second annual meeting
POCAONTAS
PHOTOCARBON

at Madrid Institute for
Advanced Studies in Nanoscience

seminar room 215
c/ Faraday, 9
Universidad Autónoma de Madrid
Campus de Cantoblanco
28049, Madrid (Spain)
Day 1 22th April

Lectures

9:30 Opening and Introduction: Current issues in organic photovoltaics
Larry Luer, IMDEA nanociencia

9:50 Time-resolved electrical studies: A simple means to identify efficiency bottlenecks in organic solar cells
Abasi Abdulimu (IMDEA Nanoscience)

10:15 Simultaneous Aromatic-Beryllium Bonds and Aromatic-Anion Interactions (II)
Ibon Alkorta, Instituto de Química Médica (CSIC) (see abstract at end of document)

11:00 Coffee break

11:30 On the Photochemical Behavior and self-assembling of Beryllium Complexes With Subporphyrazines and Subphthalocyanines.
M. Merced Montero-Campillo, Departmento de Química, Módulo 13, Universidad Autónoma de Madrid, Campus de Excelencia UAM-CSIC, Cantoblanco, 28049 Madrid (Spain) (see abstract at end of document)

12:15 Extremely Intense Ground-state Charge Transfer Interactions in Low Bandgap, Panchromatic Phthalocyanine-tetracyanobuta-1,3-diene Conjugates
Giovanni Bottari, Departamento de Química Orgánica, Universidad Autónoma de Madrid, Cantoblanco, 28049 Madrid, Spain and IMDEA-Nanociencia, c/Faraday 9, Campus de Cantoblanco, 28049 Madrid, Spain (see abstract at end of document)

13:00 Title to be announced
Agustin Molina, IMDEA nanociencia, Madrid

13:50 Closing of day 1 and Lunch

Day 2 23th February

Hands-on workshop: Time-resolved electrical measurements: a simple way to find efficiency bottlenecks in organic solar cells

Everybody knows current – voltage (J-V) curves as a means to characterize photovoltaic devices. If measured at 1 sun irradiation, important quantities like the power conversion efficiency (PCE), but also the amount of generation and extraction losses can be obtained. However, in case you find that the problem is extraction losses, how do you distinguish the various reasons for it: (i) extraction mobility too low, carrier dwell in the active layer for too long time, (ii) recombination rate too high, carriers find counter charge before they can reach the electrode?

In this workshop we will use a state of the art measurement setup for the detection of time-resolved photocurrents and photovoltage (TPV/TPC). The measurement is simple and quick, and the evaluation of the results can be done fully automatically. In summary – a pushbutton technique that any research group focused on material science for photovoltaic devices, can build and run in their own lab.

Students can bring their own samples if available. Otherwise we will study organic solar cells made from standard P3HT:PCBM.

Learning goals of this workshop:

- What are the efficiency bottlenecks for organic solar cells?
- How can I use TPC/TPV to distinguish different reasons for extraction losses?
- How can I build a TPV/TPC setup in my own lab with simple means (and little money)?

Larry Luer has coordinated two European Networks on organic photovoltaics and natural light harvesting. Abasi Abdulimu is Marie Curie Fellow of the European network “POCAONTAS”, focused on the improvement of organic solar cells by using single-walled carbon nanotubes.

10:00 Introduction
Larry Luer, Abasi Abdulimu. IMDEA Nanociencia

10:30 Laboratory experiments
Larry Luer, Abasi Abdulimu, IMDEA Nanociencia

12:00 Evaluation of results and discussion
Larry Luer, IMDEA nanociencia

13:00 End of Day 2
Simultaneous Aromatic-Beryllium Bonds and Aromatic-Anion Interactions (II)

Ibon Alkorta, a Marta Marín-Luna, a José Elguero, a Otilia Mó, b Manuel Yáñez, b
a Instituto de Química Médica (CSIC), Juan de la Cierva, 3; E-28006 Madrid, Spain
e-mail: ibon@iqm.csic.es
b Departamento de Química, Módulo 13, Universidad Autónoma de Madrid, Campus de Excelencia UAM-CSIC, Cantoblanco, E-28049 Madrid, Spain

Aromatic and other π-system molecules have been explored theoretically as insulators between anions and cations.1 In addition, the possibility that beryllium derivatives can interact with simple π-system has been explored recently by some of us.2

In this communication, the interaction of simple beryllium derivatives (BeR2, R=H, F and Cl) with planar aromatic derivatives (naphthalene and pyrene) and curve ones (derivatives of corannulene) studied by means of MP2 and M062x computational methods will be presented. Besides, ternary complexes BeR2:Aromatic:X– have been considered where the aromatic system is located, acting as insulator, between the beryllium derivatives and the anion (Cl– and Br–). The energetic, geometric and electron density properties of the systems have been explored.3

Figure 1. Molecular graph of the BeCl2:pyrene, BeCl2:pyrene:Cl– and BeH2:corannulene:Cl– complexes.


Extremely Intense Ground-state Charge Transfer Interactions in Low Bandgap, Panchromatic Phthalocyanine-tetracyanobuta-1,3-diene Conjugates

Giovanni Bottari and Tomás Torres

Departamento de Química Orgánica, Universidad Autónoma de Madrid, Cantoblanco, 28049 Madrid, Spain
and IMDEA-Nanociencia, c/ Faraday 9, Campus de Cantoblanco, 28049 Madrid, Spain
e-mail: giovanni.bottari@uam.es

A cycloaddition-retroelectrocyclization reaction between tetracyanoethylene and two zinc phthalocyanines (Zn(II)Pcs) bearing one [1] or four [2] aniline-substituted alkynes has been used to install a strong, electron-accepting tetracyanobuta-1,3-diene (TCBD) between the electron-rich Zn(II)Pc and aniline moieties (Figure 1). A combination of photophysical, electrochemical, and spectroelectrochemical investigations with the Zn(II)Pc-TCBD-aniline conjugates, which present panchromatic absorptions in the visible region extending all the way to the near infrared, show that the formal replacement of the triple bond by TCBD has a dramatic effect on their ground- and excited-state features. In particular, the formation of extremely intense, ground-state charge transfer interactions between Zn(II)Pc and the electron-accepting TCBD were observed, something unprecedented not only in Pc chemistry but also in TCBD-based porphyrinoid systems.¹

Similarly, preliminary results on the incorporation of TCBD units in subphthalocyanine (SubPc) conjugates will also be presented.²

Figure 1. Molecular structure of electron donor-acceptor Zn(II)Pc-TCBD-aniline conjugates 1 and 2.

[1]. M. Sekita, B. Ballesteros, F. Diederich, D. M. Guldi, G. Bottari, T. Torres Submitted manuscript.


On the Photochemical Behavior and self-assembling of Beryllium Complexes With Subporphyrazines and Subphthalocyanines.#

M. Merced Montero-Campillo,* Al Mokhtar Lamsabhi,* Otilia Móa and Manuel Yáñez*a,*

*Departmento de Química, Módulo 13, Universidad Autónoma de Madrid
Campus de Excelencia UAM-CSIC
Cantoblanco, 28049 Madrid, Spain
*Tel: +34 91 497 49 53, e-mail: manuel.yanez@uam.es

Structures of beryllium subphthalocyanines and beryllium subporphyrazines complexes with different substituents are explored for the first time. Their photochemical properties are studied using Time-Dependent Density Functional Theory calculations and compared to boron related compounds for which their photochemical activity is already known. These beryllium compounds were found to be thermodynamically stable in vacuum and present similar features to those of boron-containing analogues, although the nature of bonding between the cation and the macrocycle presents subtle differences. Most important contributions to the main peak in the Q band region arise from HOMO to LUMO transitions in the case of subphthalocyanines and alkyl subporphyrazine complexes, whereas a mixture of that contribution and a HOMO-2 to LUMO contribution are present in the case of thioalkyl subporphyrazines. The absorption in the visible region could make these candidates suitable for photochemical devices if combined with appropriate donor groups. Dimers of beryllium subphthalocyanine alone or complexed with water and pyridine are analyzed, in which Be-aza N intermolecular interactions are observed, a different behavior to that observed for beryllium phthalocyanines.