

# **Activity Report 2009**





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### INTRODUCTION

MATGAS 2000 AIE, known as MATGAS, is a non-profit organization, born as a joint venture among 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 **MAT**erials and **GAS**es, for different applications. As the demand for energy is expected to grow, clear steps should be taken towards reducing the emission of  $CO_2$  (and other greenhouse gases). One way of doing it is by developing technologies to efficiently capture it, transport it and use it in an environmentally safe manner, as well as searching for alternative energies and processes, for a sustainable development. **MATGAS**, as a center of excellence in  $CO_2$  and sustainability, is working in different angles of this complex problem, combining in a synergetic manner modeling with experiments. We do these developments in close contact with our strategic partners, with other researchers and with final users.

**MATGAS** provides an open framework and environment for creative discussions and advance of research in close contact with the industrial world.





## MatGas

- Partners
- People at MATGAS
- MATGAS Laboratories



MATGAS is a nonprofit economical interest group among the company Carburos Metálicos - Air Products Group, the Spanish National Research Council (CSIC) and the Autonomous University of Barcelona (UAB).

Our main objective is to contribute to the research and development of technologies related to  $CO_2$  and sustainable energies, empowering the synergy among entrepreneurship, research and education sectors.

THREF PARTNERS - ONE GOAL

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

Air Products Today: 21,000 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, April 2009

From bottom to top and from left to right:

Emili de la Serna, Joaquim Torres, Abel Roigé, Jordi Andreu, Aurora Aguilera, Javier Rodríguez-Viejo, Anna Roig, Lourdes Vega, Erwin Zwicky, Jordi Marquet, María Nikolou, María Mercadé, Montse Salas, Thomas Roussel, Ricardo, Raúl Solanas, Roberta Pacciani, Albert Moreno, Ignasi Salvadó, Jaume Capell, Aida Al-Nehlawi, Sonia Guri, Oriol Ossó

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### **MATGAS** Staff

Director:	Dr. Lourdes Vega	(CM-APCI)
Vice-directors:	Dr. Anna Roig Dr. Javier Rodríguez-Viejo	(CSIC) (UAB)
Executive Assistant:	Mrs. Montserrat Salas	(CM-APCI)
Project Managers:	Mr. Joan Comas Dr. Ignasi Salvadó	(CM-APCI) (CM-APCI)
Project Assistant:	Mrs. María Mercadé	(MATGAS)
Project Coordinators:	Dr. Sonia Guri Dr. Maria Nikolou Dr. Oriol Ossó	(CM-APCI) (CM-APCI) (CM-APCI)
Project Supervisor:	Mr. Joaquim Torres	(CM-APCI)
Technical Coordination:	Dr. Raquel Ramirez Mr. Javier Rubio Mr. Raul Solanas	(UAB) (CSIC) (CSIC)
Research Associates:	Dr. Roberta Pacciani Dr. Óscar J. Prado	(CM-APCI) (MATGAS)
Research Assistant:	Mrs. Aida Al-Nehlawi Mr. Santiago Builes Mr. Pedro López-Aranguren Mr. Oriol Vilaseca	(PhD Student) (PhD Student) (PhD Student) (PhD Student)
Technology Watch/web:	Mr. Jaume Capell	(CSIC)
Suppport to projects/web:	Mr. Albert Moreno	(CSIC)
Documentation and SAP:	Mrs. Aurora Aguilera	(CM-APCI)
Maintencance and workshop	Mr. Emili de la Serna Mr. Toni Pons Mr. José Rodríguez	(CM-APCI) (CSIC) (CSIC)



#### **MATGAS** Laboratories

The research carried out at MATGAS is focused on CO<sub>2</sub> and other energy related issues, including hydrogen and alternative energies. 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 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, 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 nanoscale. The equipment includes SPM techniques (AFM and SNOM), particle size determination tools, micro-Raman scattering, n a n o c a l o r i m e t r y, a n d 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, with 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 CO<sub>2</sub> capture and the behavior of selected ionic liquids.

In addition to these labs MATGAS also offers an energy laboratory which is under expansion and a high bay area for the construction and testing of new prototypes.



## **R**ESEARCH **A**CTIVITIES

- Scientific Projects and Contracts
- MATGAS Conferences
- Meetings and Conference Contributions



SOST-CO2 –CENIT project, 1st General Assembly held in MATGAS

2010 ->CDTI	Acronym: Title: Objectives:	<b>SOST-CO2 – CENIT project</b> New industrial and sustainable uses of CO2 The main objective of the project is to develop CO2 utilization technologies, complementing capture technologies, as an alternative to the geological storage only. 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.
	Budget:	26.26 Million euros. Leader: Carburos Metálicos, Air Products Group.
	Consortium:	15 companies, 28 research centers
	Status:	Started in 2008, ending in 2011
	MATGAS	Three partners / Three different ways of participation: - CM/APCI: Leader of the Consortium - CSIC: 8 contracts in the consortium - UAB: 2 contracts in the consortium
	MATGAS	Lead the technical management part of the project
	MATGAS	Has been contracted by three other companies as a Research Center expert in CO2 capture and applications

The project is developed by a significant consortium comprising 16 companies and 27 research centers. The consortium will unit efforts for four years.

CONS	SORTIUM I	ED BY:	CA ME Grup	RBUROS TALICO	S S ets	
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Fundación it ma 🔇	AIMPLAS		IBVF			ΓΟ
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Rey Juan Carlos	nalitat de Recorca en Energia de Catatar atalanía institute for Coergy Resear	UPC			Cantha Tanana Ia Photocolor	igen aus at Diante y Industriar de Raturias



Acronym:	NOMOCELL
Title:	Nanostructured organic materials for highly efficient plastic
	solar cell applications
Objectives:	Further enhance the efficiency of plastic solar cells towards
	10%-15%, the predicted range for economically viable market
	uptake of this technology.
PI:	M. Campoy (CSIC)
Members:	M. Garriga (CSIC), and J. O. Ossó (CM-APCI, MATGAS)

Acronym:	ENAPROMAT
Title:	Rational design of processes and materials for energy and
	nanotechnology applications
Objectives:	The systematic improvement of selected processes and materials, related to energy and nanotechnolgy, by a combination of molecular modeling techniques with advanced expertimental techniques. The three particular objectives are: 1) the use of alternative solvents for different applications, including ionic liquid and supercritical fluids, 2) systematic search for new adsorbents for selective separation, with special emphasis on CO2 and other greenhouse gases and 3) design, characterization and applications of nanoparticles and other materials for different industrial applications
DL	
PI:	L.F. Vega (IVIAIGAS, CSIC)
Members:	C. Domingo (CSIC), R.M. Marcos (URV), F. Llovell (CSIC)

Acronym:	<b>Torres Quevedo awards</b> These grants are given from the Spanish government to companies to hire PhDs to start or reinforce research areas of interest to the company. It covers approximately 50% of their salary for 3 years.
Title: Objectives:	Applications and control of gases in the food industry Coordination of different research projects related to the application of gases in the food industrial sector. The projects will be in the areas of (a) Modified Atmosphere Packaging (MAP), (b) $CO_2$ utilization for desinsectation, (c) aromatic compounds detection in $CO_2$ , and (d) development of microsensors for wine analysis.
PI:	S. Guri (CM - APCI, MATGAS)
Title: Objectives:	Photocatalytic Reactors for $CO_2$ reduction Design, construction, and modeling of photocatalytic reactors for $CO_2$ reduction for the production of syngas and other added-value products. The project combines management tasks with R&D activities to design photocatalytic reactors for $CO_2$ reduction.
PI:	I. Salvadó (CM - APCI, MATGAŚ)

## Generalitat de Catalunya www.gencat.cat

Title:	Consolidated Group from the Generalitat of Catalonia
	2009 SGR 666
Objectives:	To support the research carried out by quality groups, as
	approved by the catalan Government
PI:	L. F. Vega (MATGAS, CSIC)
Members:	C. Domingo (CSIC), R. M. Marcos (URV), F. Llovell (CSIC), T.
	Roussel (CSIC)

## **INFITERS** INDUSTRIAL CONTRACTS

Title:	Acidification of water effluents from power plants
	refrigeration systems through CO <sub>2</sub> .
Objective:	Physico - chemical characterization of water
IP:	S. Guri (CM-APCI)
Members:	L. Vega, E. Rodriguez (Iberdrola), J. Lafuente (UAB) and O.
	Prado (MATGAS)
Company:	Iberdrola
Starting date:	01/OCT/08
Duration:	3 years

CO <sub>2</sub> enriched atmospheres for poultry packaging.
Evaluate the different CO <sub>2</sub> concentration on microbiological
and physico-chemical properties of poultry meat.
S. Guri (CM-APCI)
A. Al-Nehlawi (MATGAS), A. Corujo (Nutreco) and C. Martin
(Nutreco)
Nutreco
01/JAN/08
3.5 years

Title:	Design & Assembly of a demonstration unit to blend and
	inject CO <sub>2</sub> at high pressure.
Objective:	Design a demo unit for expanding new polymers by $CO_2$
	injection.
IP:	J. Torres (CM - APCI)
Members:	J. Fauquier, M. Gómez, and E. Cuesta (LINPAC).
Company:	LINPAC
Starting date:	01/JAN/08
Duration:	2 years



Acronym:	ICREA JE (Junior Enterprise)
	This project is externally funded by the Catalan government
	through a prestigious award given to O. Ossó and Carburos
	Metálicos. The objective of these grants is to promote the
	incorporation of brilliant researchers to the industry section
	and thus facilitate the transfer of knowledge between the
	public and private sectors.
	It provides approximately 50% of Oriol's salary for 5 years.
Title:	Organic semiconductors for photovoltaic applications
Objectives:	Improve organic cells efficiency by controlling their structure
	and morphology at the nanometer scale.
IP:	J. Oriol Ossó (CM - APCI)
Members:	F. Schreiber <sup>1</sup> , E. Barrena <sup>2</sup> , H. Dosch <sup>2</sup> , and J. Puigdollers <sup>3</sup> .
	<sup>1</sup> Universität Tübingen, Tübingen, Germany.
	<sup>2</sup> Max-Planck-Insitut für Metallforschung, Stuttgart, Germany.
	<sup>3</sup> Universitat Politècnica de Catalunya, Barcelona, Spain.





## EC FUNDED PROJECTS

Acronym:	SUPERGREENCHEM –Marie Curie Research Training Network
Title:	Green Chemistry in Supercritical Fluids: Phase Behaviour, Kinetics and Scale-up
Objectives:	To solve a key technical issue that is limiting the use of Supercritical Fluids (SCFs), namely the relatively poor solvent power of many SCFs, which can spoil the economics of otherwise highly attractive processes. The network will target four areas of SCF chemistry (i) reactions with gases (e.g. hydrogenation, oxidation, hydroformylation, etc), (ii) reactions in mixed SCF/lonic liquid solvent systems, (iii) polymerisation and (iv) biocatalysis. These four areas are linked by a fifth, common theme of high-pressure phase equilibria.
Acronym:	PROTEC
litle:	biodegradable polymers targeting medical applications
Objectives:	The main objective of the project is to develop supercritical CO2 processing technologies for the production of biodegradable polymers for medical applications.
Acronym:	COSY
Title:	Complex Solid State Reactions for Energy Efficient Hydrogen Storage

Objectives: To reach a fundamental understanding of the sorption kinetics in Reactive Hydride Composites and related systems through three different strategies: empirical studies, model systems and a theoretical/modeling approach.

#### Acronym:

#### SURFACE T

Title: Objectives: Sustainable Surface Technology for Multifunctional Materials To develop an innovative supercritical carbon dioxide (SCCO2) surface technology, applicable to existing and new high performance functional products. This should lead to procedures that enable the creation of complex surface structures, enabling the production of unique product characteristics in relation to composition, purity, and effectiveness. MATGAS activity is focused on:

- to assess on selection and screening of solvents from a legal and safety point of view.
- to participate on the selection of real and model products to work on.
- to pevelop a view cell in collaboration with CSIC.
- to enlarge our scaling capabilities by mounting a 16L high pressure vessel into the pilot plant.

### **S**EMINAR SERIES ON CO2 AND RELATED ISSUES

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 CO2 capture, utilization and energy issues associated to environmentally benign energy technology.

Several international experts on CO2 capture, sequestration, utilization and energy connected issues (including hydrogen) have been invited and will be invited to participate at 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.

#### Prof. Dr. Rafael MOLINER

Coordinator: Chemical Science and Technology Area (CSIC), Zaragoza, Spain «Using of Hydrogen/Natural Gas mixtures: A strategy to introduce Hydrogen into the transport sector» SEPTEMBER 22nd 2009

#### Prof. Dr. John DENNIS

Department of Chemical Engineering and Biotechnology, University of Cambridge, UK «Chemical Looping Combustion one answer to separating carbon dioxide from fuel gas» JULY 14th 2009

#### Prof. Dr. José Luís GARCÍA FIERRO

Instituto de Catálisis y Petroleoquímica, CSIC, Madrid, Spain «An Outlook on the Carbon-Free Hydrogen Production Technologies» JUNE 17th 2009

#### Dr. Mario GARMA OBREGÓN

Process Engineering Department SE de Carburos Metálicos, SA – Air Products Group, Madrid, Spain «A Gas Company view of CO2 Manufacturing: Process descriptions and requirements for the food grade market» MAY 21<sup>st</sup> 2009

#### Dr. ÓSCAR PRADO

Department of Chemical Engineering (UAB) / MATGAS 2000 AIE, Spain «Biofiltration: a reliable and economical technology for the treatment of gaseous pollutants» MARCH, 5th 2009

#### Prof. Dr. Vicente J. CORTÉS

Director, CO2 Capture Programme / CIUDEN, Fundación Estatal Ciudad de la Energía, Ponferrada, Spain «CO2 Capture technologies» JANUARY, 28 th 2009

#### Dr. Jara IMBERS QUINTANA

University of Nottingham, UK «Mathematical modelling, from Nanotechnology to Mediterranean Lakes» JANUARY, 15th 2009

#### Prof. Joan Ramón MORANTE

IREC, Catalonia Institute for Energy Research, Barcelona, Spain Tailoring metal oxides and other semiconductors nanostructures for enhancing their interactions with chemical and photons. NOVEMBER, 28th 2008

#### Dr. Roberta PACCIANI

Department of Chemical Engineering and Biotechnology, University of Cambridge, UK «An improved Ca-based solid sorbent for clean energy from coal» OCTOBER 30<sup>th</sup> 2008

## **O**THER SEMINARS HELD IN MATGAS

#### Dr. Ignacio PAGONABARRAGA

Department of Fundamental Physics, University of Barcelona «Control and structure formation in internally driven colloids» FEBRUARY 24<sup>th</sup> 2009

#### Dr. Thomas ROUSSEL

Centre de Recherche en Matière Condensée et Nano-Sciences (CRMCN) «How can we Control the Porosity of Carbon Materials? – Application to Hydrogen Storage –» JANUARY 21<sup>st</sup> 2009

#### Prof. Jordi MARQUET

Vice-Rector for Strategic Projects Director «Parc de Recerca UAB (PRUAB)» Knowledge and Technology Transfer in the UAB Sphere. The model of the «Parc de Recerca UAB» NOVEMBER, 11th 2008

### MEETINGS HELD IN MATGAS

2<sup>nd</sup> General Assembly of the Consortium CENIT SOST-CO2 Project «New industrial and sustainable uses of CO2» JULY 21<sup>st</sup> 2009

Meetings of the **technical and executive committees of the CENIT SOST-CO2 project**. The technical and executive committees of the CENIT project, including the technical leaders of all activities and the responsible of the execution of the project, lead by CM-APCI were held at MATGAS. MAY 29<sup>th</sup> 2009

MATGAS held the 1<sup>st</sup> Spanish-Norwegian Seminar on Carbon Capture and Storage (CCS), organized by the Spanish CO2 Platform and the Norwegian Embassy. The workshop put together industrial and academic experts in the field, as well as politicians involved in the area. There were several presentations and fruitful discussions for collaborations. MAY 26<sup>th</sup> 2009 **Technical Water Day**, organized by Bulk Southern Europe. This was a workshop organized by the business area in collaboration with MATGAS (Sonia Guri). The workshop dealt with different water applications our company offers. The speakers were experts from our company and outside invited speakers. The commercial and marketing teams gave support to the technology team. More than 50 potential customers attended the workshop. MARCH 31<sup>st</sup> 2009

Meetings of the **technical and executive committees of the CENIT SOST-CO2 project**. The technical and executive committees of the CENIT project, including the technical leaders of all activities and the responsible of the execution of the project, lead by CM-APCI were held at MATGAS. MARCH 2<sup>nd</sup> 2009

## MEETINGS AND CONFERENCE CONTRIBUTIONS

## OUTSIDE INVITED TALKS

«CO2 as resource in the renewable carbon cycle» <u>L.F.Vega</u> Invited lecture Curso de Fronteras de la Energía, Benasque, Spain JULY 5 –  $10^{\text{th}} 2009$ 

«Molecular Simulation and Theory as Reliable Tools to Design Products and Processes» L.F. Vega Invited lecture in the Reference Network on Theoretical and Computational Chemistry - New Trends in Computational Chemistry for Industry Applications, Barcelona, Spain JULY 6 – 7<sup>th</sup> 2009

«Is CO2 as awful as it looks like? » <u>I. Salvadó</u> Invited talk in the Social Barcelona Tech Summer Sessions (b\_TEC) JULY 8<sup>th</sup> 2009

«New Industrial Uses of CO2» <u>L.F. Vega</u> Invited lecture in V Barcelona tech summer sessions (b\_TEC), energy water mobility, Barcelona, Spain JUNE 29 – JULY 3<sup>rd</sup> 2009

«Ionic Liquids: modelling, characterization and design for specific industrial applications» <u>L.F. Vega</u> Plenary lecture in the 24<sup>th</sup> European Symposium on Applied Thermodynamics, Santiago de Compostela, Spain, JUNE 27 – JULY 1<sup>st</sup> 2009

«Insights Into Mesoscopic, Micro-heterogeneous and Fluctuating Systems by Molecular Modeling and Simulations» L.F. Vega Invited lecture in the 17th Symposium on Thermophysical Properties Boulder, USA JUNE 21- 26<sup>th</sup> 2009 «Predicting the behaviour of Interfacial Properties of Binary Mixtures by a Molecular Modeling Approach»

L.F. Vega, Andres Mejía, Oriol Vilaseca

Invited lecture in the 17th Symposium on Thermophysical Properties Boulder, USA

JUNE 21- 26<sup>th</sup> 2009

«Modified atmosphere packaging. Opportunities for seafood & ready to eat products» <u>S. Guri</u>, L. Romero II Conference about MAP, Organized by CM– APCI, Santiago de Compostela, Spain JUNE 18<sup>th</sup> 2009

«MATGAS: A Research Centre on CO2 and Energy» <u>I. Salvadó</u> Invited talk at the Forum Empresarial d'Energies Renovables, organized by PIMEC Innovation MAY 14<sup>th</sup> 2009

«MATGAS food technology offer»

<u>S. Guri</u>

Invited talk at FITECH, in the frame of the Barcelona Food Technology (BTA) MAY  $12^{th}$  2009

«Water re -use and disinfection. Advanced oxidation, HiPOX technology» <u>S. Guri</u>

I Conference about gases for water and sludge treatment, Organized by CM– APCI at MATGAS, Barcelona, Spain MARCH 31<sup>st</sup> 2009

«Modified atmosphere packaging of food» <u>S. Guri</u> Thermoforming advanced course. Organized by EMO Service. Barcelona, Spain FEBRUARY 25<sup>th</sup> 2009

«MATGAS' opportunities and future collaborations» <u>L.F. Vega</u> Invited talk by the director of the Chemistry Department of the Autonomous University, Barcelona, Spain FEBRUARY 27<sup>th</sup> 2009 «Scientific Research in Private Companies» <u>L.F. Vega</u> Invited talk at the National Meeting of Young Researchers (CSIC), held in Barcelona, Spain FEBRUARY 25<sup>th</sup> 2009

«MATGAS, CENIT SOST-CO2» <u>L.F. Vega</u> Invited talk to present the CENIT SOST-CO2 program as the technical coordinator at the 1<sup>st</sup> Assembly of the Spanish Platform of CO2. Madrid, Spain FEBRUARY 13<sup>th</sup> 2009

«MATGAS Research Center» FLUCOMP, Madrid, Spain L.F. Vega FEBRUARY 5<sup>th</sup> AND 6<sup>th</sup> 2009

«Roundtable on CO2 capture and sequestration» <u>Dr. L.F. Vega</u> Roundtable held at the British Embassy, organized by the British Association for CO2 capture and storage and the Spanish CO2 Association. NOVEMBER 6th 2008

«Carbon dioxide as a resource» <u>Dr. L.F. Vega</u> Plenary lecture as part of the VIII Seminario Internacional sobre Cambio Climático, Nuevas tecnologías contra el cambio climático, Organized by GAS NATURAL and the Ministry for Environment of Spain NOVEMBER 5th 2008,

## **O**RAL **P**RESENTATIONS

«Polydispersity indexes of liniar polymer melts from rheological measurements» <u>R.M. Marcos</u>, L.F. Vega. XII Congreso Internacional en Ingeniería de Proyectos, 8 – 10 July, Badajoz, Spain «Characterizing the Solubility of Gases in Ionic Liquids through a Molecular Based Equation of State»

J. Andreu, L.F. Vega

 $24^{th}$  European Symposium on Applied Thermodynamics: ESAT 2009, 27 June – 1<sup>st</sup> July, Santiago de Compostela, Spain

«The Influence of the Force Field Used in Simulations in the Adsorption Behavior of Carbon Dioxide» S. Builes, <u>L.F. Vega</u>

17th Symposium on Thermophysical Properties, 21 – 26 June Boulder, USA

«Characterizing the Solubility of Gases in Ionic Liquids through a Molecular Based Equation of State»

J. Andreu, L.F. Vega

17th Symposium on Thermophysical Properties, 21 – 26 June Boulder, USA

«Rational Design of Ionics Liquids for Specific Applications: Equilibrium and Transport Properties from Soft-SAFT and Molecular Dynamics Simulations» J. Andreu, L.F. Vega

9º Encontro Nacional de Química Física -1st Iberian Meeting on Ionic Liquids, University of Aveiro, 15 – 16 June, Aveiro, Portugal

«The Performance of a Novel Synthetic Ca-Based Solid Sorbent Suitable for the Removal of CO2 and SO2 from Flue Gases in A Fluidised Bed» <u>R. Pacciani</u>

20th International Conference on Fluidized Bed Combustion, 18 – 21 May, Xi'An, China

«Wave-guiding effects in a single ZnO nanowire» <u>F. Güell</u>, J. O. Ossó, A R Goñi, L. Vega, A. Cornet, J.R. Morante European Conference on Lasers and Electro-Optics, 14 – 19 June, Munich, Germany

«Actividades de investigación relacionadas con fluidos supercríticos. MATGAS como centro de excelencia en CO2. Sinergia modeladoexperimentación en temas relacionados con CO2 y energía» L.F.Vega

Tercera reunión de expertos en tecnologías de fluidos supercríticos, 4-6 February, Madrid, Spain

## **POSTER PRESENTATIONS**

«Transport properties of ionic liquids and their mixtures with water and  $\operatorname{CO2}$ »

J. S. Andreu and L. F. Vega

XVI Congreso de Física Estadística, 10 - 12 September 2009, Huelva, Spain.

«Influence of the flexibility of the force field model on the adsorption of greenhouse gases»

S. Builes, A. Olivet, and L. F. Vega

XVI Congreso de Física Estadística, 10 - 12 September 2009, Huelva, Spain.

«Phase and interface behavior of pure compounds and binary mixtures with soft-SAFT coupled with density gradient theory»
<u>O. Vilaseca</u>, R. M. Marcos, and L. F. Vega
XVI Congreso de Física Estadística, 10 - 12 September 2009, Huelva, Spain.

«Wave-guiding effects in a single ZnO nanowire» <u>F. Güell</u>, J. O. Ossó, A R Goñi, L. Vega, A. Cornet, J.R. Morante European Conference on Lasers and Electro-Optics, 14 – 19 June, Munich, Germany

«Assisted self assembly of solution derived CeO, 9Gd0, 1O2-y interfacial nanostructures on mechanically modified perovskite type substrates» J. Zabaleta, M. Gibert, J. O. Ossó, P. Abellán, F. Sandiumenge, N. Mestres, T. Puig, X. Obradors EMRS Spring Meeting, 8 – 12 June, Strasbourg, France

«Direct imaging of the visible emission bands from individual ZnO nanowires by near-field optical spectroscopy» <u>F Güell</u>, J O Ossó, A R Goñi, A Cornet and J R Morante EMRS Spring Meeting, 8 – 12 June, Strasbourg, France

«Optimization of organic bulk heterojunction solar cells – The benefits of mixing»

<u>M. Neophytou</u>, I. Etxebarria, U. Munecas, J. Ajuria, M. Campoy, J. O. Ossó, A. Roigé, C. Waldauf, S. Choulis, R. Pacios EMRS Spring Meeting, 8 – 12 June, Strasbourg, France «SNOM and STXM characterization of Pentacene-Perfluoropentace heterojunctions»

J. O. Ossó, S. Kowarik, A. Hinderhofer, A. Gerlach, U. Heinemeier, L. F. Vega, F. Schreiber

EMRS Spring Meeting, 8 – 12 June, Strasbourg, France

«Synergistic effect of modified atmosphere packaging and use of food additives for the preservation of corn cakes» <u>A. Al-Nehlawi</u>, S. Guri Second International Congress on Food Safety (SAFE consortium), 27 – 29 April, Girona, Spain

«MATGAS - Investigación y equipamientos - Laboratorio de fluidos supercríticos» <u>R.Solanas</u>, J.Torres, L.F.Vega Tercera reunión de expertos en tecnologías de fluidos supercríticos, 4-6 February, Madrid, Spain

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## PUBLICATIONS

PATENTS

## **A**RTICLES IN **J**OURNALS

- Capturing the Solubility Minima of n-Alkanes in Water by Soft-SAFT
  L. F. Vega, F. Llovell and F. J. Blas
  Journal of Physical Chemistry B 113, 7621-7630 (2009)
- 2.- Bulk soft magnetic materials from ball-milled Fe77Nb7B15Cu1 amorphous ribbons
   J. Torrens-Serra, R. Bruna, S. Roth, J. Rodriguez-Viejo and M. T. Clavaguera-Mora
   Intermetallics 17, 79-85 (2009)
- 3.- Structural and magnetic characterization of FeNbBCu alloys as a function of Nb content
   J. Torrens-Serra, P. Bruna, S. Roth, J. Rodriguez-Viejo and M. T. Clavaguera-Mora
   Journal of Physics D-Applied Physics 42, (2009)
- 4.- Supercritical-Fluid-Assisted One-Pot Synthesis of Biocompatible Core(gamma-Fe2O3)/Shell(SiO2) Nanoparticles as High Relaxivity T-2-Contrast Agents for Magnetic Resonance Imaging
   E. Taboada, R. Solanas, E. Rodriguez, R. Weissleder and A. Roig
   Advanced Functional Materials 19, 2319-2324 (2009)
- 5.- Selective Paraffin Removal from Ethane/Ethylene Mixtures by Adsorption into Aluminum Methylphosphonate-alpha: A Molecular Simulation Study
   M. C. Kroon and L. F. Vega
   Langmuir 25, 2148-2152 (2009)
- 6.- Synthesis and optical spectroscopy of ZnO nanowires
  F. Güell, J.O. Ossó JO, A.R. Goni, A. Cornet and J.R. Morante
  Superlattices and Microstructures 45, 271-276 (2009)
- 7.- Glass transition in vapor deposited thin films of toluene
   E. Leon-Gutierrez, E; G. Garcia, M. T. Clavaguera-Mora, J. Rodríguez-Viejo
   Thermochimica Acta, 492, 1-2, pp. 51-54 (2009)
- 8.- Direct imaging of the visible emission bands from individual ZnO nanowires by near-field optical spectroscopy
  F. Guell, J. O. Ossó, A. R. Goni, A. Cornet and J. R. Morante
  Nanotechnology 20, (2009)

- 9.- Synthesis and optical spectroscopy of ZnO nanowires F. Güell, J.O. Ossó, A.R. Goñi, A. Cornet, J.R. Morante Superlattices and Microstructures 45, 271-276 (2009)
- Crystallisation of Amorphous Germanium Thin Films
   G. Garcia, A. F. Lopeandia, A. Bernardi, M. I. Alonso, A. R. Goni, J. L.
   Labar and J. Rodriguez-Viejo
   Journal of Nanoscience and Nanotechnology 9, 3013-3019 (2009)
- 11.- Organo-modified silica aerogels and implications for material hydrophobicity and mechanical properties
   L. Martin, J. O. Ossó, S. Ricart, A. Roig, O. Garcia and R. Sastre
   Journal of Materials Chemistry 18, 207-213 (2008)
- 12.- An accurate direct technique for parametrizing cubic equations of state Part III. Application of a crossover treatment
   F. Llovell, L. F. Vega, D. Seiltgens, A. Mejia and H. Segura
   Fluid Phase Equilibria 264, 201-210 (2008)
- 13.- Carbon nanotube-TiO2 hybrid films for detecting traces of O-2
   E. Llobet, E. H. Espinosa, E. Sotter, R. Ionescu, X. Vilanova, J. Torres, A. Felten, J. J. Pireaux, X. Ke, G. Van Tendeloo, F. Renaux, Y. Paint, M. Hecq and C. Bittencourt
   Nanotechnology 19, (2008)
- 14.- In situ nanocalorimetry of thin glassy organic films
   E. Leon-Gutierrez, G. Garcia, A. F. Lopeandia, J. Fraxedas, M. T. Clavaguera-Mora and J. Rodriguez-Viejo
   Journal of Chemical Physics 129, (2008)
- 15.- Tuning in-plane magnetic anisotropy in (110) La2/3Ca1/3MnO3 films by anisotropic strain relaxation
  I. C. Infante, J. O. Ossó, F. Sanchez and J. Fontcuberta
  Applied Physics Letters 92, (2008)
- 16.- Exciton-phonon coupling in diindenoperylene thin films
   U. Heinemeyer, R. Scholz, L. Gisslen, M. I. Alonso, J. O. Ossó, M. Garriga, A. Hinderhofer, M. Kytka, S. Kowarik, A. Gerlach and F. Schreiber
   Physical Review B 78, (2008)

- Uniaxial anisotropy of organic thin films determined by ellipsometry
   U. Heinemeyer, A. Hinderhofer, M. I. Alons, J. O. Ossó, M. Garriga, M. Kytka, A. Gerlach and F. Schreiber
   Physica Status Solidi a-Applications and Materials Science 205, 927-930 (2008)
- 18.- Interfacial effects on the thermal conductivity of a-Ge thin films grown on Si substrates
   J. Alvarez-Quintana, J. Rodriguez-Viejo
   Journal of Applied Physics, 104, 7, pp. 074903 (2008)

## PATENTS

Title:	Process for erradication of pests in an agricultural product
Inventor:	J. Riudavets, C. Castañé, C. Alomar, S. Guri, J. Sánchez
Applicant:	S.E. de Carburos Metálicos, SA
Number:	(EP08382036.5) - European Patent
Year:	2008

## PhD THESIS AND OTHER RESEARCH WORKS

#### PhD thesis defended in MatGas financed by MatGas projects - CSIC student

Title:	Molecular Modeling of SF6
Author:	Dr. Aurelio Olivet
Director:	Dr. Lourdes F. Vega
Grade:	Excellent cum laude

Thermal transport in low dimensional structures and films.
Dr. Jaime Álvarez
Dr. Javier Rodríguez-Viejo
Excellent cum laude

#### Diploma of Advanced Studies (PhD studies), financed by MatGas projects

Title:	Modeling of ionic liquids and CO2
Author:	Jordi S. Andreu (CSIC-MATGAS)

- Director:
- Dr. Lourdes F. Vega
- Title: Interfacial properties of important relevant fluids Author: Oriol Vilaseca (MATGAS) Dr. Lourdes F. Vega Director:
- Modeling of CO2 adsorbents Title: Author: Santiago Builes (CSIC-MATGAS)
- Director: Dr. Lourdes F. Vega

#### **Research training at MATGAS**

Final Engineering Project student. Materials engineering

Student:	Mr. Abel Roigé Godia
Title:	Organic photovoltaic cells
Supervisor:	Dr. Oriol Ossó

Undergrad UAB student in training in MatGas under industrial training education.

Student: Title:	Ms. Silvia Donnici Synthesis and characterization of materials for CO2 photoreduction
Supervisor:	Dr. Oriol Ossó
Student: Title:	Mr. Joan Atcher Synthesis and characterization of materials for CO2 photoreduction
Supervisor:	Dr. Oriol Ossó
Student: Title:	Ms. Laura Cabana Synthesis of carbon/transition metall oxide composites by SCF drying and electrochemical characterization
Supervisor:	Dr. Lourdes Vega and Dr. Rosa Palacín
Student: Title:	Mr. Ricardo Noe Rodríguez Strategies to integrate CO2 capture and utilization technologies
Supervisors:	Mr. Joaquim Torres
Student: Supervisors:	Pablo Gago Ferrero Dr. Lourdes F. Vega (CM/APCI) and Prof. Javier Rodriguez-Viejo (UAB)

**ERASMUS Students** 

 Student: Mr. Guilherme Coelho
 Title: Biopolymers – verification of its applicability in modified atmosphere packaging
 Project presented at the «Escola Superior de Biotecnologia, Universidade Católica Portuguesa, Porto» achieving a 18/20 qualification.
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Student:Ms. Laura WojtasTitle:Nutritional ScienceSupervisor:Dr. Sonia Guri





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