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Editorial



Carbon Conference (Madrid, 1-6 July 2018)

I would like to thank the members of the Spanish Coal Group for their excellent work at the CARBON 2018. The work of all the members of the Executive Committee, Local Organizing Committee and members of the Scientific Committees has made possible the success of our conference. Thank you very much to everyone. I am very proud of all of you. Moreover, I would like to thank all the participants for attending our conference and especially the authorities that assisted to the inauguration table, Mrs Menéndez, President of the Spanish National Research Council, Mrs Villegas, General Director of the Spanish State Research Agency, Mr Garesse, Rector of Universidad Autónoma de Madrid, Mr Carrasco, Vicepresident of Spanish Carbon Group and Program Committee Chair. Also other authorities like the presidents of the Local Organizing Committee, Mr. Gillarranz and Mr. Rodriguez, presidents of the Carbon associations, the vicepresidents of Spanish National Research Council and members of the Carbon community in general as well as our sponsors.

We were lucky enough to organize

Carbon 1994 in Granada, Andalusia, and Carbon 2003 in Oviedo, Asturias. This year we have brought the Carbon 2018, conference in Madrid the capital of the country.

Since the First Carbon meeting in 1953 in Buffalo USA, where only four papers were resented, the Carbon family has grown a lot and this week we will have the chance to attend more than 800 presentations. We have received 706 participants from 55 different countries of all continents, more than 200 being students.

The motto chosen for this edition was "Bonded by Carbon", which symbolized the organizers' desire that once again the carbon scientific community have found the opportunity to share knowledge and experiences in the conference and to build new collaborations.

Plenary lectures have been delivered by Research Prof. Menéndez, from the Spanish National Research Council, Prof. Cazorla from the University of Alicante, Prof. Gotgosi, from Drexel University, USA, Prof. Prato, Università di Trieste, Italy and Prof. Cheng from the Shenyang National Laboratory for Materials Science, China.

Prof. Menéndez talked about the “State of the art and future perspectives of traditional carbon materials and new carbon forms”. She has emphasizes the recent discovery of new carbon forms such as graphene presages a revolution in the field, although she has mentioned that this expected tendency is still only observed at a scientific level. An interesting and detailed discussion of the worldwide evolution at an industrial and scientific level of traditional carbon materials and the new carbon forms has been presented.

Professor Cazorla plenary focused on “The surface (electro) chemistry of carbon materials about the role of oxygen and nitrogen heteroatoms”. He has summarize all they have learnt about Surface Electrochemistry of carbon materials, focusing in O and N functionalities, paying special attention to: electrical conductivity, wettability, electroactivity and reactivity with the electrolyte and the solvent.

Professor Gotgosi talked about “Transformative synthesis of carbon based materials from graphene to nanotubes and Mxenes”. His plenary provided fundamental insights and describe approaches to realizing non-equilibrium carbon materials via solid state transformation of carbides. Examples of electrochemical energy storage applications were presented. Professor Prato plenary focused on the “Synthesis, Properties and Applications of functionalized Carbon Nanoforms”. He presented the organic functionalization of various types of nanocarbons, including carbon nanotubes, fullerenes and, more recently, graphene and carbon nanodots. The chemical functionalization represents an important and versatile tool for tuning the chemical and physical properties of carbon nanostructures (CNS).

Professor Cheng talked about the “Graphene Materials: Fabrication and Use in Electrochemical Energy Storage”. They have fabricated different types of graphene materials , such as graphene oxide (GO), reduced GO, graphene nanosheets, graphene films and single crystal domains, and 3D graphene networks, and from them they have prepared various graphene -based hybrid electrode materials by mechanical mixing, coating, hydrothermal deposition, and in-situ synthesis. These hybrid electrode materials showed desirable electrochemical properties in terms of long cycling life, good high rate capability, and high reversible capacity.

This conference has also included an awards ceremony, where the merit of our colleagues will be acknowledged by different associations. What's more 3 satellite courses have been organized. As well as that, the participants have the opportunity to present their communications to be published in one of the special issues of the journal: Carbon, Electrochimica Acta and Nanomaterials.

I hope our participants had experienced an unforgettable week in Madrid and we hope they had time to discuss and interact with one another, as well as to visit the city.



María Jesús Lázaro
President of the Spanish Group of Carbon
Chair of the Carbon 2018 Conference

Electrochemical Applications of Carbon Materials: a recent perspective from The World Conference on Carbons 2018

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Abstract

This article analyzes the contributions on the Electrochemical Applications Topic presented in the last World Conference on Carbon 2018. The subject and relative proportion of these contributions are proposed to be an objective indicator of worldwide current research activity in the field. Moreover, some of the new findings and trends on carbon materials for supercapacitors, batteries and fuel cells are discussed.

Resumen

El presente artículo analiza las contribuciones sobre “Electrochemical Applications Topic” de los materiales carbonosos presentadas en el último congreso mundial World Conference on Carbon 2018. Se propone utilizar la temática y proporción relativa de estas contribuciones como un indicador objetivo de la actividad investigadora actual en este campo. Además, se discuten algunos de los nuevos avances y tendencias sobre los materiales carbonosos en supercondensadores, baterías y pilas de combustible.

1. Introduction

Carbon materials represent a wide, unique, and one of the most versatile families of materials, exhibiting different allotropic forms, dimensionality, morphology-conformation-dimension, crystalline structure, porous texture, and surface chemistry. All these features make

carbon materials to display several extraordinary properties for multiple industrial applications and technologies. Consequently, research on the field of carbon materials generates significant interest in multidisciplinary fields.

At present, many indicators may be useful to describe the state of the art on carbon materials. For example, the number of scientists and research groups on carbon materials; markets of conventional as well as novel carbon materials; the annual number of articles and impact of journals related to carbon science, and so on. Moreover, national and international conferences may constitute exceptional thermometers of local or worldwide research activity in the field.

Since it was born in 1956, the World Conference on Carbon is an international conference of the highest authority in this field. This annual meeting, sequentially organized by the Asian, European and American Carbon Societies, gathers the rich and multidisciplinary community of scientists and technologists working on the preparation, characterization and study and application of carbon materials. Although the participation may be partly conditioned by geographical issues, the analysis of the communications presented in this meeting may provide an objective view of the state on the art on carbon materials research.

One of the exceptional properties of carbon materials is their electrical conductivity, which mainly arises

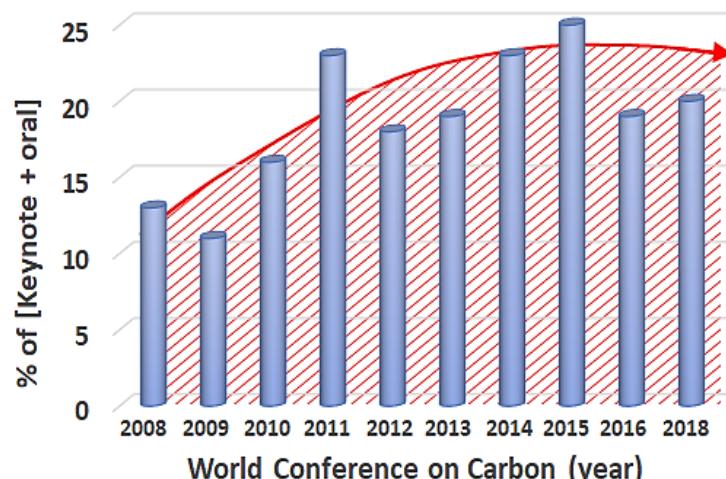


Figure 1. Evolution of the relative importance of the topic on “Electrochemical Applications”, expressed as the % of keynote+oral presentations on this topic, for the last 10 years of The World Conference on Carbon. *sometimes the Topic referred to as Energy storage and conversion, Energy, etc.; data of 2017 not available.

Figura 1. Evolución de la importancia relativa de la temática de “aplicaciones electroquímicas”, expresada como % de presentaciones tipo keynotes+orales sobre esta temática, durante los últimos 10 años en el congreso mundial de los materiales carbonosos. *adquiriendo en ocasiones otros nombres, como Almacenamiento y conversión de energía, Energía, etc.; datos del año 2017 no disponibles.

from the delocalized π electrons in condensed aromatic rings, as well as their dimensions, order and/or crystalline assembly. This and other characteristics, together with a variable electrochemical activity for different processes and reactions, make carbon materials exceptional candidates to be used as electrodes, electrocatalysts or electrocatalysts supports in multiple electrochemical applications.

The present and potential impact of electrochemical applications of carbon materials may be incalculable. From the scientific point of view, in the last 10 years the relative importance of the topic on "Electrochemical Applications" within The World Conference on Carbon has significantly grown and seems to stabilize (Figure 1). During this period (2008-2018), it has been considered the most, second most and third most relevant topic (in number or % of keynote + oral communications) in The World Conference on Carbon on 4, 4 and 1 occasions, respectively; thus, remarkably beating the other most important topics of this conference, such as nanocarbons, graphene or porous carbons. This work analyzes the contributions related to the Electrochemical Applications Topic presented in the last World Conference on Carbon 2018 in Madrid.

2. Electrochemical applications Topic in The World Conference on Carbon 2018

Last July 2018, the World Conference on Carbon was held in Madrid. As it can be observed in Figure 2A,

the topic on "Electrochemical applications" was the major among the different types of communications, i.e. keynote, oral and poster communications. In fact, even two sessions of oral communications on this topic were simultaneously carried out in different rooms.

Among the different subjects on this topic, energy storage on supercapacitors (SCs) clearly prevailed, followed by energy storage in batteries (BATTs) and energy conversion in fuel cells (FCs) (Figure 2B). It is worthy to mention that one of the keynotes was dedicated to SCs and BATTs, and another to electrocatalysis in FCs and CO_2 electroreduction, so they have been accounted as 0.5 in the figure. Details on the research of these 3 main applications are provided below (sections 3-5).

Other electrochemical applications of carbon materials arise also great interest (Figure 2B). The utilization of carbon materials in electrochemical (bio)sensors or as support of different electrocatalysts are among the most establish ones. Particularly, the electro-reduction of CO_2 is currently on the rise, so part of the keynote lecture of Prof. Bandosz (see section 5) was related to the influence of nanopores to syngas and CH_4 formation. Other interesting topics deal with the use of electrochemical techniques to process carbon materials, like the electrochemical exfoliation of graphite or the electrochemical functionalization of carbon surfaces.

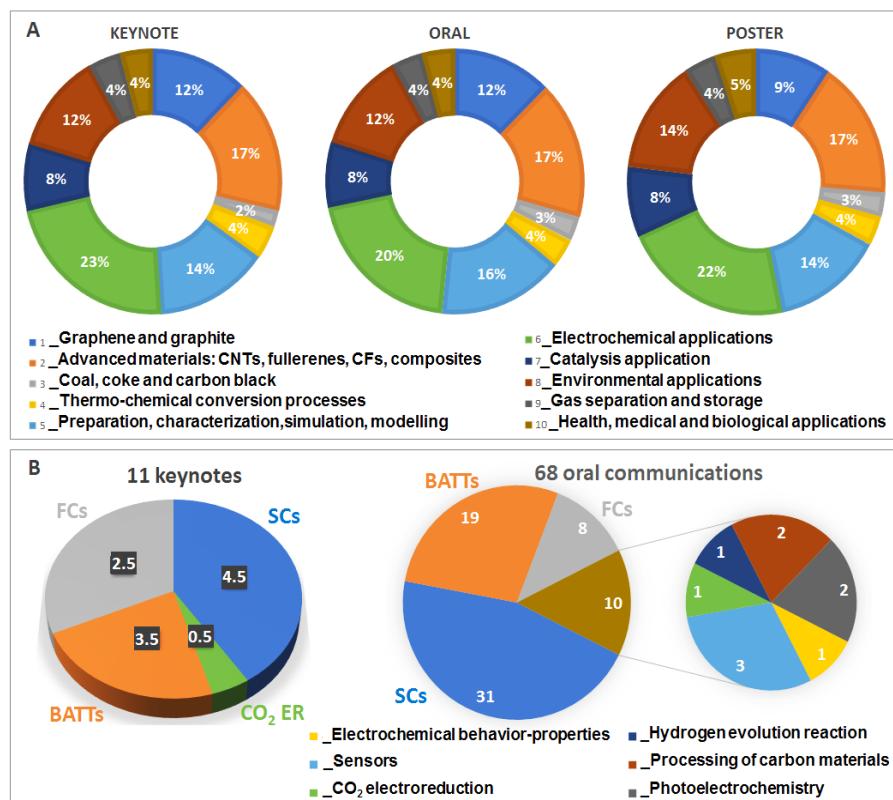


Figure 2. Distribution of (A) the different topics (%) and (B) the different electrochemical applications (number) within keynote-, oral- and poster-type communications in The World Conference on Carbon 2018.

Figura 2. Distribución de (A) las diferentes temáticas (%) y (B) las diferentes aplicaciones electroquímicas (número) en las comunicaciones tipo keynote, oral y póster en el congreso mundial de los materiales carbonosos 2018.

3. Research on Supercapacitors

The increase in energy density without compromising durability is one of the most challenging and hottest topics on SCs research. Significantly, the 4 keynote communications related to SCs in CARBON 2018 were devoted to this. Prof. Frackowiak (*Poznan University of Technology*) presented the latest results of her group on novel approaches for extending the capacitor voltage in aqueous electrolytes, including (i) the use of neutral electrolytes (sulfates, nitrates, iodides, etc.); (ii) selection of two different electrolytes (different pH) for positive and negative electrodes; and (iii) modifying the pH of positive and negative electrodes by ammonia treatment of carbon surfaces. Through these strategies, operating voltages of up to 1.8 V can be reached.

Major attention was paid into the study on ageing mechanisms of SC carbon electrodes, a topic that was the subject of two keynotes and part of the other two. Prof. Shiraiishi (*Gumma University*) presented the last results on the durability and degradation mechanism of seamless AC electrodes in organic medium. Post mortem analysis of these electrodes indicated that the deposition of electrolyte decomposition products is the cause of the capacitance decline upon cycling at high voltage. On the other hand, the keynotes of Prof. Beguin (*Poznan University of Technology*) faced the study of this mechanism by electrochemical on-line (in-situ) mass spectroscopy, enabling to monitor the release of gases during operation. It was concluded that the ageing mechanism of electrodes strongly

depends on the carbon material and the electrolyte type.

Nevertheless, the most represented subject on SCs (22 % of communications) tackled the preparation and study of nitrogen-doped carbon materials. N-functionalities have been proved to increase the pseudocapacitance, electrical conductivity or electrochemical stability of electrodes in these devices. In another keynote, Ms. M.J. Mostazo-López presented the collaborative research between the groups of Profs. Morallón and Cazorla-Amorós (both from *University of Alicante*) with Prof. Balducci (*CEEC, Jena*) that demonstrated the positive effect of these N-functionalities on the durability of high surface area (capacitance) AC in non-conventional electrolytes with large operation voltage, like Pyr14BF₄/PC and Pyr14TFSI/PC.

On the other hand, other relevant research topics on SCs are the preparation and electrochemical characterization of novel electrode materials from biomass (21 % of communications) and composites (11 % of communications); or the study of ion adsorption on nanopores during charge/discharge (15 % of communications). Related to this last topic, it can be stressed the research on carbide-derived carbon materials, and the benefits of N-doping when used in ionic liquid (EMIM-BF₄), presented in a keynote by the group of Prof. Presser (*Saarland University*); and the new findings on the anomalous co-ion association of ionic liquids in carbon nanopores.

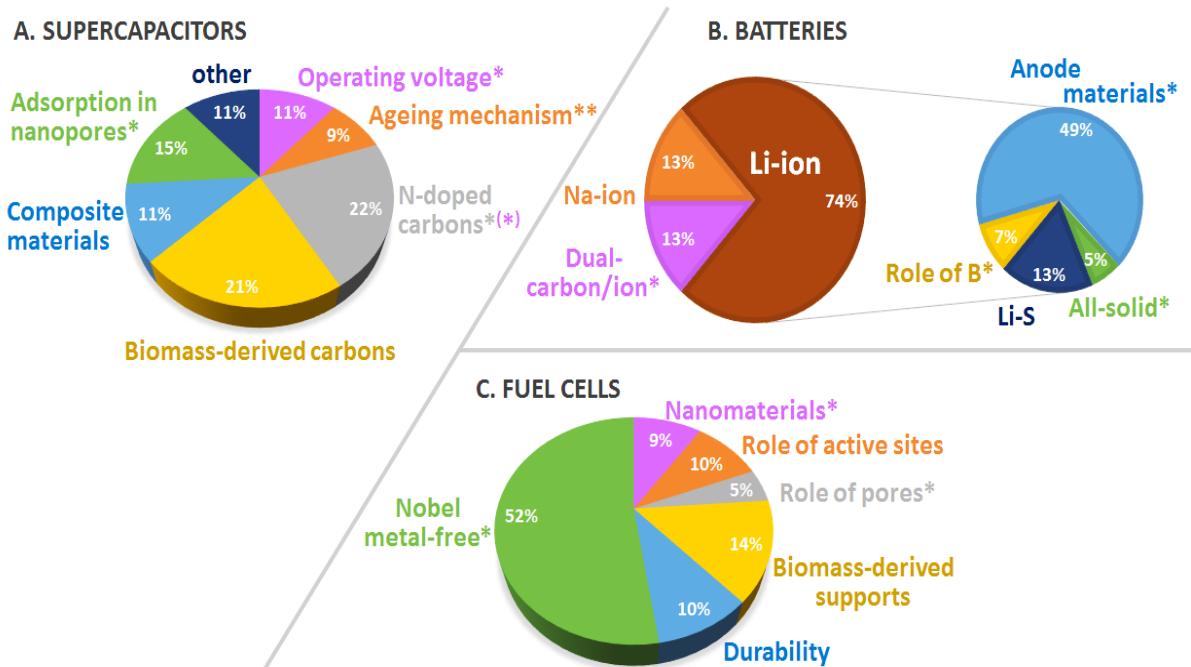


Figure 3. Distribution of different research subjects (%) among the keynote + oral communications on supercapacitors (A), batteries (B) and fuel cells (C) in The World Conference on Carbon 2018. Asterisks refer to keynote presentations, which may involve one or two different research subjects.

Figura 3. Distribución de diferentes temas de investigación (%) en las comunicaciones tipo keynote y orales sobre supercondensadores (A), baterías (B) y pilas de combustible (C) en el congreso mundial de los materiales carbonosos 2018. Los asteriscos hacen referencia a presentaciones tipo keynote, que pueden abarcar uno o dos temas de investigación distintos.

4. Research on Batteries

Regarding the application of carbon materials in batteries (Figure 3B), most research (ca. 75 %) is related to lithium-ion batteries (LIBs), which currently constitute the state-of-the-art technology for various small-scale and large-scale applications. Within this field, the design and study of new anode materials is the major focus of research (49 %). In their keynote presentation, the group of Prof. Presser showed the performance of silicon oxycarbides (SiOC) as anode material for LIBs, exhibiting high capacities (up to 922 mAh/g) and capacity retentions (83% after 100 cycles). In another keynote, Prof. Kawaguchi (Osaka Electro-Communication University) presented recent results on the electrochemical intercalation of Li into B-doped carbon materials. Different techniques reveal an interaction between intercalated Li ions and B atom, so these materials can show higher reversible capacity (up to 540 mAh/g) and the higher rate capability than commercially available graphite. Moreover, advanced LIB technologies always receive great expectation. In a keynote communication, the group of Prof. Moriguchi (Nagasaki University) analyzed the charge/discharge properties of SnO₂-embedded nanoporous carbons in all-solid-state LIBs. Other works were dedicated to the lithium sulfur (Li-S) battery systems, using novel carbon-sulfur based cathode materials, which potentially offer significant advantages over metal oxides-based LIBs for high-energy density storage devices.

On the other hand, the conference witnessed the growing interest in alternative battery technologies with advantages in terms of cost and sustainability, such as Na-ion batteries and the so-called dual-ion or dual-carbon batteries (with 13 % of communications both). In the case of Na-ion batteries, most work is devoted to the study of anode materials, e.g. hard carbons. Respect to dual-ion or dual-carbon batteries, the group of Prof. Winter (University of Münster) presented an overview on the promises, challenges and limitations of this technology. Besides, in a keynote communication, they analyzed the effect of the graphitization degree of non-graphitic and graphitic carbons on their anion uptake capability as cathodes for dual-ion batteries. It has been found that the specific discharge (de-intercalation) capacity remarkably increases with the degree of graphitization.

5. Research on Fuel Cells

CARBON 2018 compiled an outstanding progress on fundamental-mechanistic aspects for the Oxygen Reduction Reaction (ORR) catalyzed by carbon materials. Thus, two keynotes and one oral communications were dedicated to study and discuss the role of pores, N-doping and active sites, respectively, on the ORR performance.

Prof. Bandosz (*The City College of New York*) emphasized the role of nanopores in the ORR for carbon free of heteroatoms and metals. The onset potential of the ORR was found to depend on the

size of ultramicropores. An enhancement in the ORR performance owing to adsorption forces in small pores was concluded and the involved mechanisms were discussed.

Dr. D. Sebastián presented the advances of the group of Prof. Lázaro (*Instituto de Carboquímica*) on noble metal-free electrocatalysts based on N-doped carbon. They effect of N content on the ORR activity of metal-free or M (Co or Ti)-doped reduced graphene oxide (rGO) was analyzed. An optimum nitrogen doping of ca. 10 wt.% was found, and the presence of transition metals (Co and Ti) synergistically contributed to the positive shift of potential for ORR.

A systematic study on the influence of active sites on a wide range of different metal- and heteroatoms-free carbon materials was presented by Dr. A. Gabe from the groups of Profs. Morallón and Cazorla-Amorós (*University of Alicante*). A linear relationship between ORR activity and carbon-oxygen gasification reactivity was found, emphasizing the effect of the active surface area (ASA).

Apart from the significance of these fundamental works, most communications in the field of fuel cells were focused on the preparation and characterization of novel ORR electrocatalysts (Fig. 3C), highlighting metal noble-free and N-doped carbons (with 52 % of communications) and the development of simpler synthetic methods and/or by using more sustainable carbon precursors (14 % of communications). Moreover, a keynote by Prof. Mingbo Wu (*China University of Petroleum*) was related to the electrocatalytic performance of petroleum coke-based carbon nanomaterials.

6. Conclusions

The analysis of the contributions on *Electrochemical Applications Topic* presented in the last World Conference on Carbon 2018 indicates that: (i) the increase in energy density through different strategies, highlighting the use of N-doped carbons, the analysis of ageing mechanisms and the development of biomass-derived carbon electrodes prevail in SCs research; (ii) the design and study of new anode materials for LIBs dominates the research on batteries, while emerging Na-ion and dual-ion or dual-carbon technologies present promising perspectives to solve some of the problems associated to LIBs; (iii) related to FCs, the understanding of the role of pores, N-doping and active sites on the ORR performance of carbon materials has been greatly progressed.

Catalytic applications of Carbons, main issues discussed during The World Conference on Carbon 2018

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Carbon Materials found many interesting applications in catalysis and subsequently there were many papers that were discussed in this topic during the Carbon 2018 conference, including 4 keynotes, 27 oral and 38 poster presentations, a total of 69 papers. The first keynote was given by Juan Matos, from University of Concepción, to show the advances in the production of solar fuels using efficient carbon-based photocatalysts. The second one, by Akira Takatsuki, described the use of oxidized carbon powder as catalysts for the hydrolysis of cellulose, that constitute a promising method for the selective conversion of cellulose to glucose. Zhao Quingshan presented the third keynote lecture, in which it was presented a novel nitrogen-doped porous carbon supported Pd nanoparticles as an efficient catalyst for C-N allylation coupling reactions. In this work, the porous carbon material was prepared by a hard template-oriented method and using inexpensive petroleum asphalt as raw material, and urea as nitrogen source. It was shown how the N-doped carbon material induced a uniform dispersion of Pd catalysts and adjust the electronic environment of the catalytic sites. The fourth keynote was given by Diego Garcés, and described the use of carbon materials as co-catalysts and as catalytic supports for biomass upgrading processes, considering the route of cellulose to biogenic aldehydes with further transformation of those aldehydes into long chain hydrocarbons and chemicals via aldol condensation and hydrogenation. The use of the carbon materials as co-catalysts enhanced the mass transfer of the aldehydes from aqueous to organic phase improving reaction rates and limiting further transformation of the aldehydes into humics. Carbon based supports such as carbon nanofiber of high surface area graphites improved the performance of the catalysis during the aldol condensation step. This better performance was explained in terms of a more appropriate basic sites distribution and in the interaction of the reactants with the carbon surface.

Some of the oral presentations were on the use of carbon materials as catalysts for the oxygen reduction reaction (ORR), since the use of carbon cathode catalysts in polymer electrolyte fuel cells instead of the present platinum catalysts is attracting increasing interest. In this sense, several presentations described promising results with the use of nitrogen containing carbon materials containing transition metal-nitrogen coordination structures (M-N-C materials), including CNTs and graphenes. Another important issue that covered by some of the oral presentations was the photocatalytic processes. The use of carbon materials as additives to semiconductors has been proven as an effective strategy for enhancing the photocatalytic performance of the semiconductor with the resulting hybrid semiconductor/carbon material typically

displaying an enhanced catalytic performance under sunlight. During the conference, papers on the use of graphene oxide on photocatalytic water splitting was presented, as well as an ecotoxicity risk assessment for the photodegradation of synthetic and industrial wastewater using TiO₂ and TiO₂/carbon photocatalysts. Also a presentation described the use of Cu/carbon spheres as catalyst for the CO₂ photo electrochemical reduction. Another group of papers described the use of carbon materials as catalysts for different biomass waste upgrading processes, such as sugar hydrogenation on Ru supported carbons, dehydrogenation of alkanes on nanostructured carbons, hydrolysis of biomass on modified carbon xerogels, or cellulose conversion into sugars. In this sense, also presentations focused on the preparation of catalytic materials from waste valorization such as Pd catalysts supported on activated carbons from lignin. As well as these oral presentations, the 38 posters also focused in this main topics (electrochemical and photochemical catalytic applications of carbon materials and on the upgrading of biomass waste). Also some of them focused on the synthesis of carbon materials with acid properties for esterification and condensation reactions, as well as alcohol decomposition.

Thus, all these papers showed the potential of carbon materials as catalysts, catalytic supports and as co-catalysts in some of the most important catalytic processes that have to be developed during the next years in order to cover the energy, environment, and sustainable issues that the humanity should face. The papers presented during the Carbon Conference have shown how these versatile materials found hundreds of applications in electrochemistry and in photocatalysis, as well as other classical applications, such as acid-based catalysts, that are also important for waste valorization.

Graphene and Graphite main discussions during The World Conference on Carbon 2018

Isabel Suelves. *Instituto de Carboquímica (ICB)*

The communications included in this topic dealt with aspects related to the preparation, modification, characterization and properties of both graphene and graphite, but also included works about some applications of these materials in different fields like, conversion and storage of energy, catalysis, medicine or biology, among others.

From the 89 works finally presented in this topic, 42 were presented in Tuesday's Poster Session and 47 as Oral Communications, in six sessions that took place from Tuesday to Friday. The Oral sessions were chaired by: Dr. Nidia C. Gallego from Oak Ridge National Laboratory (USA), Prof. Javier Narciso Romero from Alicante University (Spain), Prof. Milo Shaffer from Imperial College London (UK), Prof. Manuel J. Pérez-Mendoza from Granada University (Spain), Prof. Mauricio Terrones from Penn State University (USA), Dr. Wolfgang Maser from ICB-CSIC (Spain), Dr. Indrek Kulaots from Brown University(USA) and Dr. Luiz Depine de Castro President of the Brazilian Carbon Association.

Among the oral presentations, the following ones were selected as keynotes:

- “Rosin-mediated ultraclean transfer of graphene and related two dimensional materials” presented by Jinhong Du from the Institute of Metal Research, Chinese Academy of Science (China).
- “Doped graphene: synthesis and superior molecular sensing” presented by Mauricio Terrones from Penn State University (USA).
- “Just add water and table salt: new perspectives on the electrochemical exfoliation of high quality graphene” presented by José María Munuera Fernández from INCAR-CSIC (Spain).
- “Graphitization of activated carbon obtained from local biomass (babassu) and their electrochemical properties” presented by Bartolomeu Cruz Viana Neto from Universidad Federal de Piauí (Brasil).
- “Nanographenes by solvent-free syntheses - the mechanochemical Scholl reaction” presented by Sven Grätz from the Technische Universität of Dresden (Germany).
- “Carbon-coupled plasmonic sensors: from quantum coupling to subwavelength resonant strain sensors” presented by Morteza Aramesh from ETH-Zurich (Switzerland).

Some of the works presented in this topic are being included in the Special Issue “Graphite, Graphene, Advanced Carbon Materials and Nanostructured Carbon-Based Composites and Selected Papers from Carbon 2018” of Nanomaterials (MDPI Journal).

Scientists from more than 20 countries, belonging to over 50 different Universities and Research Institutions, showed their work in the different topic sessions. Thanks to the great effort of all participants, chairpersons and speakers involved in oral and poster sessions, very interesting discussions were held throughout the week on the latest research being developed on graphene and graphite.

Carbon 2018, Topic 9: Gas separation and storage

Materiales de carbón para la separación y almacenamiento de gases

Fabián Suárez García. Instituto Nacional del Carbón (CSIC)

En el Topic 9 se agruparon aquellos trabajos sobre la utilización de distintos materiales de carbono para la separación y el almacenamiento de gases. A pesar de que en esta temática se agrupan algunas de las aplicaciones más relevantes para los materiales carbonosos porosos y que están siendo objeto de una intensa investigación, tan solo 34 trabajos seleccionaron este Topic. De todos estos excelentes trabajos, 15 se presentaron como orales, de los cuales 2 fueron seleccionados como Keynote por el Comité Científico. Los trabajos mostraron los últimos avances en la separación y purificación de gases, en el almacenamiento de hidrógeno y metano y en la captura de CO₂. Dentro de este Topic, un importante número de trabajos abordaron el efecto del vapor agua en la separación y almacenamiento de otros gases de interés, poniendo de relevancia la

importancia de determinar la capacidad de adsorción de agua por los materiales porosos, ya que este vapor está presente en muchas de las corrientes gaseosas a tratar. Así, la Keynote titulada "The state of water adsorbed in carbon nanopores" y presentada por la Profesora Krisztina Lázló de la Universidad de Budapest, Hungría, mostró el efecto del tamaño de poro y de la química superficial en el mecanismo de adsorción del vapor de agua. La otra keynote seleccionada: "Highly selective adsorptivities of porous carbons for water and oxygen isotopes" fue presentada por el Profesor Katsumi Kaneko de la Universidad de Shinshu, Japón. En esta ponencia, se mostró la capacidad de los carbones porosos para la adsorción selectiva de unas formas isotópicas sobre otras. Esto permite la separación y concentración de isótopos de gran interés, como ¹⁸O₂.

Carbon for health, medical and biological applications

Reseña de los trabajos presentados en Carbon 2018, Topic 10

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El topic 10 contó con un total de 40 contribuciones, de muy diversas nacionalidades de Asia, Europa y América, y de gran interés y relevancia científica en el campo de la síntesis y el desarrollo de diferentes materiales de carbono, como carbones activados, nanofibras y nanotubos, materiales compuestos, fulerenos, grafenos y sus derivados y "carbon nanodots", para su aplicación en ingeniería de tejidos, biosensores y sistemas bioelectrónicos para la detección de compuestos biológicos, sistemas de hemoperfusión extracorpóreos, etc. Casi la mitad de estas contribuciones, el 43%, se presentaron en forma de presentación oral, repartidas en distintas sesiones orales del jueves 5 y viernes 6 de julio y el resto en forma de cartel, en la Sesión de Posters del miércoles 4 de julio. Entre ellas, caben destacar las 2 conferencias invitadas (keynotes) que impartieron el Dr. Volodymyr Kuzmenko, de la Universidad Tecnológica de Chalmer, sobre la aplicación en ingeniería de tejidos de tintas viscosas conductoras imprimibles en 3D para la proliferación de redes de crecimiento de células neuronales preparadas a partir de nanotubos de carbono y celulosa nanofibrilada, y el profesor Sergey Mikhalovsky, de la Universidad de Brighton, sobre la aplicación en sistemas de hemoperfusión extracorpórea para la eliminación selectiva de compuestos relacionados con problemas de sepsis de materiales compuestos basados en grafeno que permiten la adsorción rápida de citoquinas pro-inflamatorias.

No podemos olvidar la extraordinaria conferencia plenaria que el profesor Maurizio Prato, de la Universidad de Trieste y del CIC BiomaGUNE, impartió el viernes 6 de julio en el marco de este Topic 10 y que estuvo dedicada a la síntesis, propiedades y aplicaciones de nanoformas de carbono funcionalizadas, en la que destacó el proceso de síntesis de "carbon nanodots" dopados con nitrógeno, de tamaño extremadamente reducido, con rendimientos cuánticos de fluorescencia muy altos y con una elevada capacidad de ser funcionalizados debido a la gran abundancia de grupos amino. Otra parte importante de esta charla estuvo centrada en las interacciones de estas nanoestructuras de carbono con las células y tejidos biológicos (sistema inmune, sistema nervioso y barreras biológicas) y en sus aplicaciones biológicas.

Carbon 2018, Topic 2: Advanced Carbon Materials

Resumen de los trabajos presentados durante Carbon 2018

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Francisco Javier Narciso Romero. *Universidad de Alicante*

Ignacio Martín Gullón. *Universidad de Alicante*

Topic_02, Advanced Carbon Materials, compiled all those communications received within the topic of nanomaterials (nanotubes, nanofibers, etc.), fullerenes, carbon fibers or carbon composite materials, among others. 148 contributions were presented from Monday to Thursday: 8 keynotes, 56 oral communications and 84 in the form of poster. These communications represented a total of 27 countries, being China, Korea, Japan and Spain, with 21, 16, 16 and 13 contributions, respectively, the most representative countries. By continents, Asia with 68 and Europe with 53, were the most represented. These contributions ranged from fundamental aspects to theoretical developments, combining from classic materials, such as carbon fibers, which seem to revive a new apogee, to latest generation of materials with nanometric and highly hierarchical structures. The 8 keynotes dealt with very different matters: the use of some solid polymers to be directly transformed into carbon nanotubes by plain heat-treatment; a new approach to nanotube processing based on reductive charging to form pure nanotubides which can be easily

purified or optionally functionalized; routes to obtain carbon fiber reinforced thermoplastics with extremely high mechanical properties, good thermal stability and good recyclability for automotive application; optimization of the spinning process parameters (e.g., mass and energy transfer, phase changes or fluid flow behavior) for the production of carbon nanotube fibers; experimental verification, using flow visualization techniques, of the flow circulation at inlet and outlet of horizontal quartz tube reactors; chirality effects in the structure of nanotubes grown according to shape and solid-state nature of nanoparticles "sides"; preparation and characterization of lignin-derived carbon fibers produced by electrospinning and study of their potential application in adsorption, catalytical and electrochemical processes; and findings about the effects of fiber length distribution in chopped rayon fibers at different stages of processing and also some insights into melt, flow and cure behavior of phenolic resin obtained from implementation of several advanced techniques.

Thermo-Chemical Conversion Process, papers on The World Conference on Carbon 2018

Francisco Carrasco. *Universidad de Granada*

The communications included in this topic dealt with all the thermo-chemical conversion processes (combustion, gasification, pyrolysis, torrefaction) for converting carbon-containing fuels into another more valuable products including carbon materials, fuel gas and chemicals. The topic covered different aspects going from the optimization of the conversion process itself, to the kinetic determination and process modelling, the characterization of the final products and the environmental aspects related with the processes.

The topic included 13 oral communications and 16 posters, and was divided in two sessions chaired by Prof. Diego Cazorla from the University of Alicante (Spain), Dr. Francisco García-Labiano from CSIC (Spain), and Dra. Carmen Clemente from the Technical University of Madrid (Spain). Scientists from 15 countries were represented in this topic.

Among the oral presentations, the following ones were selected as keynotes:

- “CO₂ capture by chemical looping processes using c-fuels” presented by Francisco García Labiano from the Consejo Superior de Investigaciones Científicas, CSIC (Spain).
- “Modelling cellulose conversion to kerogene: a pathway of reversible rare events” presented by

Pierre-Louis Valdenaire from the Massachusetts Institute of Technology, MIT (USA).

Although this topic represents a small niche within the usual CARBON conference researchers, the organizing committee wanted to include here the most relevant research related with the different thermo-chemical processes and the new tendencies in this area. Considering the interest awakened by the assistants and relevance of the works there presented, the result can be considered satisfactory.

Aplicaciones Medioambientales de los materiales de carbono, resumen de los trabajo presentados durante el World Conference on Carbon 2018

Tomás Cordero. Universidad de Málaga

El Topic 8 del congreso trató sobre las aplicaciones medioambientales de los materiales de carbono. Entre los temas tratados destacaban aquellos dedicados a la adsorción en fase gas y acuosa, la oxidación húmeda de contaminantes, la fotocatálisis y la preparación de materiales carbonosos mediante procesos y materias primas sostenibles.

Las intervenciones orales se agruparon en las mañanas de los días 3 a 6 de Julio y en la tarde de los días 3 y 4 de Julio, siendo presentadas en la sala 3. Se presentaron 55 intervenciones orales acompañadas por 6 keynotes sobre la preparación de materiales carbonosos magnéticos para oxidación húmeda catalítica, fotocatalizadores híbridos para la eliminación de contaminantes en fase líquida, nanocomuestos de carbón mineral para la adsorción de mercurio de las aguas residuales, las novedades en la preparación de fibras carbono a partir de poliacrilonitrilo, síntesis de materiales carbonosos a partir de las lejías negras del proceso kraft y la síntesis de carbonos nanoporosos usando líquidos iónicos para preparar la adsorción de contaminantes emergentes.

En la sesión de pósters se presentaron más de 80 contribuciones, las cuales estuvieron expuestas el 4 de Julio. Los asistentes pudieron discutir los resultados con los autores de las contribuciones en la sesión de pósters desde las 5 a las 7 de la tarde.

KEYNOTES

- Rui Ribeiro
- Ana Amorós-P
- Sergey Mikhalovsky
- Masaaki Yoshikawa
- Luis Felipe Chazaro-Ruiz
- Ana Sofía Mestre

CHAIRS de las distintas sesiones:

- Juan Matos
- Vanessa Fierro
- René Rangel
- Ma Teresa Izquierdo
- Andrzej Kotarba
- Semih Eser

Award Ceremony at Carbon 2018

M. Victoria Martínez Huerta. Instituto de Catálisis y Petroleoquímico (ICP). mmartinez@icp.csic.es

During Award Ceremony at The Word Conference on Carbon 2018, a series of awards to researchers, who have contributed significantly to the scientific and technological advances in carbon in recent years, were presented. The ceremony was presided over by the chair of the Spanish Carbon Group (GEC), Dr. Maria Jesus Lazaro Elorri, and accompanied by Prof. Malcom Heggies to present the Brian Kelly Award, Prof. Alain Penicaud of the Francophone Carbone Society (SFEC) to present the Young Researcher Award and Dr. Mauricio Terrones to present the Carbon Journal Prizes.

European Carbon Association (ECA) Award

The European Carbon Association (ECA) Award, created in 2009, recognises a significant contribution to the European carbon science community carried-out by a scientist from around world, or a remarkable service to the worldwide carbon community carried-out by a scientist from Europe. The award is made on the recommendation of the ECA Award Committee and seeks to honour "Remarkable service to the carbon science community". This year seven persons have been nominated and the European Carbon Association has decided to honour Professor François Béguin with the ECA Award 2018.

Prof. Béguin is a person world-wide known to the

carbon community, especially those dealing with carbons for the application in energy conversion/storage and environment protection. He is the author of 300 original papers published in high rank international journals and several review articles or book chapters, as well as co-editor of relevant books dealing with energy storage and conversion systems using carbon materials. The professional career of Prof. Béguin was related for many years to the Centre de Recherche sur la Matière Divisée, CNRS-Université d'Orléans. As a leader of carbon research group and the Director of CRMD he strongly contributed to the creation there the laboratory which was opened to students and researchers from different countries. Since 2011 he has shared his knowledge and experience in the field of carbons for energy conversion/storage systems amongst students and postdocs at the Poznan University of Technology (Poland). Professor Béguin has served for several years to the carbon society the chair of the French Carbon Group, acting actively for the sake of ECA. In 2005 he launched a series of very successful conferences on Carbon for Energy Storage and Environment Protection (CESEP). All in all Prof. Béguin is a dedicated professional and he has offered a lot the Carbon community.

Dr. M^a Jesús Lázaro Elorri gave the diploma to Professor François Béguin, who then proceeded to give a short talk about his excellent scientific contribution to the carbon community.

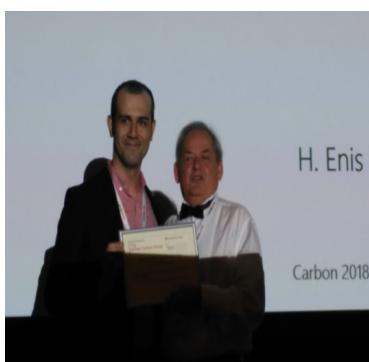


Brian Kelly Prize (British Carbon group)

This annual award was established in 1996 by the British Carbon Group in memory of Brian Kelly, who was a world authority both on the physics of graphite and on irradiation damage in solids. Brian Kelly was born and educated in Wales and spent most of his career working for the United Kingdom Atomic Energy Authority, UKAEA.

The award is intended as a travel grant for students and early career researchers with up to ten years postdoctoral experience to attend the annual World Carbon Conference. This year the Award Committee of the British Carbon Group has nominated Dr. H. Enis Karahan with his paper on "Factors influencing the antibacterial activity of graphene oxide beyond materials physicochemistry". Dr. Karahan works at the Nanyang Environment and Water Research Institute in Nanyang Technological University. He does research in Carbon Materials, Molecular Assemblies, Colloids & Surfaces, and Nano-Bio Interfaces including Antimicrobial Nanotechnologies.

The award was given by Professor Malcom Heggie. Dr. Karahan then proceeded to give a short talk about his research work.



Francophone Carbone Society (SFEC) Young Researcher Award

This award recognises significant contributions to carbon science or carbon technology made by a "young", non-tenured, scientist or engineer, regardless of his/her country of origin and citizenship, when this work has been conducted in a laboratory from a country whose official language is French, or

by a citizen from a country whose official language is French and whose awarded work has been carried-out anywhere in the world. The laboratory may be academic and public, or from a private company.

This year the SFEC Award Committee has nominated Dr. Alicia Gomis Berenguer. She incorporated as PhD fellow to INCAR-CSIC (Oviedo, Spain) in 2013 where he developed research activities related to exploring the photochemical activity of nanoporous carbons for energy conversion and environmental remediation. After obtained her PhD in 2016, she joined as post-doctoral researcher to POR2E group in CEMHTI-CNRS (Orléans, France) where she develops work focused on optimizing the nanoporous carbon layout in a controlled way to achieve stable carbon photocatalyst and photoelectrodes with high efficiency for solar energy conversion.

The award was given by Dr. Alain Penicaud. Dr. Gomis then proceeded to give a short talk about her scientific career.



Carbon Journal Prize

The journal Carbon and its publisher Elsevier are awarding the Carbon Journal Prize, given for "an outstanding Ph.D. thesis in carbon material science and technology". The selection was made based on the quality and importance of the Ph.D. research, and preference also was given to thesis research that had led to at least one publication in the journal Carbon.

The winner of the Carbon Journal Prize for 2018 is Dr. Md Julker Nine. The committee has also recognised Dr. Nithya Subramanian, Dr. Youfeng Zhang, and Dr. José Francisco Vivo Vilches for a second-place in the international 2018 Carbon Journal Prize competition.



Dr. Mauricio Terrones gave the award to Dr. José Francisco Vivo Vilches, who was the only prize-winner to attend the congress. Dr. Vivo then proceeded to give a short talk about his research work.

Student Prize: Nitrogen doped activated carbons as electrocatalysts for the oxygen reduction reaction

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Introduction

One of the main challenges for the development of fuel cells is the generation of new catalysts for the oxygen reduction reaction (ORR) that takes place in the cathode. The most common materials are based on platinum and other noble metals, but they show drawbacks, such as their high cost, low availability and vulnerability to CO-poisoning, that strongly affects the durability of the device. An alternative to the current state-of-the-art catalysts is the use of metal-free carbon materials doped with different heteroatoms, such as nitrogen, since its presence can modify the electron-donor properties of the carbon and provide a redistribution of electronic density, producing an increase of the electrocatalytic activity for the ORR. However, the role of the different nitrogen functional groups is not still well understood.

In this work, N-doped activated carbons have been prepared by chemical polymerization of aniline over activated carbons with well-developed microporosity followed by thermal post-treatments of the polyaniline/activated carbon composites at different temperatures. The role of surface chemistry on their electroactivity towards ORR has been extensively studied.

Materials and Methods

Activated carbon (AC) was produced by chemical activation of anthracite with KOH as activating agent (4:1 ratio) at 750°C for 2 hours. PANI/AC composite was prepared by chemical polymerisation of aniline (70mM) with ammonium persulfate solution in 1M HCl. The obtained PANI/AC composite was submitted to thermal treatments at a heating rate of 5°C/min up to 600 and 800 °C under N₂ atmosphere (200mL/min, 1h) to produce N-doped activated carbons, named as N-AC_600 and N-AC_800. Porous texture of the samples was characterized by N₂ adsorption/desorption at -196 °C. XPS analyses were performed in a VG-Microtech Multilab 3000 spectrometer (Al anode). TPD experiments were carried in a TGA-DSC instrument (TA Instruments, SDT Q600 Simultaneous) coupled to a mass spectrometer (Thermostar, Balzers, BSC 200).

The electroactivity of the materials for the ORR was evaluated by using a rotating-disk electrode, equipped with a glassy carbon disk (5.61 mm diameter) and a platinum ring electrode, in alkaline electrolyte (0.1 M KOH). A platinum wire was used as counter electrode and a reversible hydrogen electrode (RHE) immersed in the same electrolyte as reference electrode. The

catalyst was deposited on the glassy carbon disk by using a dispersion of each carbon material in ethanol and Nafion. The materials were characterized by linear sweep voltammetry in O₂ saturated 0.1 M KOH electrolyte at different rotation rates (400 – 2025 rpm) and at a scan rate of 5mV/s. The potential of the ring electrode was kept constant at 1.5 V (vs RHE) during all measurements.

Results and Discussion

Table 1 summarizes the main physicochemical properties related to the surface chemistry and porous texture of the samples. The polymerization of aniline over AC produces the attachment of nitrogen (mainly amines) and oxygen functionalities (CO and CO₂ evolving groups), as well as a decrease of the apparent surface area and micropore volume. The thermal treatments produce the decrease of nitrogen and oxygen groups due to the elimination of surface functionalities. Moreover, the nitrogen groups in the PANI/AC composite are selectively converted into pyridones/pyrroles and pyridines (Figure 1a) as consequence of carbonization of polyaniline through cross-linking and condensation reactions¹. In addition, some part of the microporosity of the pristine carbon material is recovered after the heat treatments because of the removal of surface functional groups. Thus, two different activated carbons with high microporosity but different surface chemistry are obtained.

The role of the nitrogen groups on the ORR was thoroughly analysed in alkaline medium. Figure 1b shows the LSV curves obtained for the pristine carbon material (AC) and N-doped activated carbon at 800°C (N-AC_800) and Table 1 compiles the onset potential (E_{onset}) and the number of electrons involved in the ORR for all samples. The chemical modification of the carbon material AC produces some changes in the electrocatalytic activity of the samples. The formation of polyaniline over AC decreases the electroactivity because of the generation of detrimental surface functionalities. However, some beneficial effects are observed for the heat-treated N-doped activated carbons (N-AC_600 and N-AC_800). First, an increase of the number of electrons involved in the reaction was detected for both heat-treated carbons due to the presence of nitrogen groups, such as pyridones, that favors the 4e⁻ pathway for the production of H₂O. The best performance was found for the activated carbon heat treated at 800 °C, which also evidences an improvement on the E_{onset} up to 0.90 V.

These improvements are mainly consequence of the formation of nitrogen groups with high electroactivity at this temperature² along with an increase of conductivity.

Sample	N _{XPS} (At. %)	CO ₂ TPD (μmol/g)	CO TPD (μmol/g)	S _{BET} (m ² /g)	V _{DOR} ^{N2} (cm ³ /g)	E _{onset} (V vs RHE)	n (at 0.3 V)
AC	0.3	520	2400	3460	1.19	0.81	2.9
PANI/AC	6.0	1320	3560	1460	0.54	0.78	2.6
N-AC_600	4.7	380	1860	2290	1.03	0.80	3.3
N-AC_800	2.0	210	740	2330	1.04	0.90	3.4

Table 1. Physicochemical and electrochemical properties of the samples.

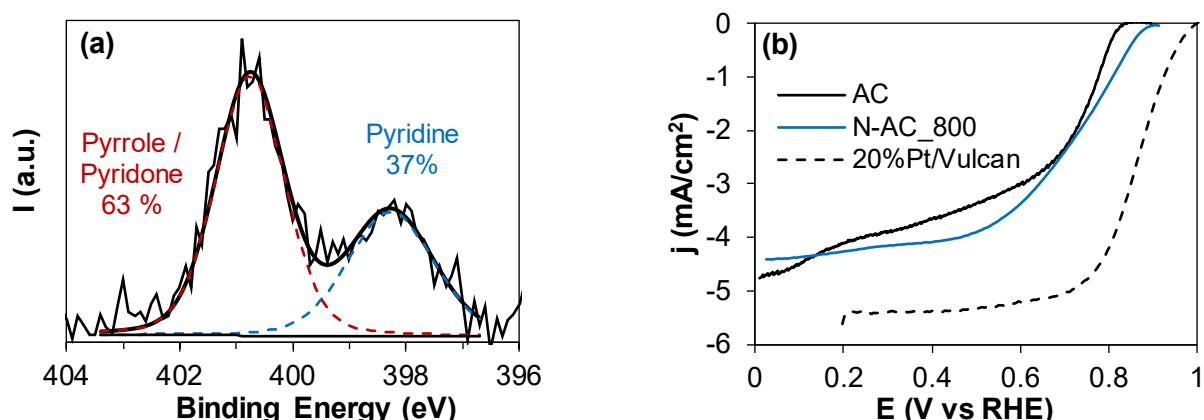


Figure 1. (a) N1s XPS spectrum obtained for N-AC_800, (b) LSV profiles obtained for AC (black), N-AC_800 (blue) and Pt/Vulcan (dashed line) at 1600 rpm. 5 mV/s.

Conclusions

Carbon-based electrocatalysts with high apparent surface area and different nitrogen content were prepared by polymerisation of aniline and post-heat treatments. Their performance towards ORR evidenced an improvement of the electrocatalytic activity towards ORR related to the generation of nitrogen groups at high temperatures (pyrroles, pyridones, etc.).

Acknowledgment

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References

- [1] Kuroki S, Hosaka Y, Yamauchi C. A solid-state NMR study of the carbonization of polyaniline. Carbon 2013; 55:160-167
- [2] Quilez-Bermejo J, Gonzalez-Gaitán C, Morallón E, Cazorla-Amorós D. Effect of carbonization conditions of polyaniline on its catalytic activity towards ORR. Some insights about the nature of active sites. Carbon 2017; 118: 62-71

Student Prize: Fe-Catalyzed graphitic carbon materials from biomass resources as anodes for Lithium-ion batteries

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Introduction

The ongoing raising environmental and economic concerns have currently lead the research community to investigate the use of biomass-derived carbons as electrodes for lithium-ion batteries (LIBs) with the main aim of sustainability management. However, carbons from the pyrolysis of most biomass resources are considered hard or non-graphitizing since subsequent heat treatment does not lead to perfectly ordered graphitic domains even when heat treated at temperatures above 2400°C^[1]. When tested as anode materials for LIBs, they deliver a limited capacity due to the cross-linked and disordered structure, suffer from a large irreversible capacity in the first charge/discharge cycles and a large voltage hysteresis on the potential profile.

An alternative pathway for developing synthetic graphitic materials from non-graphitizing carbons consists of the catalytic graphitization by the prior addition of a transition metal into the raw precursor [2, 3]. The graphitization can be induced *in situ* during pyrolysis within a solid carbon template from temperatures below 1000 °C, with enhancements in crystallinity and electronic conductivities with increasing treatment temperature. In this work, a renewable biomass precursor, a medium density fibreboard (MDF) recycled-wood, was graphitized by means of an iron catalyst at temperatures between 850 °C and 2000 °C and systematically studied as anode materials for LIBs. The microstructural parameters are correlated with the anodic behaviour, compared with high-temperature soft and hard carbons without catalyst up to 2800°C.

Materials and Methods

MDF wood pieces were first impregnated with 1.0 M FeCl_3 solution and then submitted to a pyrolysis process up to peak temperatures ranging between 850 °C and 2000 °C (Fe content ≈11.6 wt. %). The remaining Fe catalyst was removed by ultrasonic stirring in concentrated HNO_3 . The crystallinity and microstructural parameters were evaluated by SEM, TEM, Raman spectroscopy and Nitrogen adsorption/desorption measurements. Electrochemical investigations were carried out in a three-electrode set-up. Carbon electrodes consisted of 90 wt. % graphitized carbons, 5 wt. % Na-CMC as binder and 5 wt. % Super C65 as conductive agent. Galvanostatic and cyclic voltammetry experiments were carried out in a potential range between 0.02 and 1.5 V vs. Li/Li⁺.

Results and Discussion

The graphitization process starts at ≈700 °C when Fe is used as a catalyst, showing a microstructure characteristic of catalyst particle cores surrounded by several curved and ordered graphitic shells^[2]. After acid etching, Fe particles are almost completely removed from the material (content 0.4 wt. %), leaving hollow ordered carbon nanostructures. Raman measurements (*Figure 1.a*) of catalyzed samples reflects a progressive improvement in the degree of structural order and crystalline orientation with increasing treatment temperature, observable by an enhancement of the G peak intensity with respect to the intensity of the D_1 band, along with the narrowing of the full-width at half-maximum of the G peak. By fitting Raman spectra using pseudo-Voigt line shapes, the degree of graphitization ($\alpha = I_G / (I_G + I_{D_1})$) was estimated and compared in *Figure 1.b* as a function of temperature with non-catalyzed carbons and a reference soft carbon (petroleum coke^[1]). Non-catalyzed MDF samples do not reflect any abrupt development in the crystalline structure even when heat-treated up to 2800 °C ($\alpha \approx 0.4$), while when using Fe as catalyst, values close to 0.7 are reached at 2000 °C, achieving comparable but slightly lower values than petroleum coke samples ($\alpha \approx 0.8$ at 2000°C).

When used as anode for LIBs, an increasing structural order within the carbon structure goes along with an increase in specific capacity of more than 50% within the range of temperatures investigated herein (*Figure 1.c*). *Figure 1.d* shows the effect of the treatment temperature on specific reversible capacities of MDF when using Fe as catalyst^[2], compared with the usual trend of soft and hard carbon up to 2800°C^[1].

Without the effect of any catalyst, the trend is clear: a decrease up to ≈2000 °C due to the release of remaining surface functional groups, followed by a slight increase up to 2800°C due to the improved structural order (maximum reversible capacity of ≈160 $\text{mAh} \cdot \text{g}^{-1}$ and ≈310 $\text{mAh} \cdot \text{g}^{-1}$ for hard and soft carbons, respectively). However, by using Fe, the capacity increases directly from 1000°C as the graphitization has already begun at this temperature. Fe-catalyzed sample at 2000 °C delivered a remarkable specific capacity of 307 $\text{mAh} \cdot \text{g}^{-1}$, a value up to twice as much as that of non-catalyzed MDF-derived carbons at the same temperature and comparable to synthetic graphite derived from petroleum coke precursor at higher temperatures (≈2600-2800 °C).

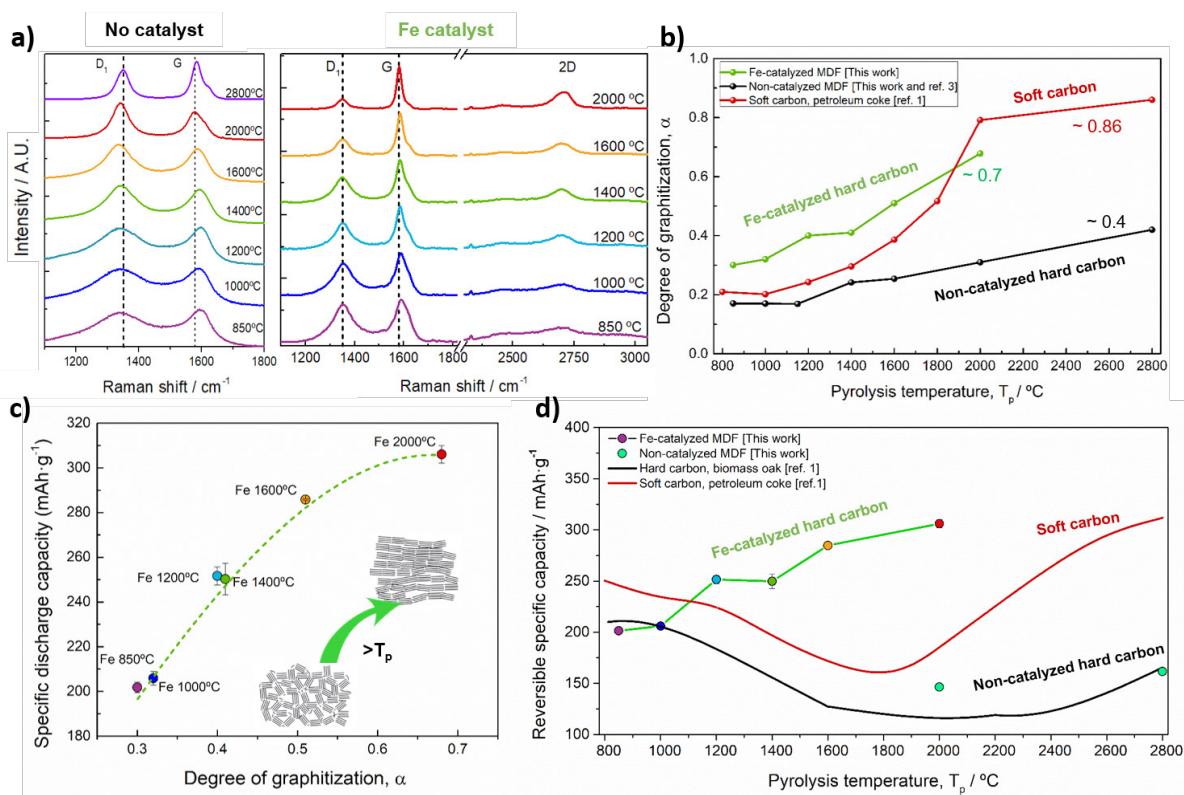


Figure 1. a) Raman spectra of Fe- catalyzed and non-catalyzed MDF carbons; b) Degree of graphitization vs. pyrolysis temperature ^[2]; c) Reversible capacity of Fe-graphitized MDF-derived carbon as a function of degree of graphitization from Raman fitting and d) Reversible specific capacity vs. pyrolysis temperature compared with soft and hard carbons ^[1]. Electrolyte: 1.0 M LiPF₆ in 3:7 EC/EMC+ 2 wt. % VC.

Conclusions

Graphitized carbon materials from biomass resources were successfully synthesized at moderate temperatures by means of an iron catalyst, and their electrochemical performance as anode materials for lithium-ion batteries (LIBs) was systematically investigated. An enhancement in the degree of graphitization was corroborated by Raman analysis with increasing treatment temperature. Fe-catalyzed MDF sample at 2000 °C delivered a specific discharge capacity of 307 mAh·g⁻¹ as anode for LIBs, a value comparable to synthetic graphite derived from soft carbons at higher temperatures (\approx 2600-2800 °C). The results reported here demonstrate that the catalytic graphitization of biomass resources, by a low cost and environmental friendly process using iron as a catalyst, is a promising synthesis route to develop synthetic graphitic anode materials for LIBs.

References

- [1] O. Fromm, A. Heckmann, U.C. Rodehorst, J. Frerichs, D. Becker, M. Winter, et al., Carbons from biomass precursors as anode materials for lithium ion batteries: New insights into carbonization and graphitization behavior and into their correlation to electrochemical performance, Carbon 128 (2018) 147-163.
- [2] A. Gomez-Martin, J. Martinez-Fernandez, M. Ruttert, A. Heckmann, M. Winter, T. Placke, et al., Iron-Catalyzed Graphitic Carbon Materials from Biomass Resources as Anodes for Lithium-Ion Batteries, ChemSusChem 0(0).
- [3] A. Gutiérrez-Pardo, J. Ramírez-Rico, A.R. de Arellano-López, J. Martínez-Fernández, Characterization of porous graphitic monoliths from pyrolyzed wood, Journal of Materials Science 49(22) (2014) 7688-7696.

Student Prize: In situ electron microscopy studies of carbon particulate matter oxidation and filtration

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Introduction

As the global requirements for energy continue to rise ¹, emissions from combustion of fossil fuels have increased as well. When released into the air, carbon particulate matter (PM) is an especially harmful by-product of incomplete combustion as it is harmful to human health and is a major contributor to pollution and climate change ². To minimize emissions, and design new filtration technologies, a better understanding of the underlying mechanisms of PM formation and oxidation is required. Apart from emitted carbon, Carbon PM is also a crucial and useful industrial product - with a wide variety of applications in materials science, pharmaceuticals, and electronics. The Combustion Research Lab at the University of Toronto has therefore applied real time imaging of reactions inside an environmental transmission electron microscope (ETEM) to study the underlying mechanisms behind carbon particulate matter formation, oxidation, and reactivity.

Experimental Methodology

The study of nanomaterial presents many challenges; as the microscopes capable of the resolution needed to see the nanoscale reactions traditionally required a vacuum environment around the sample. The vacuum environment limits research to either a reacting bulk sample outside the microscopes, or simply imaging “snapshot” of a non-reacting nanomaterial. Through a partnership with Hitachi Higher Technologies Canada and Norcada Inc. – we have been able to develop and run high temperature in-situ tests on carbon nanomaterials inside of a high-resolution environmental transmission microscope. These experiments have focused on studying how changing combustor designs affects PM reactivity, how we can develop new catalysts, and how we can further apply this technique for synthesizing new nanomaterials.

The ETEM technique relies on a customized transmission electron microscope (Hitachi HF3300) suitable for gas injection into the sample area, a microelectromechanical (MEMS) heating substrate where the sample is deposited, and high sensitivity gas and temperature control systems. The HF3300 was also equipped with secondary electron imaging and energy-dispersive X-ray spectroscopy (EDX). Functioning together, this platform allowed for tests up to 1000°C and 1Pa of gas surrounding the sample as it was visualized and analysed for morphological and chemical changes in conditions representative of flames or exhaust gases.

In situ nanomaterial experiments are run in 4

stages; material synthesis, sampling, imaging, and post processing. The carbon PM synthesis is accomplished with a diffusion flame with the variation of a specific parameter (e.g. fuel, temperature, or pressures, etc.). By controlling a single variable per study, its effect on the particles generated and their reaction pathways can be studied. The particles are then extracted from the combustor through a rapid injection of a substrate into the flame. The substrates are held in the flame from 20 to 100ms, and the sample deposits on the substrate surface through thermophoresis. The sampling is done directly on a TEM-transparent MEMS microchip, and high-speed imaging ensures minimal flame disruption and proper sampling location. With the samples collected, the MEMS chip is connected to the gas and heating systems and inserted into the ETEM for imaging.

The goal of the imaging in the ETEM is to create an atmosphere as similar as achievable to the real world conditions the particles would undergo in engines, exhaust streams, and reactors. The samples are first heated up to the reaction temperatures, gas mixtures are injected, and any reactions are captured by transmission electron microscopy, secondary electron microscopy, or EDX. The different imaging techniques give us information on the sample’s internal nanostructure (TEM), surface properties (SE), and elemental composition (EDX) – all potentially changing as the sample reacts. Combining this real time imaging with other more traditional methods such as thermal gravimetric analysis provides an extra degree of confidence in the new technique that we are not fundamentally changing the reaction pathways with the microscope electron beam and allows us to acquire a complete picture of the nanoparticle evolution during reactions.

Finally, the experimental videos are post processed with video and photo analysis tools such as ImageJ and Photoshop CC. This post processing allows us to measure particle size changes, filter out background generated by the substrate, and more clearly track the reaction mechanism. The conventional post processing follows: conversion to 24bit colour, thresholding, background elimination, and colour blending. The colour blending applies a colour enhancement to the particle, based on the luminance of the base image and the hue and saturation of the blend colour. This preserves the grey levels in the image and is useful for colouring monochrome images and for tinting colour images.

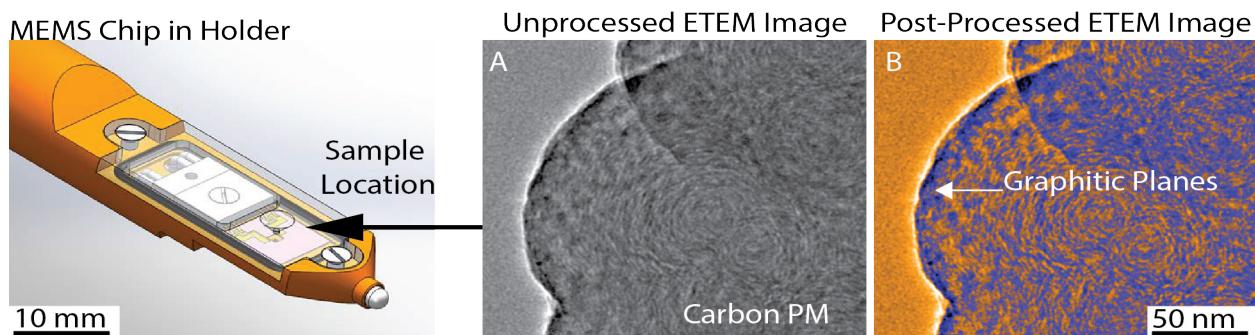


Figure 1. A: Holder Assembly B: Unfiltered sample image C: Filtered Image (purple sample, orange substrate)

Results

Studies have been carried out on the effects of combustor pressures, aftertreatment temperatures, and fuel chemistry on soot reactivity. Real time imaging of carbon particle oxidation was carried out to establish the mechanisms – confirming previously held hypothesis (e.g. how the particles grow protective graphitic “protective shells”⁵), along with

discovering new pathways such internal oxidation shown in Figure 2. New nanomaterials and catalysts have also been synthesized and tested in the ETEM - as the technique highlights how active the materials are and how they respond to environmental changes. These findings allow for cleaner combustor design, as well as fine tuning industrial carbon production to generate carbon PM with specific properties.

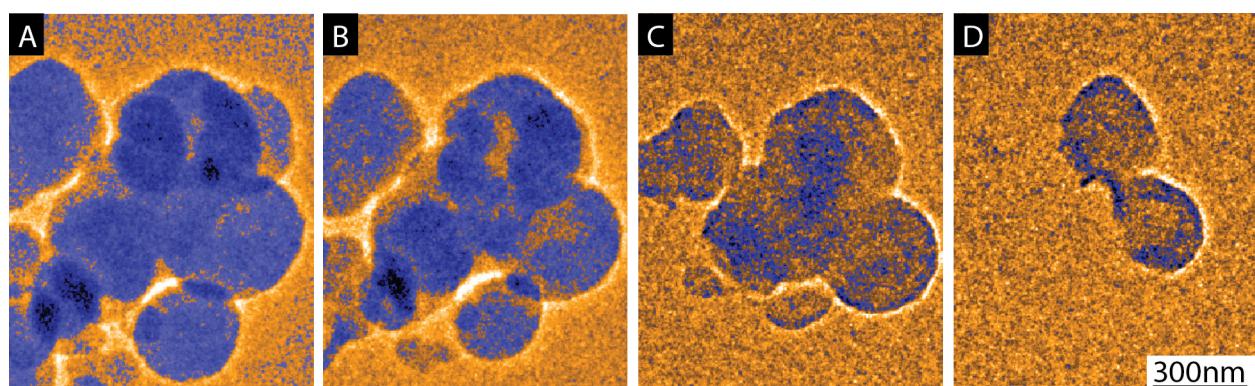


Figure 2. Oxidation pathways shown for a carbon PM particle aggregate

Conclusion

The real time nanoparticle reaction imaging techniques developed provide a powerful workbench for studying carbon particulate matter reactions, restructuring, and chemical changes. The findings allow researchers and our industrial partners to devise novel strategies for controlling emissions or modifying and creating new nanomaterials with specific properties, behaviour, and structure.

Acknowledgment

The authors would like to thank Hitachi Canada and Norcada Inc. for their continued support with the development of this new technique, and NSERC Canada for project funding. We would also like to thank the OCCAM- UofT team, where all the microscopy was performed on the Hitachi HF3300, as well as all our academic collaborators from UofW, KAUST, and PSU.

References

- [1] Statistics, I. *Energy use (kg of oil equivalent per capita)*. (2014).
- [2] Menon, S., Hansen, J., Nazarenko, L. & Luo, Y. Climate effects of black carbon aerosols in China and India. *Science* (80-.). **297**, 2250–3 (2002).
- [3] International Carbon Black Association. Carbon Black User’s Guide. *Carbon Black User’s Guid.* 36 (2016).
- [4] Sediako, A. D., Soong, C., Howe, J. Y., Kholghy, M. R. & Thomson, M. J. Real-time observation of soot aggregate oxidation in an Environmental Transmission Electron Microscope. *Proc. Combust. Inst.* **36**, (2017).
- [5] Kholghy, M. R., Veshkini, A. & Thomson, M. J. The core-shell internal nanostructure of soot - A criterion to model soot maturity. *Carbon N. Y.* (2016). doi:10.1016/j.carbon.2016.01.022.

Conferences sponsors

Francisco Heras. Universidad Autónoma de Madrid

Another important aspect related to Carbon2018 organization was the collaboration of many companies and organizations as conference sponsors. Carbon2018 organization offered six different sponsorship packages, three including the benefit of to have an exhibition stand during all the congress.

Finally, Carbon2018 had the participation of 15 sponsors (please, visit <https://carbon2018.org/sponsors/>), including laboratory equipment and analytical instrumentation companies, scientific journals, universities and the company in charge of technical secretariat of the conference.

As non-exhibitor sponsors, were Praxair (the well-known company of industrial gases business area), Merck (that commercialize in Europe the products catalogue of Sigma-Aldrich and other companies) and Viajes El Corte Inglés – Congresses (in charge of technical organization and secretariat of the event). In this point, we would like to take the opportunity to thank to our PCO the fantastic work during the conference and the preparation from about three years ago. As well, very valuable was the support of different journals: Sustainable Energy & Fuels and Energy & Environmental Science through the funding of best student contributions (oral and poster) prize and Electrochimica Acta (official journal of the International Society of Electrochemistry) because of the publication of a special issue with the best congress contributions in electrochemistry applications of carbon materials. The company Análisis Vínicos has two bussines areas: instrumental analysis consumables and wine production and commercialization; the company provide one bottle of and excellent Spanish red wine for each congress attendant.



By last, Universidad Autónoma de Madrid (university, to which most members of the Local Committee belongs) had a strong presence in Carbon2018 providing the folders and pens in the attendant kit and with the nice participation of the Chancellor of the University in the Opening Ceremony.

In section of exhibitor sponsors, was the scientific journal Nanomaterials, participating also with a brief presentation of the journal during the congress and the edition of a special issue of this journal, with the best contributions in carbon nanomaterials preparation and characterization, graphene and graphene-derived materials, etc. Also many companies of research equipment, as the group Iberfluid Instruments – PID Eng&Tech and Demede Engineering and Research (all these companies devoted to produce small/medium-scale custom research devices). Related to instrumental analysis, we had the presence of lesmat (representative in Spain of Quantachrome Instruments) and Surface Measure Systems and Hiden Isochema (world leaders in sorption instrumentation for research). Finally, a special recognition to Aplitec, a Spanish company dedicated to production and repair of custom glass and quartz parts and devices for research laboratory; they offered to all the attendants live demonstrations of hand making of glass parts.

The participation of all the sponsors was very important for the final congress success due to both economical support and the presence during the congress, giving a great atmosphere during the event. All the Carbon2018 Committees are very grateful to all the sponsors.





La cara social de Carbon 2018

Juan José Rodríguez, Miguel Ángel Gilarranz, Francisco Heras

Universidad Autónoma de Madrid

La motivaciones para asistir a un gran congreso como *The World Conference on Carbon* son diversas. Una de ellas es sin duda la oportunidad de reunirse con colegas y amigos para fortalecer las relaciones y las colaboraciones. Los descansos entre las sesiones científicas y las actividades sociales juegan un papel muy importante en esta cara social del congreso. En el diseño de Carbon2018 el Grupo Español del Carbón fue consciente del valor de este aspecto del congreso y se eligieron espacios y actividades que lo favoreciesen.

El hotel Marriott Auditorium Madrid ofreció unas instalaciones excepcionales para conseguir que el cóctel de bienvenida, los coffee breaks y los almuerzos se convirtiesen en momentos agradables y de intercambio. Los menús se cuidaron para dar un toque festivo a ese merecido descanso entre las sesiones de trabajo, con una oferta amplia que se fue retando para ofrecer especialidades de las diferentes cocinas del mundo (asiática, americana), pero siempre también con presencia de la cocina mediterránea y española. Como no podía ser de otra forma, también se cuidó la adaptación de los menús a las diferentes necesidades que pudiesen tener los congresistas.



Momentos de descanso y networking durante Carbon 2018

Otra de las premisas en el diseño del congreso fue organizar dos eventos fuera de la sede del congreso para no caer en la rutina y también mostrar otros aspectos de la ciudad de Madrid. El martes 3 de Julio se organizó una visita guiada en autobús en la que se recorrieron los lugares más emblemáticos de la ciudad, seguida de una visita a pie por los rincones con más encanto del Madrid de los Austrias. La visita

finalizó con una degustación de tapas en el entorno de la Plaza Mayor y las Cava. Fue todo un reto, para el que fue necesario organizar 28 grupos con sus respectivos guías, pero el resultado fue excelente.



Visita guiada por Madrid

Carbon2018 contó también con un momento más solemne con la cena de gala celebrada el Jueves 4 de Julio en La Casa de Mónico. Los asistentes pudieron disfrutar de un cóctel y una excelente cena al aire libre en los amplios jardines de una casa señorial. La ambientación y el tiempo óptimo del que pudimos disfrutar contribuyeron a hacer de la cena un momento muy especial. La parte final fue amenizada un cuadro flamenco de primer nivel, que marcó un momento mágico en el congreso y entusiasmó a los asistentes.



Momento de la cena de gala de Carbon 2018

Al igual que en el resto de facetas del congreso, el Grupo Español del Carbón quiso ofrecer un extra a los congresistas en su parte social. El esfuerzo, compartido por el Comité Organizador y Comité Local, mereció la pena. Seguro que contribuirá a que durante mucho tiempo oigamos a nuestros colegas del Grupo y de otros países comentar: ¿Te acuerdas de la Carbon de Madrid? – ¡Claro que sí, estuvo fenomenal!

International Summer School on "Carbon and related nanomaterials: Synthesis, characterization and properties"

Wolfgang Maser. Instituto de Carboquímica (ICB)



Del 23 al 27 de Julio de 2018 tuvo lugar en Jaca (Huesca) el curso internacional de verano “Nanomateriales a base de carbón y próximos en estructura: Síntesis, caracterización y estudio de propiedades” que ha sido dirigido por el Dr. Raúl Arenal (INA-LMA-Universidad de Zaragoza) y por el Dr. Wolfgang Maser (Instituto de Carboquímica, ICB-CSIC, Zaragoza).

El curso estaba dirigido a estudiantes universitarios, de máster o doctorandos de ciencias (física, química e ingeniería, preferentemente) con interés en la nanociencia y la nanotecnología. Este curso, de carácter multidisciplinar, ofreció una amplia introducción al área de los nanomateriales de carbono y otros sistemas relacionados. Se proporcionaron las bases científicas para entender tanto el comportamiento de los materiales como el análisis mediante técnicas de caracterización experimentales y teóricas. Asimismo, se subrayó la importancia de los nanomateriales de carbono en aplicaciones y productos de interés tecnológico, y se abordaron las posibilidades y estrategias para aplicar estos nanomateriales al mundo macroscópico. Los seminarios se construyeron de una manera sistemática describiendo los diferentes tipos de nanomateriales y sus principales métodos de síntesis, su química y procesado en forma de dispersiones, las técnicas más importantes para su caracterización, las técnicas de ensamblado macroscópico y por último su aplicación en los campos de la electrónica, la mecánica, los sensores, la catálisis y la energía.

La finalidad del curso era mostrar la importancia de los nanomateriales de carbono y sistemas relacionados

para el avance científico y tecnológico. Asimismo, demostrar que para hacer realidad este progreso y aprovechar el alto potencial de los nanomateriales de carbono se requiere un esfuerzo inter- y multidisciplinar, interactuando científicos y tecnólogos especializados en diferentes disciplinas. Y que, por lo tanto, estos nanomateriales son objetos idóneos para adquirir una amplia base de conocimiento científico-tecnológico.

A lo largo del curso, 10 docentes de diferentes instituciones (Instituto de Carboquímica (ICB-CSIC), Instituto de Nanociencia de Aragón (INA)-Universidad de Zaragoza, así como de las Universidades de, Murcia, Valencia, Montpellier (Francia), y Sussex (Reino Unido)), y especializados en las diversas temáticas mencionadas anteriormente, impartieron un total de 20 horas lectivas. Con ello, se consiguió iluminar de una manera muy amplia los diferentes aspectos relacionados con las nanoestructuras de carbono. El curso terminó con un examen final que permitió a los participantes obtener un total de 0,5 créditos ECTS reconocidos por la Universidad de Zaragoza.

En el curso participaron 16 alumnos, en la mayoría de los casos estudiantes de doctorado, procedentes de España, Inglaterra, Francia y de Ucrania con diferente especialización (física, química, ingeniería y materiales).

Se abrió el curso con la calurosa bienvenida por parte del director de los Cursos Extraordinarios de Verano, D. Chesús Bernal (Universidad de Zaragoza), y por los directores del curso, D. Raúl Arenal y D. Wolfgang Maser.

En el primer seminario, el investigador Dr. Wolfgang Maser (ICB-CSIC) introdujo las nanoestructuras de carbono, resaltando la importancia de los defectos pentagonales en el descubrimiento de los fullerenos, la tercera forma alotrópica de carbono y la nanoestructura de carbono que procedió a los nanotubos de carbono y grafeno. Relató las curiosidades del descubrimiento de las nanoestructuras de carbono y la importancia para sus aplicaciones. Igualmente, subrayó la simplicidad y belleza de sus estructuras, a partir de las cuales, se derivan todas sus propiedades únicas y su interés científico-tecnológico. En su segunda contribución, se desvió de las estructuras grafénicas perfectas hacia un derivado químico del grafeno, el óxido de grafeno. Tomó éste como ejemplo para destacar que también las estructuras no bien definidas pueden estimular gran curiosidad científica y atracción tecnológica. Destacó que el óxido de grafeno es una plataforma única en la que se pueden aprovechar tanto su grupos funcionales como sus dominios sp^2 para preparar nuevos materiales funcionales y arquitecturas macroscópicas.

En la ponencia del Dr. José Miguel González (ICB-CSIC), los participantes aprendieron de la existencia de otras formas de nanoestructuras de carbono, como son los nanocuernos, las nanocápsulas, las nanocebollas, los nanoribbons, los nanodiamantes y los puntos cuánticos de grafeno y de carbono. Explicó sus estructuras, los métodos de fabricación (curiosamente, en la mayoría de los casos, métodos "top-down", bastante destructivos e incluso explosivos) y su interés tecnológico. Aquí cabe de destacar el valor de estos materiales para aplicaciones en el campo de la (nano-)biomedicina como agentes terapéuticos, biocompatibles, sistemas de suministro específico de medicinas y de marcadores fluorescentes para la detección y tratamientos tumores, entre otros. Las aplicaciones biomédicas fueron tratadas con más detalle en su segunda ponencia. En primer lugar, abordó la importante cuestión de la biocompatibilidad y toxicidad. Aclaró que sus efectos positivos o negativos están definidos por su solubilidad, su forma y tamaño, por lo cual, es difícil, por no decir imposible, predecir, de una manera general, sus efectos adversos. Por otro lado, destacó el valor de las nanoestructuras de carbono para la rápida detección de rutas de metabolismo alterados (causa de la proliferación de células cancerígenas), para el reconocimiento de células cancerígenas y el suministro local de medicamentos, la ingeniería de tejidos y crecimiento neuronal y la teranóstica, siempre acompañado con ejemplos de su propia investigación.

El profesor Jaime Colchero introdujo las técnicas de microscopía de fuerzas atómicas. Destacó su valor único para la caracterización de nanoobjetos a nivel local (nanométrico) y para entender, por último, el funcionamiento (o el fallo) de los procesos y los dispositivos a escala macroscópica. Expuso de una manera muy clara el fundamento físico y el funcionamiento de esta técnica que se basa en las

diferentes interacciones (mecánicas, eléctricas, químicas) entre punta (sonda) y superficie del material en sus diferentes modos de uso (AFM, STM, SNOM, KPM,...). A lo largo de sus tres seminarios, resaltó la importancia de la punta misma, que se puede considerar como un laboratorio propio ("lab-on-the-tip"). Conociendo la importancia de la punta en el sistema, se puede modelar las diferentes interacciones y obtener información única sobre la mecánica, la electrónica y la química del sistema en cuestión. Con varios ejemplos, demostró que esto ayuda al mejor entendimiento de los procesos optoelectrónicos, y catalíticos a escala nanométrica y a la optimización de los respectivos dispositivos.

El Dr. Raúl Arenal, investigador ARAID (LMA-INA-Univ. Zaragoza), ofreció una amplia introducción a la técnica de microscopía electrónica de transmisión (TEM). Describió el funcionamiento de la técnica y de los diferentes modos (HRTEM, STEM, EDX, EELS, cathodoluminescence,...), que van más allá de la pura observación geométrica de un objeto a escala nano y que incluyen información sobre la composición, configuración atómica y propiedades electrónica de un material con resolución sub-atómica. Proporcionó ejemplos de su propia investigación en el campo de nanoestructuras de átomos hetero, como son los nanotubos de CN_x y BN y sistemas laminares de los dicalgenuros de metales de transición, entre otros. Con videos impresionantes también demostró la posibilidad de obtener imágenes 3D de los objetos estudiados y información sobre su composición capa por capa. La técnica igualmente sirve para estudios procesos in-situ y los cambios de un material bajo la influencia de estímulos externos, como son la irradiación con electrones y iones, la temperatura, o efectos mecánicos. Es una técnica indispensable para entender materiales y cambios de materiales a nivel de escala nano y con ello sacar conclusiones sobre el comportamiento de los materiales o dispositivos en el mundo macroscópico.

El investigador Dr. Matthieu Paillet (CNRS-Universidad de Montpellier) realizó una introducción a la espectroscopia Raman. Después de haber expuesto los fundamentos de la técnica, la llevó al campo de los nanoestructuras de carbono. Aclaró los orígenes de los varios modos vibracionales de una lámina de grafeno, dando origen a la banda D, G y 2D, y modos de respiración radiales RBM, de importancia en los nanotubos de carbono de capa única (SWCNTs). Comentó en detalle la información que se pueden obtener a partir de su posición, de su forma y anchura, y de su intensidad. Con varios ejemplos de espectros Raman de muestras bien definidas, ilustró cómo se pueden extraer conclusiones sobre un amplio rango de propiedades estructurales como son la presencia y evolución de defectos, el número de capas, la presencia de nanotubos de capa única de un tipo bien definido (diámetro y quiraldad). Hizo hincapié en que, aparte de la mera información estructural, la espectroscopia Raman de estos materiales ofrece información sobre las propiedades mecánicas (efectos de estrés) y

electrónicas (resonancia, dopaje), entre otras, a la vez que permite el estudio de efectos in-situ.

Las técnicas de caracterización fueron complementadas por una introducción a la teoría de estructuras de bandas que proporcionó información sobre la estructura electrónica de los nanomateriales. Estos seminarios fueron impartidos por el investigador Dr. Alejandro Molina de la universidad de Valencia. Después de una detallada exposición de los conceptos básicos sobre el desarrollo de las estructuras de bandas y las densidades de estados, ilustró los fundamentos de la teoría de densidad funcional (DFT) en sus varias aproximaciones de la mano del grafeno, TMDs y perovskitas. Comentó como el número de capas afecta a la densidad de estados (DOS) y al nivel de Fermi, afectando así a las propiedades electrónicas (la zona de banda prohibida, "Bandgap", y la superconductividad, entre otros). Resaltó la estrecha relación de la teoría DFT y la espectroscopia experimental, como son la absorbancia, la fotoluminescencia y la espectroscopia Raman. Aquí los cálculos teóricos, es decir la espectroscopia teórica, no sólo puede contribuir al entendimiento de las propiedades electrónicas y mecánicas de los materiales, sino que igualmente puede predecir nuevas propiedades y, así, contribuir al descubrimiento o diseño de nuevos materiales funcionales.

La investigadora Dra. Ana Benito (ICB-CSIC) ofreció una visión general sobre la funcionalización y las dispersiones de nanoestructuras de carbono. Explicó la ventaja que proporciona la curvatura en una estructura de lámina de grafeno (ángulo piramidal sp^2-sp^3) para poder aplicar conceptos de funcionalización. Destacó que en los nanotubos de carbono eso da lugar a diferentes reactividades en la punta (más reactivo) y los lados laterales (menos reactivos), en las que la funcionalización está asistida por defectos, lo cual igualmente es aplicable a las aún menos reactivas láminas de grafeno. Expuso con varios ejemplos, de trabajos propios y de la literatura más actual, los caminos de funcionalización más empleados, mencionando rutas covalentes o no-covalentes. Destacó que el valor de una determinada funcionalización siempre está relacionado con un fines específicos, como son la purificación, el desarrollo de dispersiones estables, la mejora de propiedades ópto-electrónicas (transferencia de energía, carga), y mecánicas (transferencia de carga mecánica) en dispositivos o materiales compuestos, entre otros. Enfatizó la importancia de la fabricación de dispersiones estables de las nanoestructuras de carbono con diferentes métodos para el desarrollo de nuevos materiales híbridos o compuestos funcionales, tanto con polímeros conjugados, plásticos, biomateriales o nanopartículas, de interés para aplicaciones en diferentes áreas tecnológicas.

El turno de las aplicaciones lo abrió el investigador Dr. Enrique García-Bordejé (ICB-CSIC) explicando el valor de nanoestructuras de carbono para aplicaciones en catálisis. Para esta aplicación se hace uso de la gran superficie específica de los

nanomateriales de carbono y de su porosidad. Cuando ésta está disponible en forma macroscópica (polvo, fibras, membranas, recubrimiento), es idónea para el anclaje homogéneo de metales catalíticos en forma de nanopartículas, aumentando así la superficie catalítica y contribuyendo a procesos catalíticos efectivos y más económicos con una menor cantidad de metales. Expuso varios métodos de fijación de las nanopartículas catalíticas sobre diferentes nanoestructuras de carbono. Por otro lado, demostró que las nanoestructuras de carbono en sí mismas pueden servir como sistema catalítico, evitando el uso de metales en futuras aplicaciones catalíticas. Esta investigación goza de un gran interés científico-tecnológico actual. Como la actividad catalítica depende en gran parte de la estructura macroscópica, en su segunda ponencia, hizo hincapié en varios métodos de ensamblaje de las nanoestructuras de carbono. Subrayó la necesidad de utilizar técnicas que permitan controlar el tamaño, la conectividad y la orientación de los poros y lo ilustró con varios ejemplos de estudios propios y de la literatura más actual.

Nanoestructuras de carbono para aplicaciones en las áreas de energía y sensores fue el tema de los siguientes seminarios ofrecidos por el investigador Dr. Alejandro Ansón (ICB-CSIC). Destacó de nuevo que la base para estas aplicaciones es la gran superficie específica de las nanoestructuras de carbono, su estructura porosa, y sus propiedades eléctricas. Proporcionó ejemplos de sistemas de baterías, supercondensadores y células de combustibles. Mostró que los mismos conceptos son igualmente aplicables al área de sensores, dónde, además, se hace uso de las otras propiedades funcionales únicas de las nanoestructuras de carbono, como son sus características electrónicas, ópticas, térmicas, y mecánicas. Destacó sobre todo el gran potencial de estos materiales para (bio-)sensores electroquímicos por su eficaz, rápida y selectiva detección de analitos. Son técnicas económicas y altamente competitivas con tecnologías existentes.

El Profesor Alan Dalton de la universidad de Sussex (Reino Unido) terminó la ronda de seminarios con una introducción al campo de materiales compuestos reforzados por nanoestructuras de carbono. Explicó los conceptos de relleno-matriz y las bases de la mecánica para obtener materiales compuestos reforzados mediante un material relleno. Destacó el valor de los nanomateriales de carbono y resaltó la importancia de su relación de aspecto (la relación entre anchura y largura en una hoja de grafeno, o entre diámetro y largura en el caso de los nanotubos de carbono). Demostró que la relación de aspecto es asimismo de gran relevancia para conseguir percolación eléctrica en compuestos conductores con bajas fracciones de relleno y lo ilustró con varios ejemplos de la investigación actual. En la segunda parte de su seminario ofreció rutas de ensamblaje de materiales compuestos de nanoestructuras de carbono en forma de películas mediante métodos de capa por capa.

Destacó la importancia de obtener buenas dispersiones. Demostró los conceptos de miscibilidad de disolventes y cómo los parámetros de Hansen ayudan a elegir disolventes apropiados, tanto para procesos de exfoliación, como para el procesado en forma de materiales compuestos por técnicas de capa por capa. Mostró varios videos sobre los procesos de ensamblado y algunos resultados de su propia investigación actual con aplicaciones en las áreas de fotónica y sensores mecano-ópticos acoplado con sistemas de suministro de medicamentos.

Con todo ello, a lo largo de cinco intensos días, el curso no sólo ofreció una visión general sobre las nanoestructuras de carbono y sistemas relacionados, sino, y aún más importante, la estrecha relación entre conceptos básicos en las diferentes áreas tratadas. Este hecho junto con la belleza de estas estructuras debería servir como fuente de inspiración para la investigación de los participantes.

Dado el éxito de esta primera edición, se prevé organizar nuevas ediciones del curso y contribuir así al conocimiento sobre las nanoestructuras de carbono y sistemas relacionados, desde su síntesis y procesado hacia las técnicas de caracterización y su valor en diversas aplicaciones tecnológicas.

Jaca el 27 de julio de 2018

Los organizadores

Raúl Arenal (*INA-Universidad de Zaragoza*)
Wolfgang Maser (*ICB-CSIC*)

Workshop "Carbon nano-materials and nano-composites"

Agustín F. Pérez Cadenas. Universidad de Granada

Al finalizar la Carbon 2018, del 7 al 10 de julio se celebró el workshop satélite "CARBON NANO-MATERIALS AND NANO-COMPOSITES" en el Palacio de Jabalquinto, Sede Antonio Machado en Baeza de la Universidad Internacional de Andalucía (UNIA), organizado por el Grupo Español de Carbón bajo la dirección de los doctores Agustín F. Pérez Cadenas y Francisco Carrasco Marín.

El workshop contó con la participación de importantes referentes nacionales e internacionales en el campo de los materiales de carbón, que proporcionaron una visión general del desarrollo de nanomateriales de carbono, cubriendo aspectos fundamentales y aplicados en la preparación de estos materiales a partir de diferentes precursores, su caracterización a través de un amplio espectro de técnicas experimentales, y su comportamiento en diferentes campos de aplicación. Durante las 20 horas del curso se impartieron diez conferencias por expertos internacionales en las que se presentaron los últimos avances en la producción de diferentes nanomateriales con base de carbono, tales como nanotubos y nanofibras, nanoesferas de carbono, nanocomuestos carbono/metal y carbono/no metal y grafenos. No menos importantes fueron las conferencias referentes a las aplicaciones tecnológicas de estos nanomateriales en el sector ambiental, energético y biomédico, así como en el desarrollo de nuevos materiales.

En este contexto los Profs. François Béguin y Elżbieta Frąckowiak, de la Poznan University of Technology, Polonia, se centraron principalmente en las aplicaciones electroquímicas de los materiales de carbón, impartiendo las conferencias tituladas: "Properties of nanocarbons in electrochemical capacitors implementing various electrolytes" y "Advanced materials for electrochemical capacitors", respectivamente. El Prof. Francisco José Maldonado Hódar de la Universidad de Granada nos dio una amplísima visión sobre los geles de carbón, y sus aplicaciones medioambientales, a través de la charla titulada: "Optimizing the performance of carbon gels and composites in environmental processes by fitting their physicochemical properties". Tras esta intensa mañana, el sábado continuó con una interesante visita a la monumental ciudad de Baeza.

El domingo estuvo dedicado a fines culturales, como conocer el entorno de la zona y su cultura del aceite de oliva, y por la tarde, tras una siesta obligada por el calor del estío andaluz, realizamos una visita a la vecina y también monumental ciudad de Úbeda.

El lunes se retomaron las conferencias comenzando con el Dr. Wolfgang Maser, ICB-CSIC, Zaragoza, que nos mostró el fascinante mundo de los grafenos y óxidos de grafeno con la charla titulada: "A travel through the fascinating world of graphene oxide: Challenges and Opportunities", para continuar con dos intervenciones dedicadas a los aspectos

relacionados con las aplicaciones biomédicas de los materiales de carbón, impartidas por el Prof. Maurizio Prato, Dipartimento Scienze Chimiche e Farmaceutiche, University of Trieste, Italia, y titulada: "Novel carbon-based materials and interfaces: synthesis, properties and applications", y por la Profa. Ester Vázquez Fernández-Pacheco, Departamento de Química Inorgánica, Orgánica y Bioquímica, Universidad de Castilla - La Mancha que llevaba por título: "Graphene for Bioapplications: Preparation, cytotoxicity and integration in 3D scaffolds". A continuación, la Dra. María Victoria Martínez Huerta del Instituto de Catálisis y Petroleoquímica, CSIC-Madrid, nos introdujo en el interesante mundo de la electrocatálisis mediante la charla "Carbon based nanostructure electrocatalysts for low temperature fuel cells". El lunes finalizó con la conferencia de la Dra. Dr. Zoraida González Arias, INCAR, CSIC-Oviedo, que combinaba el estudio del grafeno y los aspectos relacionados con su preparación y caracterización con diversas aplicaciones, siendo el título de su charla: "Tuning the characteristics of graphene materials towards final applications: from energy storage to composite materials".

Cabe destacar, que las noches baezanas también fueron aprovechadas por los asistentes para conocerse mejor, y en un ambiente distendido, entablar interesantes conversaciones sobre los materiales de carbono.

El último día, martes 10 de julio, comenzó con la interesante charla de la Profa. Teresa Bandosz, del City College of New York - Department of Chemistry, CUNY, USA titulada: "Enhancement in surface activity of nanoporous carbon via building their composites with GO and g-C₃N₄", para a continuación, dedicar una obligada conferencia a otros aspectos relacionados con el medio ambiente, y la producción de combustibles mediante energía solar. Así la charla "Nanoporous Carbon-based materials for the Environmental Remediation and Solar Fuels Production" fue impartida por el Prof. Juan Matos Lale, Grupo de Materiales Híbridos y de Carbono, Área de Bio-Energía UDT, Universidad de Concepción, Chile. El workshop finalizó con una mesa redonda donde se resumieron los aspectos expuestos más importantes, se debatió y discutió acerca del futuro de estos materiales, y dónde también se comentaron algunos de los mecanismos actuales para poder establecer líneas de colaboración futuras.

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