin films were obtained with 2D tunnel. The highest specific capacitance was observed in 3M $Mg(NO_3)_2$ up to 100 $mFcm^{-2}$. The cycling stability test shows a loss of specific capacitance lower than 10 percent after 5000 cycles.

Keywords: Thin films of δ-MnO_2, Micro-supercapacitors, Energy Storage.

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ESD2023_36

Investigating the Role of Oxygen Vacancies in Manganese Oxide Thin Films for Enhanced Energy Storage

C. Bohórquez[1*], Y. Esqueda[1], and A. K. Cuentas[1]

[1] *Centro de Nanociencias y Nanotecnología de la UNAM, Km 107 Carretera Tijuana-Ensenada, CP. 22800 Ensenada, B.C. Mexico*

**bohormar@ens.cnyn.unam.mx*

As the demand for efficient energy storage solutions continues to grow, the exploration of novel materials and their electrochemical properties becomes imperative. This study focuses on investigating oxygen vacancies in manganese oxide thin films and their impact on energy storage applications. MnO thin films were prepared using atomic layer deposition (ALD) in a Beneq TFS 200 reactor, to ensure precise control over film thickness and composition. As a precursor Bis(ethyl-cyclopentadienyl) manganese [$Mn(CpEt)_2$] was used, and deionized water (H_2O) as the oxidizing reagent[1]. High-purity nitrogen (N_2), with O_2 traces below 10^{-6} ppm, was used to purge and carry gases [2,3]. Then, these films were electro-oxidized by cyclic voltammetry in 1M Na_2SO_4 electrolyte to obtain MnO_2 with the crystalline structure of birnessite.

Cathodoluminescence (CL), Raman, and UV-visible (UV-VIS) spectroscopies measurements were used to comprehensively analyze the optical and structural properties of these films before and after electrochemical oxidation. The CL results are observed in the spectra of the film before and after 1,000, 2,000, and 3,000 cycles of electrochemical oxidation. The spectrum associated with the MnO film before electrochemical oxidation shows the highest intensity. The appearance of a strong CL signal can be attributed to the unique properties of the deposited MnO film, which usually becomes amorphous when freshly deposited by atomic layer deposition (ALD). The amorphous nature of the film probably results in a higher density of defects and structural imperfections, which can act as efficient radiative recombination centers, leading to the highest intensity observed in the CL spectrum. The spectrum associated with the MnO_2 film after electrochemical oxidation, shows a decreased intensity compared to the MnO deposited film. This reduction in CL intensity indicates a change in the luminescent properties in the MnO_2 film due to the alteration of its crystalline structure, and defect density due to the oxidation process. When the electro-oxidation cycles increase, there is a shift in the spectrum towards lower energy, indicating a change in oxygen vacancies. As a reference, the substrate is also characterized and does not show strong CL signals compared to the manganese oxide films.

Raman spectra provided insights into structural transformations, and UV-vis spectra revealed alterations in the optical bandgap. Our results demonstrate the potential of MnO_2 thin films with controlled oxygen vacancies as promising candidates for energy storage applications. This work actively contributes to the continuous research in the field of energy storage, highlighting the critical importance of gaining insights into the role of defects for enhancing the performance and efficiency of next-generation energy storage technologies.

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The effect of adding MgO nanostructures to a magnesium polymer electrolyte

Y. Gonzalez[1], E. Gonzalez[1], A., J. Guzman[1] , M. Estrada-Villegas[2], A. Espinoza-Roa[2] and E. Sanchez[1*]

[1] *Facultad de Ciencias Químicas, Universidad Autónoma de Nuevo León*

[2] *Unidad Monterrey, Centro de Investigación en Química Aplicada*

**eduardo.sanchezcv@uanl.edu.mx*

Recent research has focused on multivalent ion batteries, which promise double the energy density and enhanced safety compared to traditional lithium-ion batteries. Magnesium, due to its abundance, has emerged as a promising alternative, but faces challenges related to compatible electrolytes. A study explored the impact of MgO nanorods on the properties of a magnesium ion polymeric electrolyte. The electrolyte comprised 10% EMIm-ESO_4 and 90% $Mg(ClO_4)_2$/ PEO/PVdF blend, with varying MgO nanorod concentrations. Utilizing analytical techniques like FTIR, DTA, XRD, EIS, CV, and LSV, the modified electrolyte's properties were assessed. The most effective membrane, containing 2% MgO nanorods, exhibited a room temperature conductivity of 2.22×10^{-1} S cm^{-1}, a 1.37 V electrochemical window, and improved performance at higher temperatures, confirming successful additive incorporation.

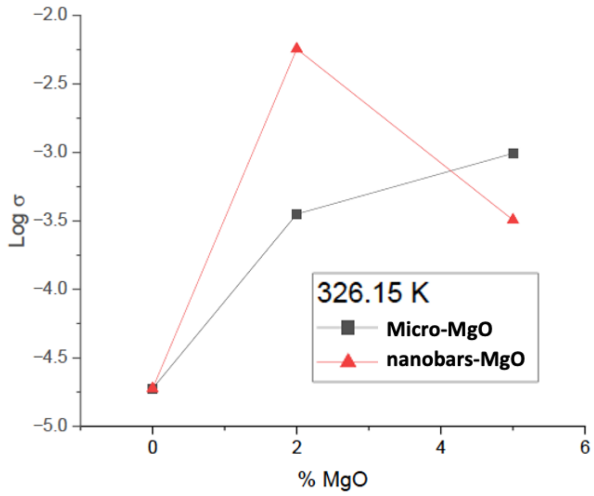

Figure 1. Effect of MgO addition vs. Log σ at 326.15 K.

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ESD2023_39

Raman Characterization of thin-layer FexOx by AP-CVD for energy storage applications

V. Parra-Elizondo[1], Abril Álvarez [2,1] Erick Hipolito[3,1], D. Pacheco-Catálan[1*]

[1] *Centro de Investigación Científica de Yucatán;* [2] *Universidad Politécnica de Chiapas ;* [3] *Instituto Tecnológico Superior Progreso*

**e-mail: dpacheco@cicy.mx*

This work presents the organometallic atmospheric pressure chemical vapor deposition (AP-CVD) synthesis of thin-layer FeOx over SS 316L substrates. This technique offers advantages such as uniform thin film growth, tunable composition, and tailored nanostructures. Integrating organometallic chemistry with CVD provides a versatile platform for synthesizing FeOx thin films with controlled stoichiometry and morphology. Key findings related to the synthesis process studied temperature depositions (600, 700, and 800 K) over 90 min time deposition and organometallic precursor ($Fe_3(CO)_{12}$ Sigma Aldrich) in two different precursor charge of 1000 and 100 mg are presented. The obtained deposits were characterized by Raman spectroscopy (Thermoscientific DRX λ=6232 nm). Temperature deposition parameters and composition show variations between phonon response modes. These changes can be associated with a mixture of oxide phases with characteristic signals of magnetite (679) and haematite (235). The results suggest that the tailored FeOx materials, produced via the proposed organometallic AP-CVD approach, offer some insight into materials tunability and can contribute to elucidating the nature of energy storage mechanisms in faradaic charge process-advancing energy storage technologies.

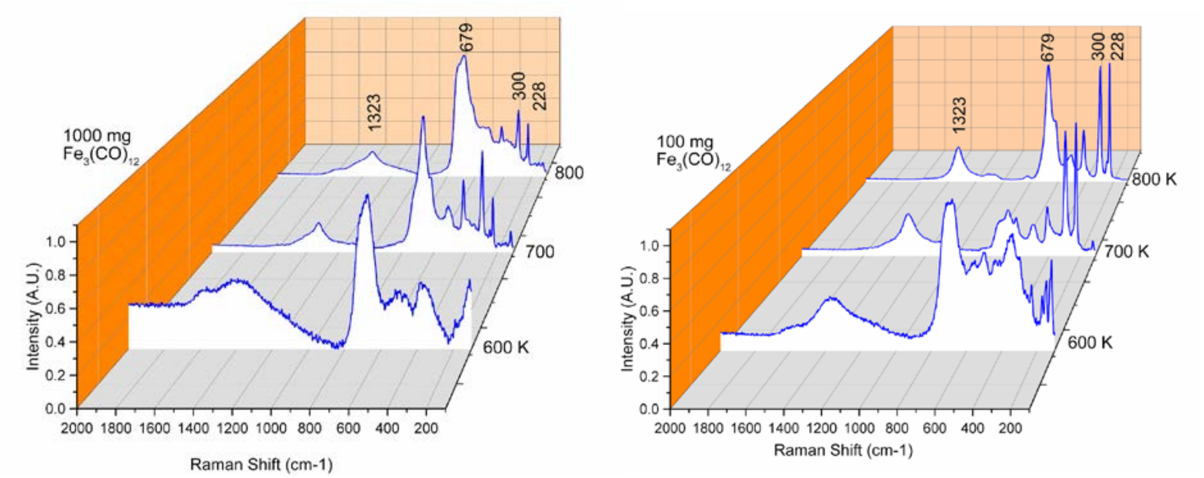

Fig. 1: Comparative Raman spectrum of thin-layer FexOx

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Synthesis of LISICON-like lithium copper (I) phosphate and its evaluation as cathode for LIBs

Sergio Alfonso Garcia-Mata[1], Salomé Maribel de la Parra-Arciniega[1*], Jesús Guzmán-Torres[1], Eduardo Maximino Sánchez-Cervantes[1]

[1] *Universidad Autónoma de Nuevo León, Facultad de Ciencias Químicas, Av. Universidad S/N, Ciudad Universitaria, 66451, San Nicolás de los Garza, Nuevo León, Mexico.*

**e-mail : salome.delaparrarc@uanl.edu.mx*

The widespread of lithium-ion batteries (LIBs) in different applications has encouraged the research to improve the energy storage capability of such devices. One way to attain that goal is to develop new cathodes with high energy density. In this sense, lithium copper (I) phosphate, Li_2CuPO_4, is a material with the LISICON crystal structure that has been proposed as a candidate due to its theoretical energy density being higher than the corresponding to other cathodes. Nevertheless, the scarce available experimental studies on Li_2CuPO_4 show an inconsistent degree of lithium-ion intercalation that is far from its theoretical capacity [1]. Aiming to improve the capability of Li_2CuPO_4 as an intercalation cathode for LIBs, the present work studied the partial substitution of phosphorus for vanadium in the system $Li_2CuP_{1-x}V_xO_4$(x=0.0, 0.1, 0.2). The synthesis was carried out with the ceramic technique, and it was proven successful through X-ray powder diffraction and Rietveld refinement. Attempts to synthesize the product using the hydrothermal technique are discussed. The particle distribution was investigated with scanning electron microscopy obtaining particles with irregular polyhedron morphology and distribution between 100 nm and 10 µm. Coin-type batteries were prepared using the synthesized samples as the active material in the cathodes. The galvanostatic cycling of the assembled batteries demonstrated the deintercalation of lithium ions at 3.75 V vs. Li/Li^+, which agrees with the available literature [2]. The substitution with vanadium improved the performance of the material.

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Nanoporous carbon fibers obtained by incomplete combustion of cotton fabric waste

I. L. Alonso-Lemus[1], F. J. Rodríguez-Varela[2], C. R. Garcia[3] and M. A. Garcia-Lobato[4*]

[1] *Conahcyt-Cinvestav. Grupo de Sustentabilidad de los Recursos Naturales y Energía. Ramos Arizpe, Coahuila. C.P. 25900.*

[2] *Sustentabilidad de los Recursos Naturales y Energía, Cinvestav Unidad Saltillo, Ramos Arizpe 25900, Coah., México.*

[3] *Facultad de Ciencias Físico-Matemáticas, Universidad Autónoma de Coahuila, C.P. 25020, Saltillo, Coah., México.*

[4] *Facultad de Ciencias Químicas, Universidad Autónoma de Coahuila, C.P. 25280, Saltillo, Coah., México.*

**marco.garcia@uadec.edu.mx*

Nanoporous carbon fibers (NCF) stand out for wearable supercapacitors due to their high flexibility and acceptable electrical properties [1]. Polymer fibers such as polyacrylonitrile [2], cellulose [3], etc., are typically used for obtaining them. Traditionally, raw materials are pyrolyzed under an inert atmosphere with relatively slow-heating ramps (1–5 °C/min), limiting their large-scale production. Thus, this work proposes carbonizing polymer fibers through incomplete combustion to use them as active material in supercapacitors. Particularly, the study focused on waste from cotton fibers. The process consists in three stages: 1) carbonization, 2) chemical activation, and 3) annealing heat treatment, and none of them requires the use of inert gases or slow-heating ramps. In a three-electrode cell, NCF exhibited a maximum specific capacitance of about 260 F/g within a potential window of 0–1 V using H_2SO_4 as electrolyte. Additionally, they were stable for more than 10,000 charge/discharge cycles.

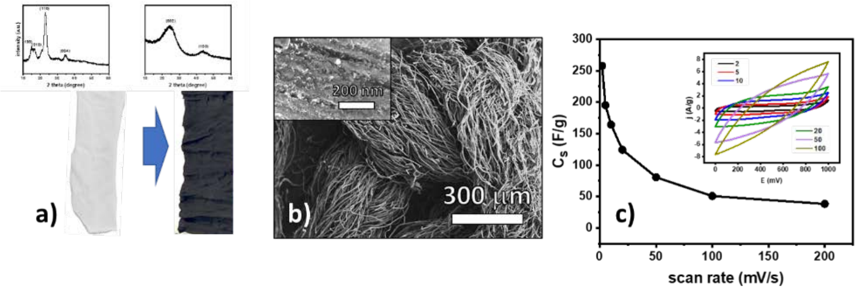

Fig. 1: a) result of carbonization of cotton fabric waste, b) SEM of nanoporous carbon fibers, c) capacitance as a function of scan rate.

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ESD2023_42

The first principal study focuses on the interface between perovskite materials and various carbon allotropes for potential applications in photosupercapacitors

J. Muñiz-Soria[1*], A. Gómez-Coronel[2*]

[1] *Instituto de Energías Renovables, Universidad Nacional Autónoma de México, Priv. Xochicalco s/n col. Centro Temixco, Morelos CP 62580, México [1]*

**jms@ier.unam.mx*, *gocoam@ier.unam.mx*

Photo supercapacitors offer a feasible option for storing energy within the same device[1]. The principal objective of this work is to study the interface between perovskite materials and various carbon allotropes, such as those used as electron transport layers, using density functional theory and Green's functionals. We have observed that the convergence in the new system (perovskite/allotrope) depends on the structural phase of the perovskite and the orientation of the carbon[2], particularly with PCBM[3] and PC71BM. In the figure 1, observed interaction between perovskite and fullerene.

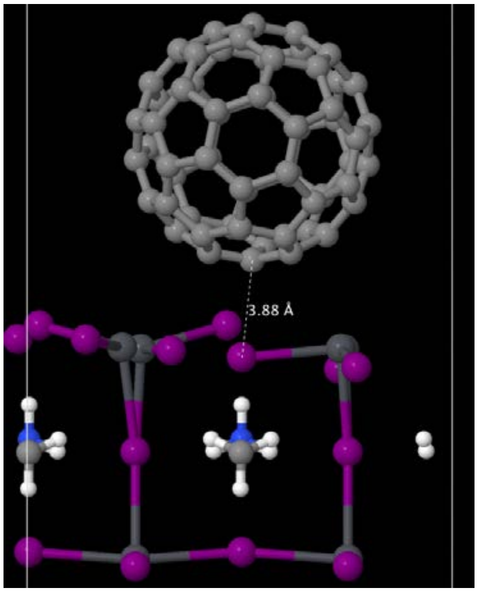

Fig. 1: Perovskite/fullerene after structure optimization in quantum espresso.

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ESD2023_43

Single lithium-ion conducting binders for high voltage LNMO electrodes studied through X-ray photoelectron spectroscopy (XPS)

J. Olmedo-González[1,3*], L. Lartundo-Rojas[2], R de G. González-Huerta[1], G. Ramos-Sánchez[3]

[1] *Instituto Politécnico Nacional-ESIQIE, Electrochemistry Research Lab, UPALM, 07738, Mexico City*

[1] *Instituto Politécnico Nacional, CNMN, UPALM, 07738, Mexico City*

[3] *Universidad Autónoma Metropolitana- Iztapalapa, IPH Department, 09340, Mexico City*

**jorgeolmedog@outlook.com*

The high-voltage spinel $LiNi_{0.5}Mn_{1.5}O_4$ (LNMO) shows great potential as material for the next generation of Lithium-Ion batteries. Nevertheless, it faces stability and cycling difficulties when operating near 5V. Here we propose the use of a single lithium-ion conducting polymer binder (SLICPB) replacing the typical binder, polyvinylidene fluoride (PVDF). The polymer is utilized to envelop the active material particles, creating a customized cathode-electrolyte interface that could potentially provide protection. Completely substituting the traditional binder with SLICPB does not add any extra weight to the electrode, which is a common problem when integrating inorganic coatings or additives into the active material or electrolyte. This approach is employed to hinder interactions with reactive anions and establish a protective layer that prevents electrolyte decomposition [1].

The characteristics of SLICPB effectively lower reactivity and decrease the release of Mn^{2+} ions, as assessed using differential electrochemical mass spectrometry (DEMS) and electron paramagnetic resonance (EPR), respectively. In this work these results are confirmed through X-ray photoelectron spectroscopy (XPS). The high-resolution C1s spectrum in the reference material with PVDF shows the formation of a signal at 290.6 eV, attributed to an intermediate compound in the degradation of the electrolyte, ethylene carbonate (EC). In relation to the decrease in Mn^{2+} leaching in SLICPB electrodes confirmed by EPR, it is worth noting that the presence of HF has been reported to promote Mn^{2+} disproportionation. Additionally, the high-resolution F1s spectrum demonstrates that the electrode with SLICPB possibly forms an interface between the B-F, although up to now there is no indication of an increase in the formation of LiF, which degrades into HF.

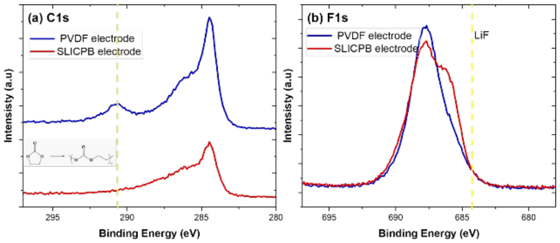

Fig. 1: a) C1s and b) F1s XPS spectra of the PVDF and SLICPB after the first charge

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Sustainable batteries with carbonaceous materials obtained from biomass, in-situ spectroscopic study of intercalation processes

Abstract

G. Rojas[1*], J. Mendoza[1] and G. Ramos[1]

[1] *Universidad Autónoma Metropolitana, Unidad Iztapalapa, Departamento de Electroquímica, 09340, Ciudad de México, México.*

**cbi2223803318@xanum.uam.mx*

The use of carbonaceous materials obtained from biomass, specifically "sargassum" from the Caribbean, in the development of sustainable batteries is an emerging research topic. However, besides the incorporation of carbonaceous materials in the fabrication of electrodes, the study of the intercalation process by spectroscopic methods is fundamental to understand the complex interplay between pososity, graphitic domains and functional groups.

Sodium ion batteries are considered a promising alternative due to the abundance and low cost of sodium. In this context, the use of biomass as a carbon source, such as sargassum, presents a unique opportunity to develop sustainable carbonaceous materials for application in these batteries.

The main objective of this research is to carry out an in situ spectroscopic study of the intercalation processes in carbonaceous materials derived from sargassum and other sources. This will provide a detailed understanding of the electrochemical reactions and structural changes that occur during the charging and discharging of sodium ion batteries.

The results of this research are expected to provide crucial information for the design and optimization of sustainable batteries with high energy storage capacity and long service life. Furthermore, the use of biomass as a carbon source is expected to contribute to the reduction of dependence on petroleum-derived materials and the use of renewable resources.

This study has the potential to open new perspectives in the field of sustainable batteries and contribute to the development of more environmentally friendly energy storage technologies.

ESD2023_46

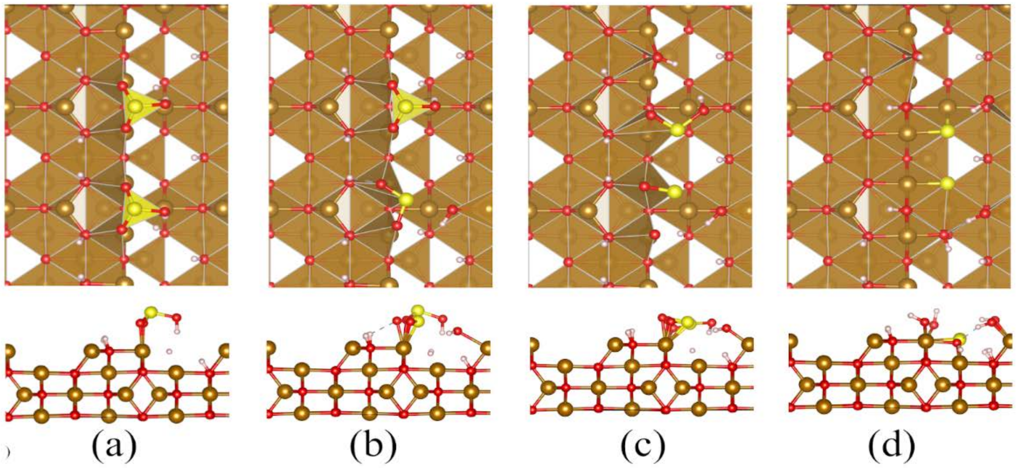
Charge transfer of Li, Na, K, and S ions in the electrolyte using Fe_3O_4 and MnO_2 surfaces as electrodes in a supercapacitor: A DFT study

Cornelio Delesma[1], Orlando Castro-Ocampo[1], Christian A. Celaya[1] and Jesús Muñiz[1*]

[1] *Instituto de Energías Renovables, Universidad Nacional Autónoma de México, Priv. Xochicalco s/n, Col. Centro, Temixco, Morelos. CP 62580, Mexico.*

**Corresponding autor. E-mail: jms@ier.unam.mx (Jesús Muñiz)*

In this work, we performed calculations using Density Functional Theory (DFT) to study the charge transfer of Li, Na, K, and S ions in the electrolyte when magnetite (MnO_2) [1] and Fe_3O_4[2] surfaces are employed as electrodes in a supercapacitor. These materials are considered pseudocapacitors because redox reactions occur on their surfaces with the active substances. In our study of the electronic structure properties and diffusion trajectories of MnO_2 and Fe_3O_4, we observed that Fe_3O_4 reduces $2SO^{2-}_3$ to form S^{2-} ions. The reaction trajectory of MnO_2 reveals a likely capacitance mechanism involving sequential redox reactions of SO^{2-}_3, SO^{2-}_2, SO^-, and finally S^{2-} ions on the magnetite surface (see Fig. 1). In the case of MnO_2, redox reactions occur with $LiNO_3$, $NaNO_3$, and KNO_3, resulting in the absorption of ions on the surface and the creation of MnOOLi, MnOONa, and MnOOK. The theoretical modeling approach allows us to understand the charge transfer of ions in the electrolyte when interacting with pseudocapacitor electrodes, which is essential for applications in energy storage devices.



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Electronic properties of Magnetite (Fe_3O_4) and transfer Mechanisms of ions at its surface

O. Castro-Ocampo[1*], Jesús Muñiz[1], Cornelio Delesma[1] and Christian A. Celaya[2].

[1] *Instituto de Energías Renovables, Universidad Nacional Autónoma de México, Priv. Xochicalco s/n, Col. Centro, Temixco, Morelos. CP 62580, México1*

[2] *Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, Km 107 Carretera Tijuana-Ensenada, Ensenada, B.C., C.P. 22800, México. 2*

**orcaoc@ier.unam.mx*

The band structure and the magnitude of the band gap in a material are pivotal factors influencing ion transfer, as the phenomena of capacitance and pseudo capacitance, in electrochemical devices like supercapacitors and batteries [1]. This work, delves into an examination of the electronic structure of magnetite, aiming to elucidate the mechanisms governing the charge-discharge reaction pathways involved in energy storage phenomena on the magnetite surface. Additionally, we introduce an initial modeling of the discharge reaction pathway.

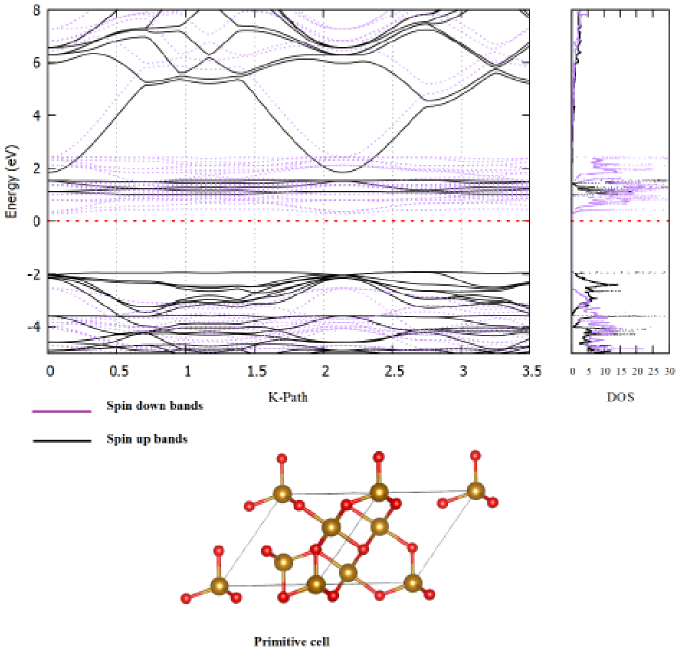

Fig. 1: Band Structure (BS) and Density of States (DOS) of the magnetite, obtained from the primitive cell showed below. Purple and black lines represent spin down and spin up values, respectively. Ferrimagnetic properties are evident.

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Understanding Li interaction in TiO2/graphene composites for high performance Li-ion battery anodes: A first principles study

Abdel Ghafour El Hachimi[1], <u>Jesús. A. Jiménez-Juárez</u>[1], Christian A. Celaya[2], Dage Sundholm, Pekka Pyykko and Jesús Muñiz Soria[1*]

[1] Instituto de Energías Renovables, Universidad Nacional Autónoma de México, Priv. Xochicalco s/n, Col. Centro CP 62580, Temixco, Morelos, México

[2] Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, Km 107 Carretera Tijuana-Ensenada, Ensenada, B.C., C.P. 22800, México

[3] Department of Chemistry, Faculty of Science, University of Helsinki, P.O Box 55, A.I. Virstasen aukio 1, FI-00014, Helsinki, Finland

*jms@ier.unam.mx

Composite materials consisting of TiO2 and graphene (TiO2/GR) have exciting properties that could make them suitable as anode material for Li-ion batteries [1-3]. Systematic DFT calculations were performed to investigate the TiO2/GR energy storage mechanism, adsorption sites and diffusion pathways of Li ions in TiO2/GR. Its interface and the region outside graphene were studied for identifying stable surface sites. The adsoprtion energies are dominated by van der Waals interactions. Li diffusion along the graphene plane was the most favorable with a diffusion energy barrier of 0.24 eV, whereas the probability of diffuison at the interface is low due to the barrier of 3 eV. The composite exhibited a higher specific charge storage capacity than other van der Waals heterostructures. The TiO2/GR interface retains a large amount of charge implying that the TiO2/GR composite shows suitable electrochemical properties for use as anode in lithium-ion batteries.

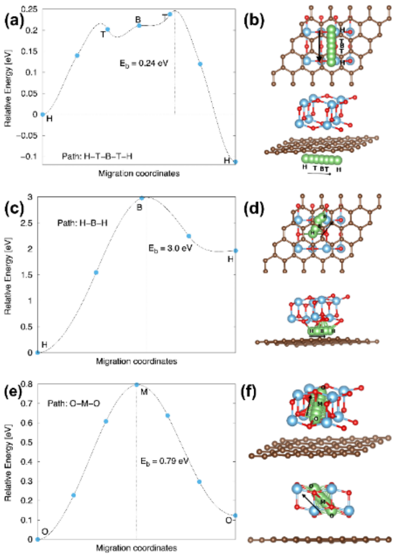

Fig. 1 : Diffusion pathways and energy barriers of the Li ions. (a) TiO2/GR/Li, (c) TiO2/Li/GR and (e) inside TiO2. Graphical representation of the minimum energy pathways of: (b)TiO2/GR/Li: H→T→B→T→H ; (d) TiO2/Li/GR: H→B→H and (f) inside TiO2:O→M→O.

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First principles study of the energy storage properties of the α-MnO_2/functionalized-graphene interface

Jesús. A. Jiménez-Juárez[1], Christian A. Celaya[2] and Jesús Muñiz Soria[1*]
[1] Instituto de Energías Renovables, Universidad Nacional Autónoma de México, Priv. Xochicalco s/n, Col. Centro CP 62580, Temixco, Morelos, México
[2] Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, Km 107 Carretera Tijuana-Ensenada, Ensenada, B.C., C.P. 22800, México
*jms@ier.unam.mx

Composite materials that combine metal oxides (MOs) with a carbon structure have been widely studied as electrodes for energy storage devices [1,2]. They show high specific energy density due to faradaic reactions on the metal oxide surface, while preserving the high electrical conductivity and stability of the carbon matrix [1]. In these hybrid materials, the nature of the interaction at the interface determines the efficiency of the charge transfer in the electrode [3]. The theoretical study of this interface is a very useful approach to understand the phenomena occuring and propose new composite materials for energy storage applications.

MnO2 has been studied as battery and supercapacitor electrode because it is inexpensive and has high energy specific density[2,4]. This metal oxide arranges in different crystal structures, in particular the α phase has received attention as electrode material due to its tunneled structure which exhibits high ionic diffusivity [5,6]

In this work, we studied graphene from a theoretical approach the energy storage properties of a composite material at the interface between α-MnO2 and graphene using DFT. The graphene surface was functionalized with different chemical groups (OH, COOH, NH2) to study the influence of the functional groups on the electronic structure of the composite material, we also studied the case of porosity on the graphene surface. The charge transfer between the metal oxide and graphene surface were calculated, and additionally we evaluated the diffusion barrior of a Li-ion at the interface. From this systematic study, we elucidate the effect that funcional groups have on the energy storage properties of the composite material.

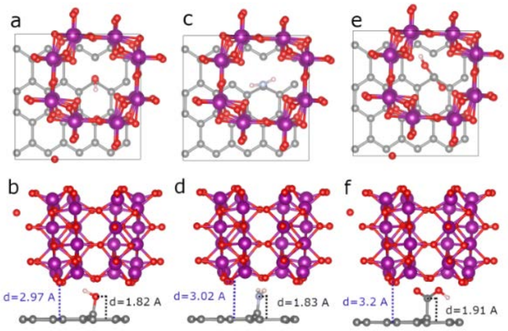

Fig. 1: Optimized structures of the interface with graphene functionalized with different groups: (a),(b)OH; (c),(d)NH2 ; (e),(f) COOH , top and side views respectively.

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Enhancing the performance of pyrolusite MnO_2 in supercapacitors by solid state incorporation of potassium cathions

E. López[1], K. Chávez[2] and E. Quiroga-Gonzalez[2*]

[1] *Faculty of Electronic Sciences, Benemérita Universidad Autónoma de Puebla, 72570 Puebla, Mexico*

[2] *Institute of Physics, Benemérita Universidad Autónoma de Puebla, 72570 Puebla, Mexico*

**equiroga@ieee.org*

The demand for more efficient energy storage devices with a sustainable approach has turned supercapacitors into a great alternative in applications where high instantaneous power is required (Paramati, Shahzad, & Doğan, 2022). Among the materials used as electrodes of supercapacitors, those based on manganese oxides are attracting much attention due to their low cost, durability, and relatively high specific capacitance. However, it is known that MnO_2 with a pyrolusite structure (β-MnO_2) has a poor performance. This work intends to study this material electrochemically before and after thermally incorporating potassium cations at 800 °C. For the present work, commercial MnO_2 and MnO_2 doped with potassium ions (K-MnO_2) were used as active material for the electrodes of supercapacitors. By Raman and XRD, it was verified that the commercial material is β-MnO_2 and that the thermally doped material is predominantly manganese oxide with a cryptomelano structure (α-$KxMnO_2$). Cyclic voltammetry measurements were performed at different scanning rates, to elucidate the electrochemical response of the materials. The results corresponding to K-MnO_2 present a higher current compared to commercial MnO_2, implying that this electrode has a higher specific capacitance, which can be attributed to a greater potassium ion insertion/extraction capacity. Furthermore, at high scanning speeds, its behavior shows that it is pseudocapacitive.

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Sulfur and Nitrogen-Doped Multiwalled Carbon Nanotubes and Graphene for Supercapacitors

Yoxkin Estévez-Martínez[1*], Enrique Quiroga-González[2], Erick Cuevas-Yañez[3], Víctor Castaño-Meneses[4]

[1] *Instituto Tecnológico Superior de Acatlán de Osorio, Tecnológico Nacional de México, 74949 Acatlán de Osorio, Puebla, Mexico.*

[2] *Institute of Physics, Benemérita Universidad Autónoma de Puebla (BUAP), 72570 Puebla, Puebla, Mexico.*

[3] *Center for Research in Sustainable Chemistry, Autonomous University of Mexico State, 50200 Toluca, Edo. de México, Mexico.*

[4] *Center of Applied Physics and Advanced Technology, Universidad Nacional Autónoma de México, 76230 Queretaro, Mexico.*

**yoxkin@gmail.com*

Research on multiwalled carbon nanotubes, graphene, and their interaction with various electrolytes and chemical compounds is driving the development of more efficient and versatile supercapacitors with potential applications in energy storage and power electronics [1][2]. In this context, this work presents a systematic study of supercapacitors based on sulfur and nitrogen-doped carbon nanotubes and graphene. The nanostructures have been characterized by elemental analysis by combustion and energy dispersive X-ray spectroscopy (SEM-EDS). Additionally, their morphology has been investigated at different stages of charge/discharge. Furthermore, their electrochemical performance has been evaluated by assembling battery half-cells with Sodium Sulfate (1 M) as the electrolyte, platinum as the counter electrode, and a Ag/AgCl reference electrode. The results indicate that doping with sulfur produces totally different electrochemical effects than doping with nitrogen. This research represents a promising approach towards tuning the energy storage mechanisms of supercapacitors for various practical applications.

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ENERGY PRODUCTION FROM BIOMASS

Carolina Pano-Azucena[1], Javier A. Arcibar-Orozco[1*], Liliana E. Arrvizu-Rodriguez[1] and Oscar E. Valdivia-Moreno[1]

1. CIATEC, Calle Omega No. 201, Col. Industrial Delta, León Guanajuato, CP 37545.

*Javier.arcibar@gmail.com

The growing global energy demand has driven the search for more efficient energy storage solutions. In this regard, lithium-sulfur (Li-S) batteries have emerged as a promising technology with high potential to address these challenges. Li-S batteries take advantage of the chemical reaction that occurs between lithium and sulfur to store and release energy, as they have a high theoretical specific capacity of 1672 mAh/g, high energy density (2600 Whk/g) being ideal for applications requiring high energy in a small space. However, Li-S batteries face significant challenges such as electrode degradation during charge and discharge cycles, polysulfide formation and migration limiting battery life and efficiency. To overcome these problems, research related to the use of activated carbons (AC) from waste as sulfur acceptors in the battery is being carried out. The present work reports the obtaining of AC from different sources including agave bagasse, tannery waste and sargassum and its modification with nitrogen groups with the aim of promoting polysulfide adsorption and improving battery efficiency. The results obtained in capacities, voltammetry and impedance show variations with the treatments made in the carbons with the insertion of the nitrogen groups, in which the porosity and surface chemistry of the carbons determine the electrochemical performance of the batteries.

Keywords: battery, polysulfides, activated carbon, tannery residue, nitrogenous groups.

Operando Raman spectroscopy of supercapacitors of carbon-coated Fe_3O_4 films

K. Chávez[1], B. Capilla[1] and E. Quiroga-Gonzalez[1*]

[1] *Institute of Physics, Benemérita Universidad Autónoma de Puebla, 72570 Puebla, Mexico*

* *equiroga@ieee.org*

Magnetite (Fe_3O_4) is one of the most studied oxides for its application as electrode of supercapacitors due to its low cost and low toxicity, besides having interesting electrochemical properties, especially when combined with porous materials such as carbon or graphite [1]. There are several methods by which carbon and magnetite composites can be made, however, in the most of the cases, the composites are prepared first (by two or more steps), and then the electrodes are prepared [2]. In this work, carbonization and electrode fabrication are performed in a single step. Nevertheless, as the electrodes have a novel structure, it is not well understood what are energy storage mechanisms involved. This work aims to give light to the understanding of these mechanisms. The film of Fe_3O_4 nanoparticles embedded in carbon, presents the synergy of both materials since they are in intimate contact. It has an overall improved conductivity and a significantly higher capacitance than the materials alone. The phenomena occuring in the electrode have been evidenced by operando Raman spectroscopy (spectra are recorded while the supercapacitor is being charged/discharged).

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Tuning the electrochemical performance of manganese oxides used as the active material of Li-ion batteries by thermal treatments: phase changes

M. L. Barrios-Reyna and E. Quiroga-González*

Institute of Physics, Benemérita Universidad Autónoma de Puebla, 72570 Puebla, México.

**equiroga@ieee.org*

In order to contribute to the development of clean and low-cost energy options, this work proposes obtaining advanced low-dimensional materials based on manganese oxides for their application as cathodes in high-speed lithium-ion batteries. The morphology, crystallinity, crystalline phases, conductivity, and mass loading of the manganese oxides affect the electrode parameters and, therefore, the electrochemical performance of the lithium-ion batteries [1-3]. In particular, we studied the influence of heat treatment on the structural and electrochemical properties of these oxides. The samples without thermal treatment present the Mn_3O_4 (hausmannite) phase, as could be evidenced by Raman and XRD. While the material is heat-treated at 600 °C/6 h in an oxygen-poor atmosphere, it is composed of the α-Mn_2O_3 (bixbyite) and Mn_3O_4 phases. On the other hand, when treating the material in an oxygen-rich atmosphere, only the α-Mn_2O_3 phase is produced, which is the most thermodynamically stable. The specific capacitance of the material composed for α-Mn_2O_3 and Mn_3O_4 phases was ~1.5 times higher than that of the samples with a pure phase (22 vs 14 Fg^{-1} of α-Mn_2O_3 and Mn_3O_4 phases, respectively). The influence of surface and diffusion-limited storage on total capacitance has been evidenced.

Keywords: manganese oxides, fast energy storage, lithium-ion batteries, phase transitions

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Metallurgical grade silicon as electrode material of lithium-ion batteries

J. Rojas[1], E. Quiroga-González[2*]

[1] *Faculty of Electronic Sciences, Benemérita Universidad Autónoma de Puebla, 72570 Puebla, Mexico.*

[2] *Institute of Physics, Benemérita Universidad Autónoma de Puebla, 72570 Puebla, Mexico.*

**equiroga@ieee.org*

A study of the performance of metallurgical grade silicon as active material of electrodes of lithium-ion batteries has been performed. The study has been carried out by means of charge and discharge galvanostatic measurements comparing between samples with different impurity contents. This allows to elucidate the effect of the presence of certain impurities in the performance of the material in batteries. Unlike other existing works, this one has the particularity of showing specifically the concentration and type of impurities in the active material.

Powders of four different metallurgical grade silicon samples were used for the present work, all silicon samples have a micro particle size. Specifically, the samples are named as follows, containing the following characteristics:

- Sample M1: Low Fe content (19.2 ppmw), purity 99.99 %.
- Sample M2: High Fe content (3344 ppmw), 99.5 % purity.
- Sample M4: Doped with P atoms, as if it were n-type Si, 99.5 % purity.
- Sample M4: Doped with B atoms, as if it were p-type Si, 99.5 % purity.

Galvanostatic cycling tests of half battery cells with metallurgical grade silicon working electrode revealed that using an n-type metallurgical grade silicon sample provides the highest specific capacity values. Compared with the non-doped samples, the boron and phosphor doped samples present the lowest coulombic efficiencies during the first cycles, but then they present the highest ones afterwards, together with the highest capacities. However, in general, all metallurgical grade silicon electrodes show a trend to maintain the capacity at values above 200 mAh/g (and above 400 mAh/g in the best case).

The existence of iron in the samples reduces the maximum capacity of the battery, but achieves higher stability, in agreement with other reports [1]. On the other hand, the presence of n-type impurities (phosphorus) allows reaching higher capacities, while the presence of p-type impurities (boron) enables higher coulombic efficiency.

The results indicate that metallurgical grade silicon can be an economical alternative of active material of battery electrodes with competitive specific capacities, despite the presence of high amount of impurities. It is also worthy to mention that the Si particles used for the present study are micron-sized, but it is desirable to have them in lower dimensions to avoid cracking while lithiated/delithiated. Then the results could be greatly improved if Si is milled into smaller particles before preparing the electrodes.

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Aqueous supercapacitors with extended operation voltage range through polyelectrolyte coating

X. León[1], César Márquez-Beltrán[1], E. Quiroga-González[1*]

[1]*Institute of Physics, Benemérita Universidad Autónoma de Puebla, 72570Puebla, Mexico.*

**equiroga@ieee.org*

The operation voltage of supercapacitors is one of their most important parameters, in addition to their capacitance. Because the capacity of the device is relatively low compared to batteries, the way to compete is to increase its voltage. The energy (Wh) depends directly on the capacity (Ah) and voltage (V). The voltage for capacitors with aqueous electrolyte is usually less than 1.1 V, limited by the nature of water, which undergoes electrolysis at 1.23 V. In this work, low-cost supercapacitors with improved properties were developed with electrodes based on activated carbon obtained from corncob [1]. After fabrication, the electrodes were coated with positively charged and negatively charged polyelectrolytes, and were assembled in a supercapacitor with an aqueous 5 M KOH electrolyte. The polyelectrolytes modified the voltage beyond the electrolysis voltage of water. This proposal represents a new sustainable alternative of extended voltage aqueous supercapacitors.

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Novel MgC_2O_4 cathode material for its application in Mg^{2+}/Li^{+} hybrid ion batteries: Synthesis and electrochemical performance

J. Guzmán-Torres, E. González-Juárez, L. L. Garza-Tovar, E. M. Sánchez-Cervantes*

Facultad de Ciencias Químicas, UniversidJ.ad Autónoma de Nuevo León, Av. Universidad S/N Ciudad Universitaria, C.P. 66451 San Nicolas de los Garza, Nuevo León, Mexico

**eduardo.sanchezcv@uanl.edu.mx*

The magnesium oxalate (MgC_2O_4) cathode material was synthesized via a dissolution route. This material exhibited higher electrochemical performance in Mg^{2+}/Li^{+} hybrid ion batteries (MLIBs) compared with magnesium ion rechargeable batteries (MIBs) that were prepared. The cell subjected to a continuous current density of 10 mA g^{-1}, achieved a high discharge capacity of 284 mAh g^{-1} at first cycle to later achieve specific capacities of 232, 205, 193 and 167 mAh g^{-1} at the 10, 20, 50 and 100 cycles (Fig. 1), remaining above the results obtained in the Mg || 0.4 M APC || MgC_2O_4 batteries. Then, the MgC_2O_4 material has the potential to be applied as a cathode in energy storage and conversion devices, such as MLIBs.

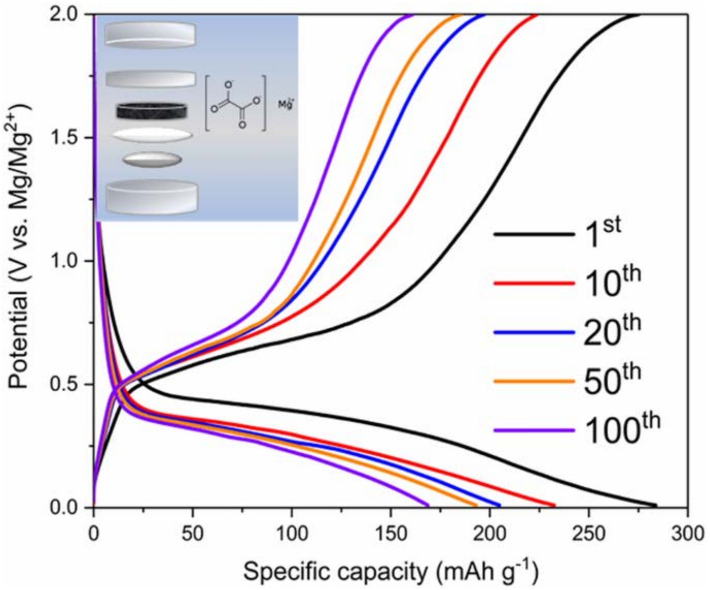

Fig. 1: Galvanostatic charge/discharge profiles at 10 mA g^{-1} of the Mg || 0.4 M APC/1.25 M LiCl || MgC_2O_4 batterie.

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Implicit solvent effect on the binding energy of the functional groups with impact in Li-S batteries

A. Ochoa-Calle[1*], G. Ramos-Sanchez[1] and I. Gonzalez[1]

[1]*Universidad Autónoma Metropolitana, Ciudad de México, México*

**ajochoacalle@gmail.com*

As a first strategy for the *in silico* experiment in the design of Li-S batteries of high specific capacity, in this work, we explore the effects of the implicit solvent that comes from theoric *ab initio* derivation with experimental parametrization and has an excellent response to the local charge of the solute in the framework of Joint Density Functional Theory (JDFT)[1]. It has taken a comprehensive set of functional groups containing boron, nitrogen, oxygen, and sulfur interacting with short and long chains of polysulfides. It is evaluated the structural and energetic stability compared to vacuum basic calculation of the several electrolytes, carbonate-based: dimethyl carbonate (DMC) and ethylene carbonate (EC) and high donor solvents: N, N dimethylformamide (DMF) and dimethyl sulfoxide (DMSO).

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Unveiling the Charging/Discharging Mechanisms of Calcium carbonate and calcium hydroxide as High Performing Electrodes of Sustainable Lithium-Ion Batteries

E. Tecpa-Flores[1] and E. Quiroga-González[1*]

[1] *Institute of Physics, Benemérita Universidad Autónoma de Puebla, 72570 Puebla, Mexico*

* *equiroga@ieee.org*

In the present work, the use of electrodes made of calcium hydroxide (, portlandite phase) and calcium carbonate ($CaCO_3$ in calcite, aragonite, and vaterite phases) as anodes in lithium-ion batteries has been analyzed. Promising results were obtained, considering that these electrodes have a higher specific capacity than those made of graphite, the material most commonly used in anodes.

XPS analyses were performed before and after lithiation. The results indicate that calcium hydroxide is the most abundant phase in the electrodes before lithiation. It is obtained from the decomposition of $CaCO_3$ into CaO and its subsequent hydration due to the humidity of the environment [1]; however there are rests of $CaCO_3$. The charge storage mechanism of the anodes consists of partially reversible conversion reactions in a potential window of 0.5 to 2.0V, related with the formation of Li_2CO_3 and Li_2O. The $Ca(OH)_2$ lithiation-delithiation process is favored over the $CaCO_3$ one. This is because this process occurs in a single stage, while the lithiation of $CaCO_3$ occurs in two stages. This is especially true for the case when charge-discharge rates are fast (5C).

The metallic Ca formed during this process reacts with the fluoride from the electrolyte used in the batteries ($LiPF_6$), forming a significant amount of fluorite (CaF_2), which is partially reversible electrochemically. This decreases the coulombic efficiency of the batteries during the first few charge/discharge cycles. This reaction is minimized when the charge/discharge process is carried out at high rates (5C), indicating that the fluorite formation reaction occurs slowly. That is why at high charge/discharge rates the battery performance is superior (Fig.1).

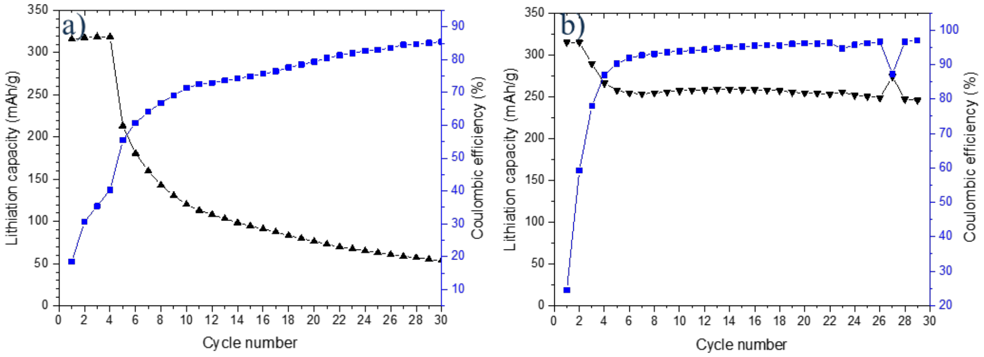

Fig. 1: Galvanostatic cycling of the anodes. Specific capacity and coulombic efficiency of the anodes at rates a) C/2 and b) 5C.

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Solar reactor for the concentration of lithium carbonate

B. Falcón-Varela[1*], C. Pérez-Rábago[1,2], R. Pérez-Enciso[2] and P. Zavala-Rivera[2*]

[1] *Instituto de Energías Renovables, Universidad Autonóma de México, Priv. Xochicalco s/n, col. Centro, Temixco, Morelos, 62580, México.*

[2] *Universidad. De Sonora (UNISON), Blvd. Rosales y Luis Encinas, Hermosillo, 83000 Sonora, México.*

**favabe@ier.unam.mx*

Using a solar simulator, energy will be irradiated to reach temperatures of 750º C inside the reactor, causing the lithium mineral within the crucible to melt. Once melted, the lithium carbonate concentration will be achieved through the electrodes, which will be present on the crucible.[1][2]
The internal part of the reactor will rotate through the magnetic force induced by the magnet embedded inside the reactor, acting on the stainless-steel cylinder. Additionally, an external magnetic stirrer will maintain a constant speed of approximately 150 rpm, ensuring a consistent and homogeneous temperature in the graphite crucible for conducting the experimentation.

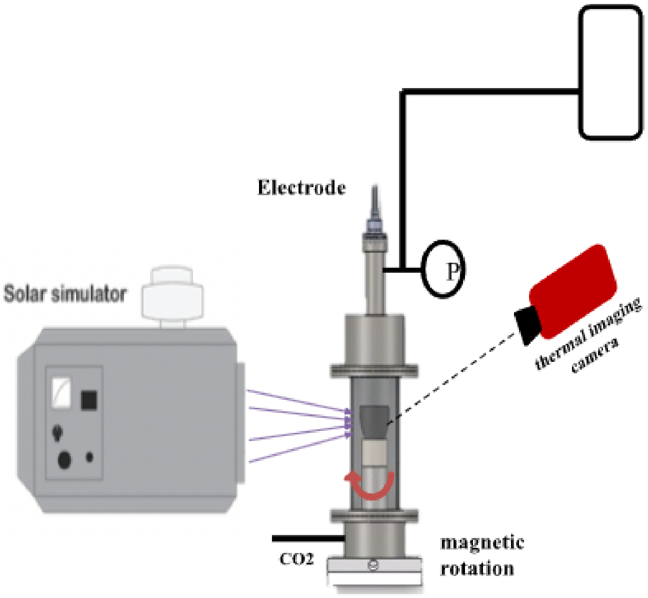

Figure 1. Experimental Setup Diagram for Lithium Carbonate Concentration in Stainless Steel Reactor with Solar simulator.

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Electrochemical and recycling protocols to guarantee the second life of lithium-ion batteries and the obtention of "Black mass"

D. Alba[1], S. Rodriguez[1], R. Pérez[1] H. Ávila[1]*, R. Suarez,[2]* G. Ramos[3]*.

[1,2] Universidad Autónoma Metropolitana-Iztapalapa, Av. San Rafael Atlixco No. 186, 09340 Mexico City, Mexico, Departamento Ingeniería de Química, [2]Departamento de Ingeniería de Procesos e Hidráulica.

[3]Consejo Nacional de Humanidades, Ciencias y Tecnologías CONAHCYT, Av. Insurgentes Sur 1582, Col. Crédito Constructor,

Benito Juárez, 03940, Ciudad de México.

1 hjap@xanum.uam.mx, 2* ruben.suarez@conahcyt.mx, 3* gramos@xanum.uam.mx,*

In Mexico 15.15 tons of lithium batteries LIBs are discarded per year [1], thus, a large amount of waste is generated. Unfortunately, the number of the recycling programs to treat the spent LIBs are scarce and even worst they usually are left in open dumps decomposing and releasing several chemical compounds that contributes to the contamination of the land.

With the purpose of decrease the contamination and also give a second life chance to the spent LIBs, in this project two main objectives are addressed: i) Design and document good practices in the collecting and treatment of LIBs to make the statistics related to their condition, the determination of physical parameters and the implementation of electrochemical protocols to obtain information that allow infer if the battery cells are suitable for the assembly of new battery packs ensuring the implementation in application of lower energy demands. ii) The implementation of methodologies to recycle non-suitable cells, the recycling methods are based on a shredding process to get a product denominated "black mass" which contain a high valuable mineral such as Li, Al, Cu, Ni, Co, and so on, besides, is possible to obtain plastics that can be used as the structure of new batteries. In the battery recycling industry, the batteries are crushed regardless of whether they can still be reused, however in this project the temperature and number of cycles were relevant factors to really analyse and conclude at what point they can be reused, also were studied the gases that LIBs generate in the environment and thus seek an alternative to reduce their impact.

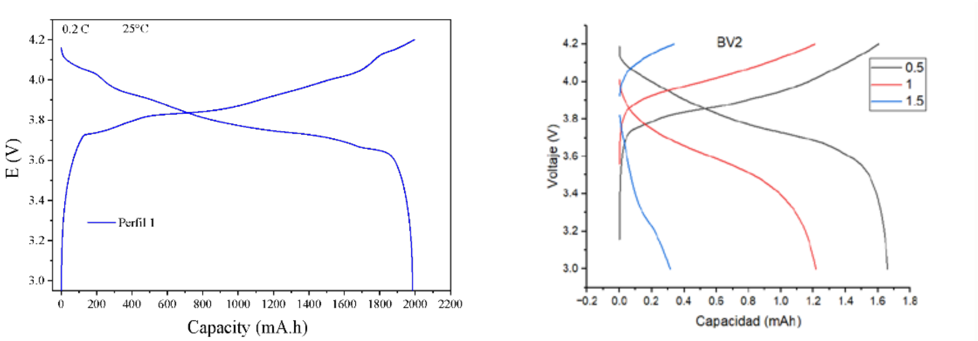

Fig. 1: Charge and discharge profiles. (left) New Battery. (right) For a discarded Battery.

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Nail Perforation Tests for the Pretreatment of Spent Lithium-Ion Batteries

O. Sánchez-Dena[1,2*], A.E. Grado-Zubiate[2] and R. Farías[2]

[1] CONAHCYT Consejo Nacional de Humanidades Ciencias y Tecnologías, Av. Insurgentes Sur 1582, Col. Crédito Constructor, Benito Juárez, Ciudad de México, 03930, México
[2] Instituto de Ingeniería y Tecnología, Universidad Autónoma de Ciudad Juárez, Av. Del Charro 450 Norte, Ciudad Juárez, Chihuahua, 32310, México
**oswaldo.sanchez@uacj.mx*

There are various alternatives to recycle spent lithium-ion batteries (sLIBs), that is, to recover lithium from the residual materials in a sLIB. Previously, it is necessary to perform an appropiate initial phase of the recycling process, known as pretreatment. It first involves an electrical stabillization (or discharge of the remnant charge in the battery), which would enable the dismantling of the sLIB with safety (minimizing fire risks from mitigation of thermal runaway) and subsequent stages of robust and fine physical separations. Some available strategies to reach electrical stabillization in gBILs are summarized in Fig. 1. Another possibility not being described in the scheme is to perform a direct physical discharge by means of perforating the battery within a safe ambient in what respects fire, explosions and inhalation of toxic gases. Ignited or not, the driven thermal runaway effect would led to an effective discharge of the battery, thus facilitating its distmantling without need of a controlled atmosphere.

In this work we report the recollection and classification of nearly 900 sLIBs as well as the observed trends after performing nail perforation tests (NPTs) to approximately 80 sLIBs outdoors, using climate conditions (air, normal pressure, room temperature). Based on these results, a prototype for an isolation chamber to perform secure NPTs will be described.

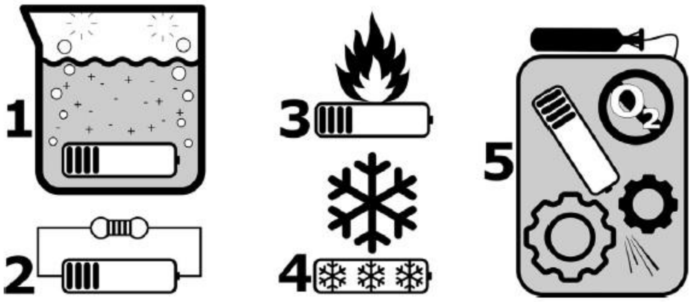

Fig. 1: Schematization of some processes to electrically stabilize a sLIB: 1. Aqueous solution with salt. 2. Direct contact with an electric resistance. 3. Thermal treatment. 4. Cryogenic treatment. 5. Direct comminution in a controlled atmosphere. *Reprinted after Sommerville et al., Sustainable Mater. Technol. 25(2020)e00197, Elsevier B.V.*

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Bi_2O_3/coal-based composites as supercapacitor electrodes

S.O. Mena-Picón[1], J.A. Díaz-Guillen[1], F.J. Rodríguez-Varela[2] and I.L. Alonso-Lemus[2*]

[1] *Tecnológico Nacional de México, Instituto Tecnológico de Saltillo, 25280, Saltillo, Coahuila México*

[2] *Cinvestav-Saltillo. Grupo SRNyE, México, Parque Industrial Saltillo-Ramos Arizpe, Ramos Arizpe, Coahuila, 25900, México.*

[2*] *CONACHYT, Cinvestav Unidad Saltillo, Sustentabilidad de los Recursos Naturales y Energía, Parque Industrial Saltillo-Ramos Arizpe, 25900 Ramos Arizpe, Coahuila, México.*

* ivonne.alonso@cinvestav.edu.mx

Energy storage is an critical topic for the electricity production from renewable sources due to the intermittency during its generation. In this regard, supercapacitors are electrochemical energy storage devices with high-power density, which can be used in transportation (e.g., electric vehicles) and backup energy systems applications. [1]

In this research two abundant resources of Coahuila, located at northeast of Mexico were evaluated as electrodes for supercapacitors: i) coal from Sabinas region and ii) bismuth oxide. On other hand, carbon-based supercapacitors are environmentally friendly, low-cost, and feasible option for large-scale production of supercapacitors [2]. Meanwhile, metal oxides can significantly increase the specific capacitance due to their pseudocapacitive storage mechanisms. In this sense, electrodes of activated coal (CMA), bismuth oxide (BO) and composites of them with a weight ratio of 1:1, 2:1 and 3:1, labelled as CMA1-BO, CMA2-BO and CMA3-BO respectively, were synthetized.

Different physicochemical characterization techniques such as XRD, FTIR, RAMAN, SEM, EDS were used to determine the structural properties, chemical composition, and morphology of the composites. Cyclic voltammetry (CV) was performed at scan rates of 100, 50, 20, 10, 5 and 2 mV/s. meanwhile charge-discharges (DC) at 0.5, 1, 5, 10, 20 and 25 A/g. Additionally, electrochemical impedance spectroscopy (EIS) was performed from 10 kHz to 100 mHz at 10 mV of amplitude.

The results indicate that CMA has a specific capacitance of 307.69 F/g at 2 mV/s, meanwhile the specific capacitance of the composite CMA1-BO increased up to 733.76 F/g at 2 mV/s, which demonstrates that coal and bismuth oxide from Coahuila have properties that make them potentially promising to be used as supercapacitors electrodes.

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Development of graphene nanobuds for energy storage: lithium-ion batteries and supercapacitors

I. Zeferino Gonzalez[1*], A.M. Valenzuela Muñiz[1], and R. Gauvin[2] Y. Verde Gómez[1]

[1] *Tecnológico Nacional de México / IT de Cancún, Av. Kabah Km. 3, Cancún, Q.R, 77500, México*

[2] *Department of Mining and Materials Engineering, McGill University, 3610 University Street, H3A 0C5, Montréal, Québec, Canada*

**e-mail : isaias.zg@cancun.tecnm.mx*

Graphene nanobud (GNB) is a carbon allotrope, which consists of the combination of covalently bonded fullerene and graphene resulting in a 3D nanostructured material with exceptional properties. Recently, our working group [1] developed this novel material through the modified chemical vapor deposition technique using toluene as a carbon source and Cu as a substrate. The direct application in lithium-ion batteries demonstrated that this hybrid material presents high electrochemical properties since the covalent integration of fullerene on the graphene surface improved Li-ion diffusion and greater Li-ion storage capacity. On the other hand, given the intrinsic properties of the graphene nanobud and its peculiar structure, this material is affordable also for applications in supercapacitors and fuel cells. The physical, chemical, and electrochemical characteristics of GNB, as well as its relevance as an advanced material for energy storage, are discussed in this work.

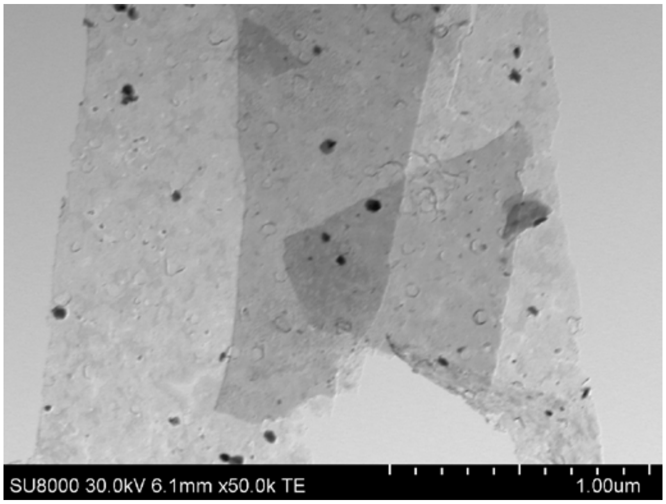

Fig. 1: SEM image of graphene nanobud (dark field mode).

Acknowledgements

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β-FeOOH and α-Fe_2O_3 as ELECTROACTIVE MATERIALS FOR BIOSUPERCAPACITORS

Eva Paola Zamora Gutiérrez[1,2], Roxana Berlanga Pérez[1,2], Francisco Javier Mendoza Martínez[1,2] Emilio Antonio García Montes[1,2], Johanna García Montemayor, Javier Osvaldo Terán Carlín, Jorge Alexis Zúñiga Martínez[1,2], Raúl Lucio Porto[1,2,*]

[1] *Universidad Autónoma de Nuevo León, Facultad de Ingeniería Mecánica y Eléctrica, San Nicolás de los Garza, 66455, Nuevo León, México*
[2] *Universidad Autónoma de Nuevo León, Centro de Innovación, Investigación y Desarrollo en Ingeniería y Tecnología, Apodaca, 66600, Nuevo León, México*

**raul.lucioprt@uanl.edu.mx*

Biosupercapitors are a new alternative to supply energy to modern miniaturized implantable biomedical devices due to a higher power and energy density and longer life cycle than micro-batteries [1-3]. Storing large amounts of energy in a device with a reduced volume, with large energy and power density and with biocompatibility is a challenging task. The key parameter to develop biosupercapacitors is biocompatibility [4]. Thus, it is mandatory that the electroactive materials, electrolytes, additives, substrates and packing components shows biocompatibility. In this work, nanostructured β-FeOOH and α-Fe_2O_3 were prepared as a potential biocompatible electrode material for supercapacitors. The charge storage process was studied by cyclic voltammetry, charge-discharge cycles, and electrochemical impedance spectroscopy. The electrochemical study also includes the effect of several neutral, acidic, and alkaline electrolytes, that includes redox electrolytes. The highest specific capacitance observed for β-FeOOH and α-Fe_2O_3 were in redox electrolytes with 124 and 185 Fg^{-1} respectively. The capacitive behavior remains at the high scan rate of 50 mVs^{-1}. The cycling stability test shows a loss of specific capacitance lower than 10 percent after 5000 cycles.

Keywords: β-FeOOH, α-Fe_2O_3, Biosupercapacitors, Energy Storage.

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LAYERED VANADIUM PHOSPHATE WITH Cu IONS IN THE INTERLAYER SPACE: INDUCING FARADAIC BEHAVIOR

Jorge Alexis Zúñiga Martínez[1,2], Raúl Lucio Porto[1,2,*], Domingo Ixcoalt García Gutiérrez, Thierry Brousse[3]

[1] *Universidad Autónoma de Nuevo León, Facultad de Ingeniería Mecánica y Eléctrica, San Nicolás de los Garza, 66455, Nuevo León, México*

[2] *Universidad Autónoma de Nuevo León, Centro de Innovación, Investigación y Desarrollo en Ingeniería y Tecnología, Apodaca, 66600, Nuevo León, México*

[3] *Institut desMateriux Jean Rouxel (IMN), Université de Nantes, CNRS,44322 Nantes*

**raul.lucioprt@uanl.edu.mx*

Layered vanadium phosphate with Cu ions in the interlayer space were prepared to study their electrochemical behavior. The charge-discharge processes were studied in three electrolytes with alkaline pH (3M LiOH, 3M NaOH, and 3M KOH) revealing that the addition of Cu ions in the interlayer space strongly modify the electrochemical mechanisms compared to pristine layered vanadium phosphate [1,2], introducing new redox processes visible at cyclic voltammograms. The specific charge arising from the double layer, pseudocapacitive, and the ion intercalation processes are extracted through the entire applied potential window, revealing that the intercalation processes are present up to 500 mVs^{-1}. Additionally, the Step Potential Electrochemical Impedance Spectroscopy (SPEIS) analysis confirms that the percentage of intercalation depends on the applied potential. The fast faradaic reactions highlight the potential for developing new intercalation chemistries to further optimize the electrochemical performance and improve the cycling stability and charge-discharge rates of layered materials.

Keywords: Layered Vanadium Phosphate, Ion Intercalation, Energy Storage,

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