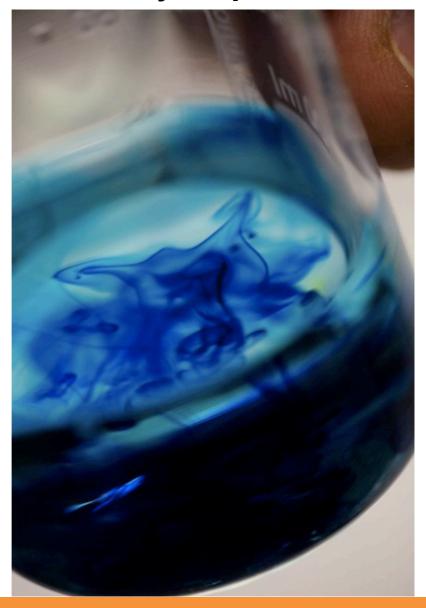
Activity Report 2011



MATGAS

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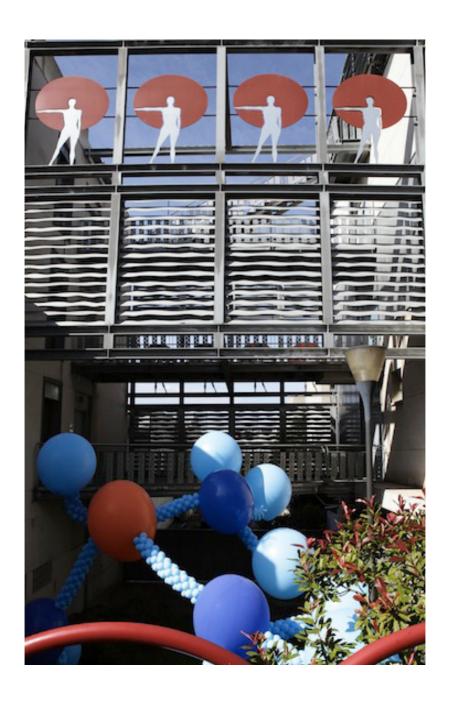
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DIRECTOR'S INTRODUCTION

MATGAS 2000 AIE, known as MATGAS, is a non-profit research organization, born ten years ago, as a joint venture between Carburos Metálicos-Air Products Group, the National Research Council of Spain (Consejo Superior de Investigaciones Científicas - CSIC) and the Autonomous University of Barcelona (Universitat Autònoma de Barcelona - UAB).

MATGAS was created to advance in the research and development of MATerials and GASes for different applications. The vision of MATGAS is to become a World-leading center of excellence that integrates research, technology development and demonstration in Energy, Sustainability and Environment, focused on greener energy solutions, including CO2 capture and application, waste treatment and alternative energies, by combining modeling and experimental approaches. We will contribute to develop energy related new technologies friendly to the environment working in different angles of this complex problem, combining in a synergetic manner modeling with experiments. As part of the sustainability commitment we use Life Cycle Assessment tools to the new processes and products we develop. We do these developments in close contact with our strategic partners, with other researchers and with final users.

Ten years have passed since the original idea of putting together a Company, a Public Research institution and a University to do R&D in a different way: with a common building, common objectives, shared capabilities and human resources. In June 2011 we celebrated the tenth anniversary of the formation of the Association; in addition to the official celebration with authorities and friends, we took advantage of this anniversary to organize a two-days international symposium in the areas of focus of MATGAS with technical presentations of world leading and recognized experts in the field and the participation of more than 300 attendees.

MATGAS has continue its activities in its area of focus along this year. We present here the annual activity report with all the notable projects, activities, events, etc. that have taken place in our organization.

Today, MATGAS provides an open framework and environment for creative discussions and advance of research and development in close contact with the industrial world. Students also benefit from this approach.

I hope you enjoy this summary and find it helpful.

In Bellaterra October 2011.

Dr. Lourdes F. Vega
Director of MATGAS



10th Anniversary of MATGAS















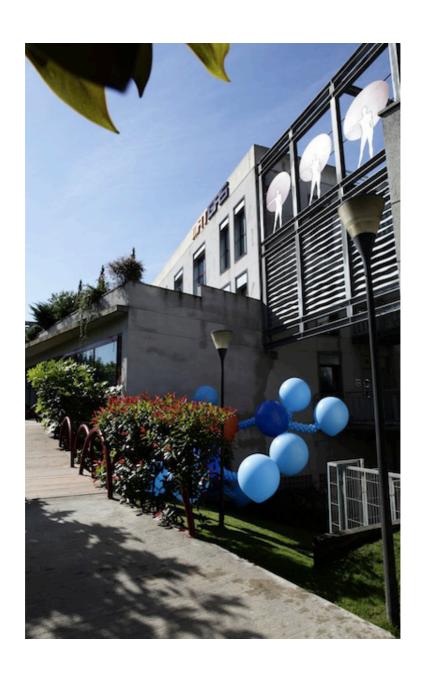
10th Anniversary in matgas

MATGAS celebrated its 10th Anniversary with a 2-day event which took place on June 1st and 2nd , 2011. The celebration begun on June 1st with a private ceremony planting a centenary Olive tree, in memory of Dr. Carlos Valenzuela, one of the founders of MATGAS, and also symbolizing the growth expected for the next years.

The official event started with a visit to the MATGAS laboratories where everyone could appreciate the evolution of the center during these 10 years as far as the facility and the last generation equipment in the six multifunctional Laboratories is concerned. After the visit the guests moved to the UAB rectorate for the rest of the celebration. A short video collecting the most important milestones in MATGAS life, as well as the present situation regarding people, projects, activities and budget opened this event. The video was followed by short presentations from the authorities: Prof. Rafael Rodrigo Montero (CSIC President); Prof. Ana Ripoll (Autonomous University of Barcelona Rector); Dr. Lluís Jofre Roca (General Director of Universities of the Economy and Knowledge Department from Catalonia Government), Dr. Lourdes Vega (MATGAS Director); and Mr. Georges Decrop (Air Products Global Marketing Director). They all emphasized the courage and vision of the three partners when they decided to start a completely and unique project, and also the importance of having a successful private-public consortium than has proven to work over these ten years, wishing MATGAS and its partners many more years of common work and success.

In ten years, MATGAS has set global benchmarks in the development and application of technologies focused on greener energy solutions, including CO2 capture and application, water treatment and alternative energies such as hydrogen and biomass, food preservation and sustainability, by combining modeling and experimental approaches. As part of this commemoration, MATGAS also organized an International Symposium on Energy Sustainability and Environment which set out the most significant advances in these fields, as well as future prospects and pending challenges in science and technology. All the invited speakers were leading researchers worldwide, both in academia and industry.

Almost 400 people participated at the celebration during these two days, including the visit at the MATGAS laboratories, the official ceremony and the International Symposium.



MATGAS

- · Three partners, one Goal
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THREE PARTNERS - ONE GOAL

Carburos Metálicos is the Spanish the leading company in the industrial and medical gases field and belongs to the multinational group Air Products since 1995.



Air Products is recognized for its innovative culture, operational excellence and commitment to safety and the environment.



Air Products Today: 18.900 employees around the world & Operations in more than 40 countries – 4 business areas: Merchant Gases, Tonnage Gases, Equipment and Energy, Electronics and Performance Materials.

http://www.carburos.com http://www.airproducts.com





The Spanish National Research Council (CSIC, Consejo Superior de Investigaciones Científicas) is a public institution devoted to research present in all the Spanish Autonomous Communities with 126 centres and over 140 associated units with universities and other institutions.

http://www.csic.es

The Universitat Autònoma de Barcelona was founded in 1968 and promotes interactivity between the university and society as an important driving force for technological, educational and ideological progress.

The UAB is able to create important links with institutions and businesses through collaborative agreements, technology transfer, work-entry programmes, professional development and continuing education programmes.

http://www.uab.cat





PEOPLE AT MATGAS

MATGAS, September 2011



MATGAS

From left to right:

Sonia Guri, Joaquim Torres, Lourdes Vega, Roberta Pacciani.

Montse Poveda, Joaquim Salleras, Joan Comas, Oriol Ossó, Emilio de la Serna
Raul Solanas, Patricio Martín, Fèlix Llovell, Aurora Aguilera, Xavier Calvo
Irene Torres, Maria Mercadé, Raquel Ramírez, Antoni Franco, Pedro López-Aranguren, Gabriel Blejman
Alicia Arce, Santiago Builes, Elena López, Sergi López, Abel Roigé.

Director: Lourdes F. Vega Vice-directors: Pedro Gómez-Romero Javier Rodríguez-Viejo **Executive Assistants:** Helena Lundquist Montse Poveda Administrative Office Manager: Joan Comas Quim Salleras **Project Manager: Project Manager Assistant:** Patricia Ruiz **Project Assistants:** Elena López María Mercadé Technical Leads: Sonia Guri Roberta Pacciani J. Oriol Ossó Joaquim Torres Laboratory Technical Coordination: Raquel Ramirez Javier Rubio Raul Solanas **Post Doctoral** Research Associates: Alicia Arce Félix Llovell Niall MacDowell Óscar Prado Research Assistant: Gabriel Blejman Santiago Builes Wounjim Chang Pedro López-Aranguren Patricio Martín Abel Roigé Oriol Vilaseca Antoni Franco Sandra Pardilla Aida Al-Nehlawi Documentation and SAP: Aurora Aguilera Maintencance and Emili de la Serna workshop:

Reception and Maintenance:

Xavier Calvo

New Employees at MATGAS



Quim Salleras

Chemical Engineering from Universitat Rovira i Virgili.

ME in organization and production engineering and management in industrial plants.

Research Project Manager.



Fèlix Llovell

PhD in Materials Science from Autonomous University of Barcelona.

Research Associate.

Expert in Molecular Modeling.



Alicia Arce

PhD in Engineering, from Seville University, Spain.

Research Associate.

Expert in Fuel Cells and Advanced Control.



Patricia Ruiz

PhD in Chemistry, from the Autonomous University of Barcelona

(UAB)Spain.

Project Manager Associate.



Santiago Builes

Master in Materials Science.

Research Assistant.

PhD Student in Simulation of materials for CO2 capture.

MATGAS Supervisor: Lourdes Vega.



Gabriel Blejman

Master in Environmental Engineering.

Research Assistant.

PhD Student in Life Cycle Assessment.

MATGAS Supervisor: Roberta Pacciani.



Xavier Calvo

Studies in Electricity as part of a formative cycle in electrotecnical installations.

installations.

MATGAS Reception and Building Maintenance.

WELCOMING NEW MATGAS EMPLOYEES



Antoni FrancoPhysics Degree from the Autonomous University of Barcelona.
Research Assistant.
MATGAS Supervisor: J. Oriol Ossó.



Montse Poveda

First cycle of a degree course in Humanities from the UPF.

Executive Technical Assistant.

MATGAS EMPLOYEES WHO LETF US IN FY2011

Several employees also left MATGAS this year to continue their professional careers in other institutions. We thank all of them for their contributions and we wish them the best for their future.



Dr. Óscar Prado, joined MATGAS in 2009 as a Research Associate. He left MATGAS in February 2011 to join UAB again. During his stay at MATGAS he took part in the SOST-CO2 project, in the field of water treatment, where he collaborated with Dr. Sonia Guri. In 2011 he went back to the Chemical Engineering department at UAB.



Ms. Aida Al-Nehlawi joined MATGAS in 2009 as a Research Assistant. She took part in the SOST-CO2 project, in the field of food preservation, collaborating with Dr. Sonia Guri. In 2011 she moved to the food technology department at UAB to continue her PhD studies.



Mr. Jaume Capell, joined MATGAS in 2005 as an ascription from CSIC for Documentation team. In 2011 he went back to CSIC.



Mr. Albert Moreno, joined MATGAS in 2008 for the IT Service department. Albert left MATGAS in 2011 and we wish him all the best for the future.



MATGAS ALUMNI DAY

1ST MATGAS Alumni Day

Alumni from the academic year 2011 at MATGAS in Barcelona came together to exchange their thoughts and experiences of their time at the research centre during their stay in training. The event on 4 February was the first of its kind at the centre.

The main goal of the event was to gather the students, their project advisors and the university professors directly involved in student programs, in a relaxed atmosphere to exchange opinions and ideas about their time at MATGAS, and their work in an industrial environment.

The event included presentations by alumni, current students, interns and student support staff on a variety of topics including individual experiences and specific student projects. Javier Rodriguez, MATGAS Vice-Director and professor at UAB, led a roundtable discussion on the issues relating to the education of students in research centers, with participation from people from industry and academy, as well as students.

A diploma was given by the Director of the School of Engineering and the Director of MATGAS to each one of the students.

4 February 2011, MATGAS, Barcelona, Spain.



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STUDENTS AT MATGAS



Pablo Ferrando
Undergraduate student from UAB, Physics.
Optical characterization of doped TiO2 nanoparticles.
MATGAS Supervisor: J. Oriol Ossó.



Sandra Pardilla
Master's thesis.
Animal and Food Science: Food Science specialty.
Improvement of quality and shelf-life of red meat in MAP using noble gases.
MATGAS Supervisor: Sonia Guri.



Albert Gustems

Material science final project student.

Study and modeling of degradation processes for PEM fuel cells.

MATGAS Supervisor: Alicia Arce and J. Oriol Ossó.



Mónica Esteban
Master project.
Materials Science and Technology.
Characterization of the behavior of elastomers for CO2 pipelines.
MATGAS Supervisor: Joaquim Torres.



Helena Nogales
Master project.
Materials Science and Technology.
Electrochemical characterization of carbon steel corrosion under dense CO2 environments.
MATGAS Supervisor: J. Oriol Ossó.



Wondwossen Bekele
Master's thesis.
Animal and Food Science: Food Science specialty.
Study on the effect of high oxygen saturation in the preservation of red meat.
MATGAS Supervisor: Sonia Guri.



Selene Gil Internship student. UAB Chemistry program. Corrosion studies of steel under supercritical CO2. MATGAS Supervisor: J. Oriol Ossó.



Sergio Soler

Internship student.

UAB Chemistry program.

Synthesis and characterization of solid materials for CO2 capture.

MATGAS Supervisor: Roberta Pacciani.



Daniel Herrera
Internship student.
UAB Chemistry program.
Characterization of the behavior of elastomers for CO2 pipelines.
MATGAS Supervisor: Joaquim Torres.



Irene Torres Alvarado
Internship student.
UAB Physics program.
Characterization of polymer electrolyte membranes for hydrogen fuel cells.
MATGAS Supervisor: Alicia Arce and J. Oriol Ossó.



French Internship student.
ENIVIL Physics program.
Study of the thermophysical and transport properties of CO2 mixtures with the soft-SAFT equation of state.
MATGAS Supervisor: Fèlix Llovell and Lourdes Vega.

Alban du Plessis de Grenedan



César Pelegrín
Internship.
Undergraduate student from UAB, Chemistry.
Synthesis and characterization of solid materials for CO2 capture.
MATGAS Supervisor: Roberta Pacciani.



RESEARCH ACTIVITIES

MATGAS Laboratories

Scientific Projects and Contracts

MATGAS Conferences

Awards, Recognitions, Contributions, Courses and Events

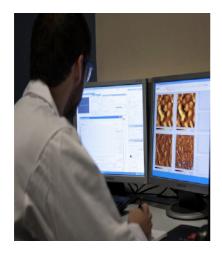
MATGAS LABORATORIES Visit them at www.matgas.org/laboratories



The research carried out at MATGAS is focused on Energy, Sustainability and Environment, with emphasis in greener energy solutions, including CO2 capture and application, waste treatment and alternative energies, by combining modeling and experimental approaches. The MATGAS laboratories offer a variety of facilities that allow from the modeling and fabrication of new materials to their physical and chemical characterization, including the test for specific applications in a variety of fields."

In the **Supercritical Fluids laboratory** research and development of new applications of supercritical fluids or fluids at high pressures and temperatures is carried out. This includes extraction and concentration of natural products, polymer impregnation, CO₂ transportation and sequestration and synthesis of new materials and catalysts. The laboratory is equipped with several high pressure reactors with different configurations and sizes, from 10ml to 16l; it also includes a pilot plant.





The Nanotechnology laboratory is a last generation lab equipped with the needed techniques for the characterization and manipulation of materials at the nanoscale. The equipment includes SPM techniques (AFM and SNOM), particle size determination tools, micro-Raman scattering, nanocalorimetry, and nanoindentation. This laboratory allows a comprehensive study of the properties of nanostructured materials, including size, mechanical, thermal, optical, structural, and electrical properties.

The Gas Reactivity laboratory is designed for the study of the reactivity and adsorption of a variety of gases into liquids or solids materials. This can be done by volumetric as well as gravimetric techniques and over a wide range of pressures and temperatures. Two magnetic microbalances with different configurations allow the gravimetric measurements under real conditions. while the volumetric measurements are done with a BET equipment. This laboratory also includes equipment for the preparation of new materials for absorption of gases by sputtering in UHV and several potentiostats for electrochemical studies.





The Computational Modeling laboratory is a permanent calculation infrastructure to provide support to MATGAS projects from a modeling perspective. Simulations performed in this lab help to obtain a deeper understanding of properties and processes at nanoscale and/or for different applications. Examples of recent projects include hydrogen storage

in carbon nanostructures, deposition of copper layers as electrical contacts in microelectronics, the optimization of nanoparticle dispersions, the design and understanding of the behavior of materials for ${\rm CO_2}$ capture and the behavior of selected ionic liquids.

The **Green Energy laboratory** offers facilities related to the study of new sustainable energies. This includes a hydrogen fuel cell test bench, several potentiostats for electrochemical characterization, and different tools for the development of water treatment processes. Equipment for the development of new technologies in the fields of photovoltaics and bioenergy are planned to be located in this lab in the coming year.



SCIENTIFIC PROJECTS AND CONTRACTS



SOST-CO2 – Vertical form fill seal machine (VFFS) for modified atmosphere packaging of food.



Public-Private Projects





Title: New industrial and sustainable uses of CO₂

Objectives: The main objective of the project is to develop CO₂ utilization technologies, complementary to capture technologies, as an

alternative to the geological storage of CO₂. This project offers a clear environmental approach, since it will not only reduce CO² emissions but it also develops technologies for sustainable energy production (e.g. biofuels and hydrogen) and new uses of CO₂ for

different applications.

PI: Dr. L. F. Vega

Status:

Budget: 26.3 Million euros.

Leader: Carburos Metálicos, Air Products Group. **Consortium:** 14 companies, 29 research centers.

Started in 2008, ending in 2011.

MATGAS Acts as the Technical Coordinator. Has been contracted by three

other companies as a Research Center expert in CO₂ capture and

applications.

The main achievements since the beginning of this project are 52 scientific articles, 7 PhD Thesis, 199 participations in Summits and conferences, 8 patents, 50 new project proposals, 9 projects accepted, 12 new processes and products and 47 work places generated.

CONSORTIUM LED BY:

CARBUROS METALICOS Grupo Air Products

More details on the project can be found at: http://www.cenit-sostco2.com







PUBLIC-PRIVATE PROJECTS





Acronym: **BIOSOS** –**CENIT** project Title: Sustainable Biorefinery

Objectives: To develop technology to design innovative and integrated

> biorefinery processes, combining energy production and bioproducts synthesis. Economic, environmental and social studies are also carried out for all the alternative processes

to guarantee feasible and sustainable solutions.

Budget: 27 Million €.

Leader: Abengoa Bioenergía Nuevas Tecnologías.

Consortium: 14 companies.

Started in September 2009, ending in September 2012. Status:

The project is divided in five different activities: Raw Materials, Sugars, Gases, Bioproducts and Sustainability. Carburos Metálicos- Air Products is one of the partners in the project, while MATGAS and the other partners, CSIC and UAB participate as contractors to develop part of the technical work.

The project is developed by a significant consortium comprising 14 companies and 29 research centers. The consortium will unit efforts for four years.

More details on the project can be found at: http://www.cenit-biosos.es

ABENGOA CONSORTIUM LED BY: Abengoa Bioenergía Nuevas Tecnologías.



EU Funded Projects





Acronym: LOLIPEM project

Title: Long-life PEM-FCH &CHP systems at temperatures ≥ 100 °C

(LoliPEM).

Objectives: To give a clear demonstration that long-life SPG&CHP systems

based on PEMFCHs working at temperatures ≥ 100°C can be developed. This is achieved based on recent knowledge on the degradation mechanisms of membranes, disclosed by some participants in this project. In order to conciliate the achievement of the main objective with the need of durability, low cost, and an easy management, several sub-objectives have been defined, concerning development of stable and less expensive membranes, development of more stable catalytic electrodes as well as physico-chemical characterizations of the

obtained products.

Budget: 3 Million €.

Coordinator: Dr. Giuseppe Barbieri, National Research Council - Institute on

Membrane Technology, CNR-ITM.

Started in February 2011, ending in February 2014. The kick-off

meeting was held on 17-18 February in Rome.

MATGAS role in this project is to perform long-term tests for the membrane developed by the other partners in hydrogen fuel cells.

Dr. Alicia Arce, an expert in Fuel Cell and Advanced Control, was hired in November 2010 to carry out the work MATGAS has committed in this project.

In collaboration with other team members she has been successfully leading this work: a hydrogen fuel cell test bench has been designed and is being assembled in the Green Energy lab. In addition, advanced control techniques are being developed to optimize fuel cell performance (efficiency and durability).



NEW FUNDED PROJECTS



Acronym: HyTECH project

Title: Hydrogen transport in European cities.

Objectives: The HyTEC project will provide a real momentum in the drive

towards commercialization of hydrogen vehicles in Europe. The overall concept is to meet the AIP aim to expand the number of existing hydrogen demonstration sites in Europe and the

real-life use of next generation fuel cell hybrid vehicles.

Budget: 27 Million €. **Leader:** Air Products Plc.

Partners: Element Energy Ltd , HyRaMP, LTI Vehicles , Centre of excellence

for low carbon and fuel cell technologies, Greater London Authority, hySOLUTIONS GmbH, LBST, Copenhagen Energy, City of Copenhagen, Hydrogen Link, Intelligent Energy Ltd, BAA Ltd, Transport for London (LBSL), Suzuki Motor Corporation and

Fraunhofer.

Status: Started in November 2011, ending in February 2014.

Acronym: SOFCOM project

Title: SOFC CCHP WITH POLY-FUEL: OPERATION AND MAINTENANCE

Objectives: Demonstrate the technical feasibility, efficiency and

environmental advantages of CCHP plants based on SOFC fed by different typologies of biogenous primary fuels (locally produced), also integrated by a process for the CO2 separation

from the anode exhaust gases.

Budget: 5.7 Million €.

Leader: Politecnico di Torino.

Other Partners: Technical Research Centre of Finland (VTT), Topsoe Fuel Cell A/S

(TOFC), Società Metropolitana Acque Torino (SMAT), National Reseach Council - Institute for Advanced Energy Technologies (CNR), Instytut Energetyki (IEN), Ecole Polytechnique Fédérale de Lausanne, Technical University of Munich (TUM) and

Università di Torino (UNITO).

Status: Started in November 2011, ending in February 2014.



Spanish Government Funded Projects







Acronym: CIUDEN

Title: Experimental characterization of SCCO2 injection into storage

materials located in Hontomín (Burgos), where the Geologic

Sequestration Development Plant will be built.

Objective: The objective of this project is to obtain detailed information

> of the reaction of CO2 with rocks under sequestration conditions, using the supercritical lab facilities and know-how.

Budget: 100.000€

MATGAS and AMPHOS 21. Partners:

Status: Started in June 2010 and finishing in October 2011.

The experimental setup to test the effects of the water displacement on the porous of the rocks by CO2 has been constructed. With this study we will be able to characterize the flow dynamics of the CO2 through the brine aguifer for CO2 sequestration.

INDUSTRIAL CONTRACTS





In addition to the public-private consortia in which Carburos Metálicos contracted MATGAS we have also been contracted by other companies to develop research and development projects.

Title: Acidification of water effluents from power plants

refrigeration systems through CO2.

Contract with Iberdrola.

PI: Sonia Guri (CM-APCI).

L. Vega, E. Rodríguez (Iberdrola), J. Lafuente (UAB) and O. Prado Members:

(MATGAS).

Started in October 2008 and finishing in October 2011. Status:

INDUSTRIAL CONTRACTS



CO2 enriched atmospheres for poultry packaging.

Contract with NUTRECO.

PI: Sonia Guri (CM-APCI).

Members: A. Al-Nehlawi (MATGAS), A. Corujo (Nutreco) and

C. Martin (Nutreco).

Status: Started in January 2008 and finishing in July 2011.



CO2-transport.
Contract with Endesa.

Partners: ENDESA and MATGAS.

Status: Started in December 2010 and finishing in

December 2011.

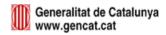


Carbon Formation
Contract with Air Products.

Status: Started in December 2010 and finishing in

December 2011.

CATALAN GOVERNMENT FUNDED PROJECTS



NEW TALENTS:

Acronym: Talent Empresa (TEM 2010) Awards

B-Type (Post-doc): Dr. Félix llovell: Use, development and improvement of various molecular modeling tools for its further application in certain

industrial processes of interest to MATGAS.

MATGAS Supervisor: Lourdes F. Vega.

A -Type (Pre-doc): Mr. Abel Roigé: Development of new nanostructured materials

for energy conversion.

MATGAS Supervisor: J. Oriol Ossó.

ONGOING TALENTS:

Acronym: Talent Empresa (TEM 2009) Awards

A -Type (Pre-doc): Mr. Santiago Builes: A combined modelling-experimental

approach to speed up the development of materials for ${\rm CO_2}$

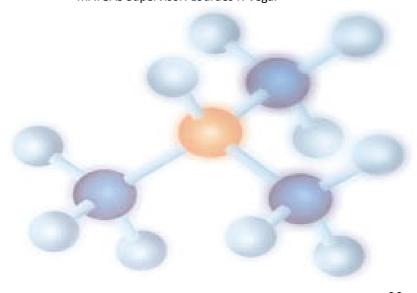
capture and utilization.

MATGAS Supervisor: Lourdes F. Vega.

B -Type (Post-doc): Dr. Raquel Ramírez: Design and optimization of new materials

for CO₂ Capture.

MATGAS Supervisor: Lourdes F. Vega.





SEMINAR SERIES ON CO2 AND SUSTAINABILITY

The objective of this series of seminars is to acquire and divulgate a solid knowledge of the state of the art in the field of ${\rm CO_2}$ capture, utilization and energy issues associated to environmentally benign energy technology and sustainability.

Several international experts on CO_2 capture, sequestration, utilization and energy connected issues (including hydrogen) have been and will be invited to participate in this series. Their expertise gives a broad perspective to the subject: from fundamental knowledge to well-developed technologies. The complementary approach enlightens the issues and challenges on this relevant topic.



Dr. Lidia LOMBARDI

Researcher, Energy Dept. "Sergio Stecco" University of Florence, Italy. "Upgrading of BIOGAS and CO2 Capture".

20 October 2010.



Prof. Juan Pedro BOLÍVAR RAYA

Vice-director of Masters and Doctorates, University of Huelva, Spain. «The valorization of inorganic wastes; the case of the TiO2 production industry».

3 November 2010.



Prof. Richard NOBLE

Alfred T. & Betty E. Look Professor of Chemical Engineering, University of Colorado, USA.

«Separations Using Room Temperature Ionic Liquids and Membranes». 22 November 2010.



Dr. Christoph MÜLLER

Head of the Energy Science and Engineering Lab, ETH, Zurich, Switzerland. «Sustainable production of hydrogen using novel chemical cycles». 2 February 2011.



Dr. Alicia ARCEResearch Associate, MATGAS, Spain.
«Advanced Control Technologies: Applications on PEM Fuel Cell Systems and CO2 Capture Systems».
11 February 2011.



Prof. Joao A.P. COUTINHO
Director of the Research Line in Biorefineries and Biomaterials, CICECO
Universidade of Aveiro ,Portugal.
«Minimizing interactions: An heterodox strategy of designing ionic liquids for gas sweetening».



Prof. Felipe J. BLAS
Department of Applied Physics, University of Huelva.
«On perturbative Monte Carlo methodologies for determining the fluid-fluid Surface tension. Application to molecular models».
27 September 2011.



8 September 2011.



Awards, Recognitions, Contributions, Courses and Events

Lourdes Vega named Physicist of Excellence

Lourdes Vega received a prestigious award in recognition of her career achievements.

Her work attracted the attention of the Spanish Collegiate of Physics (COFIS) who this year selected her for one of ten diplomas for Professional Excellence in Physical Science. The prize, which is supported by the Spanish Foundation for Science and Technology (FECYT), highlights the work of physicists who have reached a level of excellence in their profession, with this first round of honors focusing on research linked to environmental sustainability.

Palacio Municipal de Congresos del Campo de las Naciones, Madrid.

23 November 2010.



Dr. Vega inaugurated the opening ceremony of the 16 "Women in Science" exhibition in UAB.

With regards this itinerant exhibition to be held at the UAB, Dr. Vega participated with the conference "Where is the secret of scientific women? The privilege of doing what you enjoy at work".

Autonomous University of Barcelona. 8 March 2010.



The 16 "Women in Science" exhibition awarded.

The exhibition in which Dr. Vega is one of the 16 women in science, was awarded with the Special Award *Women, Science and Technology Award* in the 12th edition of the *Science in Action* Fair.

Parc Científic i Tecnològic de Lleida.

8 October 2011





Dr. Vega with other curators: Isabel Coixet (film director), Benedetta Tagliabue (architect), Santiago Ortiz (new technologies expert), Vicente Guallart (Architecture & Urban Planning) and THomas Weber (mobility).

RECOGNITIONS

Interview to Martha Collins and Lourdes Vega at Chemical Processing.

Dr. Martha Collins (Vice-president of the MATGAS Board) and Dr. Lourdes Vega (MATGAS Director) were interview by a journalist, Seán Ottewell, Editor at Large of ChemicalProcessing.com, for his contribution on an article on Companies leading their work on Sustainability, where they highlighted the work Air Products and MATGAS are doing on Sustainability and the positive influence that MATGAS had in this work.

The article was published in ChemicalProcessing.com, with the title: "Long March Toward Sustainability Begins: Companies consider reducing carbon footprint only one of the key steps necessary for sustainability." The full article can be found at: http://www.chemicalprocessing.com/articles/2010/215.html

Smart Future Minds Award

Lourdes Vega was one of the curators (Science) at the Smart Future Minds Award, from the exhibition Smart Urban Stage, organized by the automobile brand Smart.

A total of 10 finalist projects were presented during the event, as part the competition, addressing the sustainable city of the future.

The event took place from 19th May until June 2nd, in Port Vell, Barcelona, Spain. The project named TANERGY, presented by J. Bruno and M. Bruno, from AMPHOS21, sponsored by L. Vega, was the winner of the competition.

The aim of this project is to recover an obsolete postindustrial legacy and integrate it into a new urban reality focused on sustainability. It is transforming the strange and dilapidated old spaces of Les Teneries, the hide-tanning centre that was of such importance to the industrial development of the town of Vic, which became known for its fur industry. The idea is to devote these spaces to the creation of an agrofood technological research centre for the region. This reprogramming of the spaces is done by initiating energy-saving measures and researching energy crops that cannot be used as food.

Interview to Lourdes Vega

Lourdes Vega was interviewed by CTM Centre Tecnològic on its newsletter of the Boletín 09-2010 as MATGAS' Director as well as the Head of the R+D department of Carburos Metálicos.

September 2011

The full interview can be found in:

http://www.ctm.com.es/newsletter/PDF/PDF9/cast-lourdesvega.pdf



Contributions

Watermatex 2011

MATGAS, on behalf of Carburos Metálicos, sponsored the Best Oral Presentation Award of the 8th IWA Symposium on System Analysis and Integrated Assessment (Watermatex). It was held in San Sebastian, June 20-22 (Spain).

The WATERMATEX symposiums have been focused on promoting the application of a wide range of mathematical methods for solving water-related problems.



Air Products/MATGAS contribution to the program UAB in ASIA

MATGAS, on behalf of Air Products, and in collaboration with the School of Engineering at UAB, supported the trip of one of the UAB students at the UTSEUS program (Sino-European School of Technology of Shanghai University - UTSEUS).

Joel Terrades and Jesús Guerrero (students of the Engineer School, UAB) signing their agreement to go to UTSEUS, supported by Air Products through MATGAS.

They are going to complete their final year of education and develop a final project with a company. They are in contact with the AP R&D facility in Shanghai to do it. August- September 2011.











International Symposium on Energy, Sustainability and Environment.

MATGAS held an International Symposium on Energy, Sustainability and the Environment on June 1st and 2nd at its facilities in Barcelona, as part of the events organized commemorating the 10th Anniversary of the Association.

Over the two days, world-leading experts came together to unveil significant findings and explore future research prospects and challenges. Speakers included MATGAS director, Dr. Lourdes F. Vega; Professor Robert Armstrong of the Massachusetts Institute of Technology (MIT), USA; Professor Michele Aresta of the University of Bari in Italy; and Professor Andreas Züttel of the EMPA in Zurich, Switzerland.

The Symposium was closed with a roundtable focussed on Future Trends in Energy, Sustainability and Environment. This was leaded by Prof. Xavier Obradors, and focused on the different areas: Materials and Energy: Carles Miravitlles, Research Professor at ICMAB-CSIC. Hydrogen: Javier Rodriguez-Viejo, from MATGAS and the Physics Department at UAB. CO2 capture and utilization: Lourdes F. Vega, MATGAS Director and Air Products and Chemicals. Energy and Sustainability: lead by Georges Decrop, Merchan Gases, Air Products and Chemicals, Member of the MATGAS Board of Directors. The session was then open for discussions from the audience.

The closing remarks were leaded by Martha Collins, Director, Global Technology Centres, Air Products, Allentown, USA and Jordi Marquet, Director of the Research Parc, UAB, Spain.

Here is the program of the Symposium. More details can we found at the MATGAS web page http://www.matgas.org



Courses and Events

"CO2, problem or resource? A new vision of its capture, transformation and utilization"

Summer school held in the context of the SOST-CO2 project, co-financed by the CENIT project

Director: Prof. Guillermo Calleja, Secretary: Lourdes Vega

Lecturers: Prof. Vicente Cortés Galeano, Prof. Mercedes Maroto-Valer, Prof. Stefano Brandani, Prof. Andres Pérez-Estaún, Prof. Raul Sanz Martín, Prof. Michele Aresta, Dr. Sonia Guri Baiget, Dr. Concepción Domingo, Prof. Pedro Ollero de Castro, Prof. Francesc Castells Piqué, Prof. Javier Dufour Andía, Prof. Carlos López Jimeno.

Participation of 60 students from different places.

Summer School held in Aranjuez, from July 4th to 8th, 2011.

"Black Liquor Combustion and Gasification: Principles and Process Technology" Co-organized by University of Zaragoza and MATGAS.

Course held in the University of Zaragoza, from June 7th to 9th and done by Jim Frederick (Table Mountain Consulting).

SOST-CO2 Workshop 2011

The workshop was held in the Hotel El Montanyà, Resort & Spa - Seva (Barcelona). All the attendees discussed on the obtained results. Also there was a brainstorming session, in which the aim was to find and identify the most significative results since the beginning of the project and new proposals. During the session about final stage project, the attendees discussed on the action plan, chronogram and issues to focus on. At the end, took place a workshop about the project closure. 7-8 July, 2011.

Introduction to Life Cycle Assessment: a Key Tool for Industrial Ecology.

The course was co-organized by Roberta Pacciani and Javier Rodríguez-Viejo. The course aimed at giving an introduction on the LCA tool. It consisted of a first part on the basic theory of the tool and a practical part focusing on the implementation of a simple LCA project using the commercial software SimaPro. We had seven students coming from universities and companies. The lecturers came from the UAB, Inedit Innovació and Carburos Metálicos-Air Products Group. March - April 2011, MATGAS, Barcelona (Spain).

Overview and current trends in food preservation, course held in MATGAS.

The course was co-organized by Sonia Guri and Javier Rodriguez-Viejo.

The participants were given an essential overview on food preservation techniques, from packaging materials to emerging technologies through theory and practice sessions.

The professors teaching the course were from the UAB, IRTA and Carburos Metálicos-Air Products Group.

10 March to 4 May 2011, MATGAS, Barcelona (Spain).







The workshop Water Technical Day

Organized by AP Bulk Southern Europe in collaboration with MATGAS, in which a general overview of the Halia technologies including pH neutralization and advanced oxidation process (AOP) and CO2 use for water treatment were explained. Experts from AP, MATGAS and UAB participated as invited speakers. In addition, a demonstration was carried out in the MATGAS Green Energy Laboratory to show the operation of the Halia AOP reactor.

More than 40 people from academia and companies attended the workshop. 17 May 2011, MATGAS, Barcelona, Spain.







"Utilization of Biomass for the Production of Chemicals or Fuels" Co-organized by EUROBIOREF and MATGAS.
EUROBIOREF Summer School, from September 18th to 24th, 2011.



EVENTS

5th General Assembly of the SOST-CO2 project.

A meeting was held gathering 60 participants from the partners and collaborators of the CENIT "New Industrial and Sustainable Uses of CO2 – SOST-CO2" and representatives from CDTI. In this meeting there were some important presentations: Tomas Michel (CETaqua Director) presented the innovation areas of AGBAR; Roberto Mariscal (Innovation Director) presented the innovation areas of IBERDROLA and José López Domínguez (R+D+I Department) presented the innovation areas of INABENSA. Dr. Vega (Carburos metálicos R&D Director) took the advantage of the meeting to introduce to the attendees all innovation areas of Carburos Metálicos. 26 November 2010, Seville, Spain.

6th General Assembly of the SOST-CO2 project.

The meeting was held at MATGAS, gathering 40 participants from the partners and collaborators of the CENIT "New Industrial and Sustainable Uses of CO2 – SOST-CO2" and representatives from CDTI. The main purpose of the meeting was to present the results obtained in 2010 to the technical evaluator of the CDTI.

5 May 2011, MATGAS, Barcelona (Spain).



PUBLICATIONS

Publications Patents and Articles in Journals

Meetings and Conference Contributions

Oral and Poster presentations in Scientific Conferences

Publications

Books



Dr. L.F. Vega "CO2 as a resource: from capture to industrial applications" – *El CO2 como recurso: de la captura a los usos industriales* Edited by the Gas Natural Foundation, **2nd edition, 2011** ISBN: 978-84-614-1195-5.

Book Chapter

L.F. Vega, O. Vilaseca, E. Valente, J.S. Andreu, F. Llovell, R.M. Marcos: Using molecular modeling tools to understand the thermodynamic behavior of ionic liquids

Ionic Liquids, Theory and Applications, Ed. Intech.

ISBN: 978-953-307-349-1 February 2011.



PATENTS

1. Patent No.: US 7,524,533 B2.

Date of Patent: April 28, 2009.

Title: Diffusion barrier layers and processes for depositing metal films

thereupon by CVD or ALD processes.

Authors: Garg, Cheng, Norman, Machado, Ordejón.

Assignee: Air Products and Chemicals.

2. Patent No.: US 7,985,449 B2.

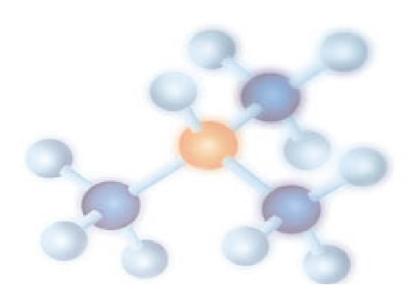
Date of Patent: July 26, 2011.

Title: Methods for depositing metal films onto diffusion barrier layers by CVD

or ADL processes.

Authors: Garg, Cheng, Norman, Machado, Ordejón.

Assignee: Air Products and Chemicals.



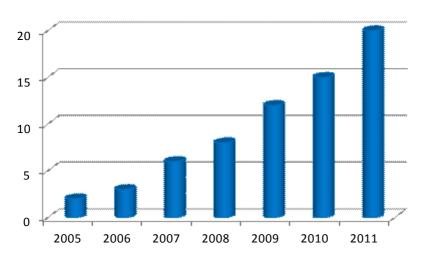
ARTICLES IN SCIENTIFIC JOURNALS

- Vilaseca, O.; Llovell, F.; Yustos, J.; Marcos, R. and Vega, L.F., 'Phase equilibria, surface tensions and heat capacities of hydrofluorocarbons and their mixtures including the critical region', The Journal of Supercritical Fluids, 55, 755 768 (2010).
- 2.- Vega, L. F. and Jackson, G. '20 years of the SAFT equation of sate recent advances and challenges', Fluid Phase Equilibria, 306, 1-3 (2010).
- Tamboli, D.; Osso, O.; McEvoy, T.; Vega, L. F.; Rao, M. and Banerjee, G., 'Investigating the Compatibility of Ruthenium Liners with Copper Interconnects', ECS Transactions, 33, 181-187 (2010).
- 4.- Domenech-Ferrer, R.; Rodriguez-Viejo, J. and Garcia, G., 'Infrared imaging tool for screening catalyst effect on hydrogen storing thin film libraries', Catalysis Today 159, 144-149 (2011).
- 5.- Ionica-Bousquet, C.; Muñoz-Rojas, D.; Jr., W. C.; Pearlstein, R.; Kumar, G. G.; Pez, G. and Palacín, M., 'Polyfluorinated boron cluster based salts: A new electrolyte for application in nonaqueous asymmetric AC/Li4Ti5O12 supercapacitors', Journal of Power Sources 196, 1626 1631 (2011).
- 6.- Llovell, F.; Valente, E.; Vilaseca, O. and Vega, L. F., 'Modeling Complex Associating Mixtures with [C-n-mim][Tf2N] Ionic Liquids: Predictions from the Soft-SAFT Equation', Journal of Physical Chemistry, 115, 4387-4398 (2011).
- 7.- Álvarez-Quintana, J.; Rodriguez-Viejo, J.; Álvarez, F. X. and Jou, D., 'Thermal conductivity of thin single-crystalline germanium-on-insulator structures', International Journal of Heat and Mass Transfer, 54, 1959-1962 (2011).
- 8.- Builes, S.; Roussel, T. and Vega, L. F., 'Optimization of the Separation of Sulfur Hexafluoride and Nitrogen by Selective Adsorption Using Monte Carlo Simulations', AIChE Journal, 57, 962-974 (2011).
- 9.- Forte, E.; Llovell, F.; Vega, L.F.; Martin-Trusler, J.P. and Galindo, A., 'Applications of a renormalization-group for potentials of variable range (SAFT-VR)' The Journal of Chemical Physics, 134, 154102 (2011).
- Domenech-Ferrer, R.; Rodriguez-Viejo, J.; Gonzalez-Silveira, M. and Garcia, G., 'In situ infrared thermographic screening of compositional spread Mg-Ti thin film libraries' The Journal of Alloys and Compounds, 509, 22, 6497-6501 (2011).

- 11.- Molina-Ruiz, M.; Lopeandia, A. F.; Pi, F.; Givord, D.; Bourgeois, O. and Rodriguez-Viejo, J., 'Evidence of finite-size effect on the Neel temperature in ultrathin layers of CoO nanograins' Physical Review B, 83, 14, 140407 (2011).
- 12.- Builes S.; Roussel, T.; Ghimbeu, C.; Parmentier, J.; Gadiou, R.; Vix-Guterl, C. and Vega, L.F., 'Microporous carbon adsorbents with high CO2 capacities for industrial applications' Physical Chemistry Chemical Physics; 13, 16063-16070 (2011).
- Sepulveda, A.; Leon-Gutierrez, E.; Gonzalez-Silveira, M.; Rodriguez-Tinoco, C.; Clavaguera-Mora, M. T. and Rodriguez-Viejo, J., 'Accelerated Aging in Ultrathin Films of a Molecular Glass Former', Physical review Letters, 107, 025901 (2011).
- 14.- López-Aranguren, P.; Saurina ,J.; Vega, L.F. and Domingo, C., 'Sorption of tryalkoxysilane in low-cost porous silicates using a supercritical CO2 method', Microporous and Mesoporous Materials, 148, 15–24 (2011).
- 15.- Pacciani, R.; Torres, J.; Solsona, P.; Coe, C.; Quinn, R, Hufton, J.; Golden, T. and Vega, L. F. 'Influence of the Concentration of CO2 and SO2 on the Absorption of CO2 by a Lithium Orthosilicate-Based Absorbent', Environmental Science & Technology, 45, 7083-7088 (2011).
- 16.- Roigé, A.; Campoy-Quiles, M.; Ossó, J. O.; Alonso, M. I.; Vega, L. F. and Garriga, M., 'Surface vs bulk phase transitions in semiconducting polymer films for OPV and OLED applications' Synthetic Metals, In press.
- 17.- Falk, A.; Ossó, J.O.; Heinemeyer, U.; Broch, K.; Scholz, R.; Gerlach, A. and Schreiber, F., 'Coupling effects in mixed pentacene:perfluoropentacene thin films studied by photoluminescence spectroscopy' The Journal of Chemical Physics ,in press.
- 18.- Llovell, F.; Vilaseca, O. and Vega, L.F., 'Thermodynamic modeling of imidazolium-based Ionic Liquids with the [PF6] anion by means of the soft-SAFT EoS' Separation Science & Technology. In press.
- 19.- López-Periago, A.M.; Pacciani, R.; Vega, L.F. and Domingo, C., 'Monitoring the effect of mineral precursor, fluid phase CO2-H2O composition and stirring on CaCO3 precipitation yield and particle size in a supercritical carbonation process'. Journal of Supercritical Fluids. Cryst. Growth Des., 2011, 11 (12), pp 5324–5332.

20.- Ayyad, O.; Muñoz-Rojas, D. and Gómez-Romero, P., 'Direct synthesis of a macroscopic array of naked Ag nanoparticles' Chem. Commun., 2011, 47, 11285-11287 (2011).

Publications



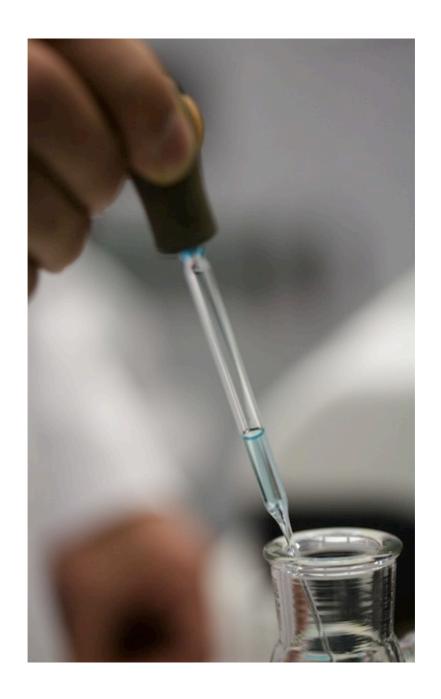
MEETINGS AND CONFERENCE CONTRIBUTIONS

OUTSIDE INVITED TALKS

- 1. "Vegetables in capture and utilization of CO₂", Sonia Guri, Seminar on The Energy of vegetables, organized by Gas Natural Foundation, Murcia, Spain, 14 October 2010.
- 2. "The challenge of capturing and utilizing CO₂", Lourdes F. Vega, Seminar at the Department of Chemical Engineering, Technical University of Denmark, Copenhagen, Denmark, 28 October 2010.
- 3. "CO₂ capture, sequestration and utilization: opportunities and challenges", Lourdes F. Vega, Departmental Seminar at the Department of Chemical and Biochemical Engineering, North Carolina State University, Raleigh, NC, USA, 15 November 2010.
- 4. "Application of the RG theory into EoSs for an accurate description of thermodynamic properties in the critical region of fluids", Fèlix Llovell, Physics Departament, Universidade de Ourense, 17 November 2010.
- 5. " $\rm CO_2$ as a resource: from capture to industrial applications", Lourdes F. Vega at Seminar $\rm CO_2$ as a Resource: Capture, storage and reutilization of $\rm CO_2$, at the Headquarter of Gas Natural in Madrid, Spain, 19 January 2011.
- 6. "Modified atmosphere packaging of food", Sonia Guri, seminar at EMO (food machinery supply) in Barcelona, Spain, 24 February 2011.
- 7. "Modeling of PEM fuel cells", Alicia Arce, seminar at the Institut de Robòtica i Informàtica Industrial, CSIC-UPC in Barcelona, Spain, 4 March 2011.
- 8. "What is the secret of women in Science? The privilege of enjoying your workplace", Lourdes F. Vega, as the inauguration conference for the itinerant exhibition "16 Women in Science", Autonomous University of Barcelona, Barcelona, Spain, 8 March 2011.
- 9. "Modified atmosphere packaging of food", Sonia Guri, seminar in the framework of the Course "Packaging and Commercial Shelf-life", organized by Integrated Safety and Prevention School Center linked to Autonomous University of Barcelona, Barcelona, Spain, 13 April 2011.

- 10. "Modified Atmosphere food Packaging Laboratory. New developments", Sonia Guri. 5th Technical Day about Modified Atmosphere Packaging of food. Organized by Carburos Metálicos, Madrid, Spain, 27 April 2011.
- 11. "On the Exploitation of MPC Formulations for Performance Enhancement of Fuel Cell Systems", Alicia Arce, seminar at the Institut d'Organització I Control de sistemas Industrials, Universitat Politècnica de Catalunya, Barcelona, Spain, 4 May 2011.
- 12. "MATGAS as a center of excellence in CO₂ and sustainability: water treatment", Lourdes F. Vega, Conference: Technical Day about the utilization of gases in water and waste water treatment, Barcelona, Spain, 17 May 2011.
- 13. "Halia® AOP Technology, Advanced Oxidation Process in water treatment", Sonia Guri. Technical Day about the utilization of gases in water and waste water treatment, organized by Carburos Metálicos- MATGAS, Barcelona, Spain, 17 May 2011.
- 14. "A tool for sustainability: what is Life Cycle Analysis?", Roberta Pacciani, XV Anniversary Conference on "Trends in Sustainability in the Chemical Industry", Zakopane, Poland, 18-20 May 2011.
- 15. "Modified Atmosphere food Packaging Laboratory. New developments", Sonia Guri. 6th Technical Day about Modified Atmosphere Packaging of food. Organized by Carburos Metálicos. Vic, Spain, 26 May 2011.
- 16. "Advances in Energy, Sustainability and Environment: MATGAS Achievements and Remaining Challenges", Lourdes F. Vega, X MATGAS' Anniversary. Organized by MATGAS, Bellaterra, Spain, 1 June 2011.
- 17. "CO₂ uses in the agri-food field and for water treatment applications", Sonia Guri and Lourdes F. Vega. VII PASCAL Conference about Environment, Safety and Quality. Organized by CEPSA, Oporto, Portugal, 2-3 June 2011.
- 18. "MATGAS Research Center and current projects", Sonia Guri and Lourdes F. Vega. Workshop on Biotechnology in application Food and non-food, Agriculture and Environment, in the VII Framework Program of 2011 KBBE call, Barcelona, Spain, 6 June 2011.
- 19. "Modified atmosphere packaging of food: adding value to food by means of new developments", Sonia Guri. Partnering Event, Innovation on food and packaging. Organized by UAB, Bellaterra, Spain, 9 June 2011.

- 20. "Present situation related to CO₂ capture and utilization", Lourdes F. Vega, invited lecture given at the workshop "Avoiding global warming: capture, valorization and storage of CO₂", organized by the School of Industrial Operation, Madrid, Spain, 9 June 2011.
- 21. "Industrial CO₂ utilization", Lourdes F. Vega, invited lecture given at the workshop "Technology trends and knowledge transfer in Energy and Environment", organized by the University Forum of Leon, Leon, Spain, 14 June 2011.
- 22. "Materials for carbon capture and utilization in the context of sustainable energy development", Lourdes F. Vega, plenary lecture given at the 25th European Symposium on Applied Thermodynamics, Saint Petersburg, Russia, 24-27 June 2011.
- 23. " CO_2 : an useful resource for the food conservation and water treatment", Sonia Guri, invited lecture given at the Summer school on CO_2 capture, transformation and utilization, Aranjuez, Spain, 4-8 July 2011.
- 24. "Utilization of CO_2 in the industrial and nowadays energetic context", Lourdes F. Vega, invited lecture given at the Summer school on CO_2 capture, transformation and utilization, Aranjuez, Spain, 4-8 July 2011.
- 25. "Utilization and valorization of CO₂", J. Oriol Ossó, Lourdes F. Vega, Summer Course The future of Carbon Capture and CO₂ storage, Andorra, Teruel, Spain, 4-6 July 2011.
- 26. "CO₂ capture, storage and utilization: a key player in the sustainable energy scenario" L.F. Vega, Invited seminar, University of Delaware, Delaware, USA, 3 August 2011.
- 27. "Molecular simulations: a tool for engineering design and optimization from molecular basis" L.F. Vega, Invited seminar, University of Delaware, Delaware, USA, 3 August 2011.
- 28. "What can we do for not having so much CO_2 in the atmosphere?: Capture and utilization of CO_2 in a sustainable world", Lourdes F. Vega, Seminar on Popular Science, "Dinner with stars conference series" (Sopar amb estrelles), Observatory Fabra, Barcelona, Spain, 7 September 2011.
- 29. "CO₂ capture, sequestration and utilization: a key player in the sustainable energy scenario", Lourdes F. Vega, Plenary lecture, Separation technologies for CO₂ Capture, College of Engineering, Swansea University, Wales, UK, 23 September 2011.



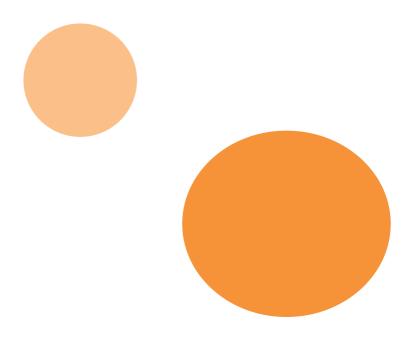
ORAL AND POSTER PRESENTATIONS IN SCIENTIFIC CONFERENCES

- 1. "Experiments and simulations of the behavior of captured ${\rm CO_2}$ on mesoporous silica". S. Builes, P. López-Aranguren, R. Pacciani, C. Domingo, L.F. Vega (oral presentation), AlChE Annual Meeting 2010, 7-12 November, Salt Lake City, UT, USA.
- 2. "Characterization of carbonaceous materials by simulations of CO₂ adsorption". S. Builes, T. Roussel, C. Ghimbeu, J. Parmentier, R. Gadiou, C. Vix-Guterl, L.F. Vega (oral presentation), AIChE Annual Meeting 2010, 7-12 November, Salt Lake City, UT, USA.
- 3. "Thermodynamic study of ionic liquids and their mixtures for separation and extraction processes using the soft-SAFT EoS". E. Valente, F. Llovell, O. Vilaseca, R.M. Marcos, L.F. Vega (oral presentation), AIChE Annual Meeting 2010, 7-12 November, Salt Lake City, UT, USA.
- 4. "Study and Implementation of Advanced Control Technologies to Maximize PEM Fuel Cell Durability". A. Arce, J. O. Ossó, C. Bordons, L. F. Vega (oral presentation), First International Workshop "Long life membranes based on PFSA & SAPs: Preparation and characterization", 17-18 March 2011, Grottaferrata, Italy.
- 5. "Integrating Life Cycle Assessment into Air Products Sustainability best practices". R. Pacciani, M. Listemann, J. Cirucci, E. Arslan, L. F. Vega, J. O'Brien, M. Collins (poster presentation), Growth Conference Poster Sessions, 6-7 April 2011, Allentown, USA.
- 6. "Keep MAP on the map!. Multidisciplinary collaboration to improve food businesses" S. Guri, S. García, L. F. Vega, D. Gamm, R. Wiktorowicz (poster presentation), Growth Conference Poster Sessions, 6-7 April 2011, Allentown, USA.
- 7. "Large scale modeling of organic molecular beam epitaxy". T. Roussel, L. F. Vega (oral presentation), E-MRS 2011 Spring Meeting 10-12 May 2011, Nice, France.
- 8. "Nanoscale in-situ characterization of thermally induced morphological changes on polymer: fullerene thin films during annealing has been". A. Roigé, J. O. Ossó, M. Campoy-Quiles, and L. F. Vega (poster presentation), E-MRS 2011 Spring Meeting 10-12 May 2011. Nice, France.
- 9. "Real-space distribution of cavity modes in single ZnO nanowires". F. Güell, A. R. Goñi, J. López-Vidrier, J. O. Ossó, L. A. Pérez, E. Coronado, A. Cornet, J. R. Morante (oral presentation). Conference on Lasers and Electrooptics CLEO 2011, 22-26 May 2011, Munich, Germany.

- 10. "Molecular Simulations of Tryalkoxysilane Functionalized Porous Silicates", S. Builes, P. López-Aranguren, C. Domingo and L.F. Vega (poster presentation), New trends in Computational Chemistry for Industry Applications, 26-27 May 2011, Barcelona, Spain.
- 11. "Grand Canonical Monte Carlo simulations of adsorption using functionalized amorphous silica", S. Builes, L. F. Vega (poster presentation), XVII Conference on Statistical Physics, FisEs11, 2-4 June, 2011, Barcelona, Spain.
- 12. "Renormalization-group corrections of White's approach for the prediction of the property fluctuations in the critical region applied to SAFT equations", F. Llovell, E. Forte, A. Galindo, and L.F. Vega (poster presentation), XVII Conference on Statistical Physics, FisEs11, Barcelona, 2-4 June, 2011, Barcelona, Spain.
- 13. "Large Scale Modeling of the Self-Assembly of Nano-Objects using a Grid Interpolation technique", T. Roussel and L. F. Vega (poster presentation), XVII Conference on Statistical Physics, FisEs11, 2-4 June, 2011, Barcelona, Spain.
- 14. "Critical, interfacial and surface properties of ionic liquids by a molecular-based equation of state", O. Vilaseca, F. Llovell, and L.F. Vega (poster presentation), XVII Conference on Statistical Physics, FisEs11, 2-4 June, 2011, Barcelona, Spain.
- 15. "Thermodynamic modeling of cross-association systems with the soft-SAFT EoS", F. Llovell, O. Vilaseca, E. Valente, N. Jung, L.F. Vega (oral presentation), 25th European Symposium on Applied Thermodynamics, 24-27 June 2011, Saint Petersburg, Russia.
- 16. "Thermodynamic modeling of alternative refrigerants", O. Vilaseca, F. Llovell, R.M. Marcos, L.F. Vega (poster presentation), 25th European Symposium on Applied Thermodynamics, 24-27 June 2011, Saint Petersburg, Russia.
- 17. "Study and Implementation of Advanced Control Technologies to Maximize PEM Fuel Cell Durability." A. Arce, J.O. Ossó, C.s Bordons and L. F. Vega. (oral presentation), Long life membranes based on PFSA & SAPs: Preparation and characterization, 17-18 March 2011, Grottaferrata, Italy.
- 18. "Real-Space Distribution of Cavity Modes in Single ZnO Nanowires", J. O. Ossó, A.R. Goñi, F. Güell, J. López-Vidrier, L. A. Pérez, E. A. Coronado, J.R. Morante, (oral presentation), BNC-b Research Meeting, 14 July 2011, Bellaterra, Spain.
- 19. "Surface vs bulk phase transitions and nanoscale conductivity measurements in semiconducting organic thin films" A. Roigé, M. Campoy-Quiles, J.O. Ossó, M.I. Alonso, M. Garriga and L.F. Vega, (poster presentation) BNC-b Research Meeting., 14 July 2011, Bellaterra, Spain.

- 20. "Molecular Simulations of Tryalkoxysilane Functionalized Porous Silicates" S. Builes , P. López-Aranguren, C. Domingo and L.F. Vega, (poster presentation) BNC-b Research Meeting , 14 July 2011, Bellaterra, Spain.
- 21. "Modeling the critical, interfacial and surface properties of ionic liquids" O. Vilaseca, F. Llovell, L.F. Vega, (oral presentation) 2nd Iberian Meeting on Ionic Liquids, 20 22 July 2011, Santiago de Compostela, A Coruña, Spain.
- 22. "Physicochemical properties of ionic liquids by a molecular-based equation of state" O. Vilaseca, F. Llovell and L. F. Vega (oral presentation) 1st International Conference on Ionic Liquids in Separation and Purification Technology, 4-7 September 2011, Sitges, Spain.
- 23. "Vapour printing: a one step method to locally control of the optical and electronic properties of organic semiconductors" M. Campoy-Quiles, D. Nassyrov, C. Müller, A. Roigé, M. Aghamohammadi, J.O. Ossó, A.R. Goñi, D. Amabilino, M. Garriga, M.I. Alonso, (poster presentation), European Conference on Molecular Electronics (ECME), 7-10 September 2011, Barcelona, Spain.
- 24. "Characterization of the black liquors pyrolysis by Computational Fluid Dynamics" P. Martín, L. Vega, J. Torres, W. Chang (oral presentation), EUROBIOREF Summer School, 18-24 September 2011, Castro Marina, Lecce Italy.
- 25. "Molecular simulations of ${\rm CO_2}$ capture using amine functionalized amorphous silica" S. Builes, L. F. Vega (oral presentation), 8th European Congress of Chemical Engineering; ICC Internationales Congress Centrum Berlin, 25 29 September 2011, Berlin, Germany.
- 26. "An Integrated Microbalance System to Evaluate High Temperature of ${\rm CO_2}$ Adsorbents in the Presence of Steam". C. Coe, R. Pacciani, L. Vega, J. Torres, P. Solsona, J. Hufton, R. Quinn, T. Golden (oral presentation), 39th Annual Conference of the North American Thermal Analysis Society, August 7-10, 2011. Des Moines, Iowa.
- 27. "Development and optimization of new materials for CO_2 capture: the importance of testing under real capture conditions". R. Pacciani, J. Torres, R. Ramirez, S. Builes, P. Lopez-Aranguren, A. Lopez-Periago, C. Domingo, L. F. Vega (oral presentation), Seminar on Separation technologies for CO_2 capture & storage, September 23, 2011, Swansea, UK.







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