

# 1st European Symposium on Computing $\Pi$ -Conjugated Compounds

*symposium* [greek: συμποσιον] = a convivial meeting, usually following a dinner, for drinking and intellectual conversation

Institute of Molecular Science (ICMol), University of Valencia, Spain

21.-23.01.2010



## Symposium CTTc

Salón de Actos,  
Institute for Molecular Sciences (ICMol)  
University of Valencia  
Poligono Coma SN  
46980 Paterna (Valencia)

### Organization:

Dr. Begoña Milián Medina  
Dr. Johannes Gierschner

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## Programme

### Thursday, 21.01.

#### 21.00 Welcome Reception & Dinner (Taberna Los Monjes, Burjassot)

Meeting Point Hotel Los Silos 20:30 h

### Friday, 22.01.

Meeting Point: Hotel Los Silos 08:20 h

#### Session A (08:50 - 10:30) - Chairman: Philippe Marsal (Marseille)

08.50 welcome address

09.00 Luis Serrano Andrés (keynote): *Quantum Chemistry, Excited States, and  $\pi$ -Conjugated Systems: New Frontiers*

09:40 Patrick Trouillas: *Antioxidant Properties of  $\pi$  Conjugated Natural Polyphenols: A DFT point of View*

10:10 Angelo Giussani: *Theoretical Study of the Photophysics of Asulam*

#### 10:30 Coffee Break

#### Session B (11:00 - 13:00) - Chairman: Juan Carlos Sancho-García (Alicante)

11:00 Enrique Ortí Guillén (keynote): *Quinoidal Oligothiophenes: Challenging Molecules with a Large Biradical Character*

11:40 Juan Aragón: *Oligothienoacenes vs Oligothiophenes: Impact of Backbone Rigidity on the Optical Properties*

12:00 Philippe Marsal: *Investigation of Probe Molecule–Polymer Interactions: a Theoretical Insight*

12.30 Yoann Olivier: *Influence of a Polymeric Dielectric Layer on Charge Carrier Mobility in Field-Effect Transistors*

#### 13.00 Lunch (at the ICMol)

#### Session C (14:30 - 16:00) - Chairman: Luca Muccioli (Bologna)

14:30 Juan Carlos Sancho-García: *A Link between Quantum and Atomistic Scales Provided by Torsion Energy Profiles*

15:00 Rubén Costa: *Light Emitting Electrochemical Cells Based on Supramolecular Interactions*

15:20 "the experimental challenge" - Larry Lüer (keynote): *Ultrafast energy and charge transfer in optoelectronic materials*

17:00 Valencia: *obvious and secret treasures*. Meeting Point: Hotel Los Silos 17:00 h

#### 21:00 Dinner (Los Sabores, Valencia)

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## Saturday, 23.01.

Meeting Point: Hotel Los Silos 08:20 h

**Session D (08:50 - 10:50)** - Chairman: Yoann Olivier (Mons)

- 08:50 Iñaki Tuñón (*keynote*): *A Computational Approach to Study Reactivity in Complex Environments: Exploring Enzymatic Catalysis*
- 09:30 Antoine Van Vooren: *Theoretical Characterization of the Dynamics of Charge Transfer Processes in Donor-Bridge-Acceptor Architectures*
- 10:00 Luca Muccioli: *Studying Molecular Rearrangements with Atomistic Simulations*
- 10:30 Mike Wykes: *A Conjugated Thiophene-Based Rotaxane: Synthesis, Spectroscopy and Modeling*

### 10:50 Coffee Break

**Session E (11:20 - 13:10)** - Chairman: Patrick Trouillas (Limoges)

- 11:20 Alfredo Sánchez de Merás(*keynote*): *Reduced Scaling using Cholesky Decomposition Based Techniques*
- 12:00 Begoña Milián Medina: *Fluorination: Ground and Excited States Properties of Conjugated Compounds*
- 12:30 Johannes Gierschner: *Conjugated Donor-Acceptor Co-Polymers by Orbital Design*
- 13:00 *closing remarks*

### 14:00 Lunch (el Palmar)

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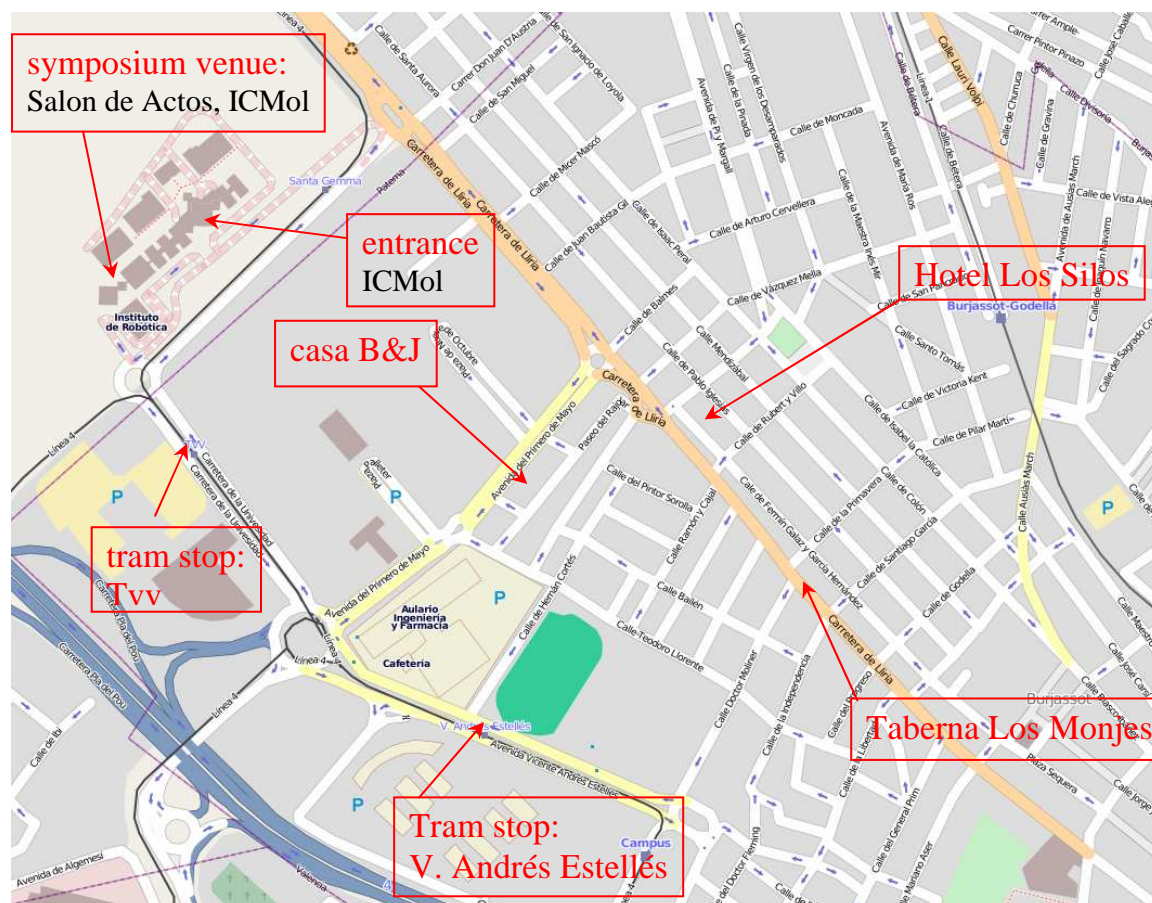
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## Street map Burjassot (Valencia)



## Addresses:

### Symposium Venue

Salón de Actos,  
Institute for Molecular Sciences (ICMol)  
University of Valencia  
Poligono Coma SN  
46980 Paterna (Valencia)

### Hotel Los Silos

Calle de Fermín Galán y García Hernández 72  
46100 Burjassot (Valencia), Spain  
Tel. +34 963 901 515

### Taberna Los Monjes

Carretera de Llíria 68  
46100 Burjassot (Valencia) Spain  
Tel. +34 96 363 28 96

### Restaurante Los Sabores

Landerer 1  
Valencia (Spain)  
Tel. +34 963926217

### Restaurante El Rek

El Palmar (Valencia), Spain

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# loSabores

## Menú

Jamón ibérico y queso

Pan con tomate

Surtido de ahumados

Choricitos a la sidra

-

Solomillo de ibérico con

Salsa de soja

-

Flan de queso

-

## Café

**Bodega básica seleccionada:**

Aguas

Refrescos

Cerveza

Vino tinto antaño D.O Rioja.

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## List of Participants

1	Aragó March, Juan	Universidad de Valencia	Spain
2	Costa Riquelme, Rubén	Universidad de Valencia	Spain
3	Gierschner, Johannes	IMDEA Nanoscience, Madrid	Spain
4	Giussani, Angelo	Universidad de Valencia	Spain
5	Gobbo, Joao Paulo	Universidad de Valencia	Spain
6	Lüer, Larry	IMDEA Nanoscience, Madrid	Spain
7	Marsal, Philippe	Université de la Méditerranée Aix-Marseille II	France
8	Milián Medina, Begoña	Universidad de Valencia	Spain
9	Muccioli, Luca	Università di Bologna	Italy
10	Nénon, Sébastien	Université de la Méditerranée Aix-Marseille II	France
11	Olivier, Yoann	Université de Mons	Belgium
12	Ortí Guillén, Enrique	Universidad de Valencia	Spain
13	Sanchez, José	Universidad de Valencia	Spain
14	Sanchez de Merás, Alfredo	Universidad de Valencia	Spain
15	Sancho-García, Juan Carlos	Universidad de Alicante	Spain
16	Sauri Péris, Vicenta	Universidad de Valencia	Spain
17	Serrano Andrés, Luis	Universidad de Valencia	Spain
18	Tonnele, Claire	Université de Mons	Belgium
19	Trouillas, Patrick	Université de Limoges	France
20	Tuñon, Iñaki	Universidad de Valencia	Spain
21	Van Vooren, Antoine	Université de Mons	Belgium
22	Viruela, Rafael	Universidad de Valencia	Spain
23	Viruela, Pedro	Universidad de Valencia	Spain
24	Wykes, Mike	Université de Mons	Belgium