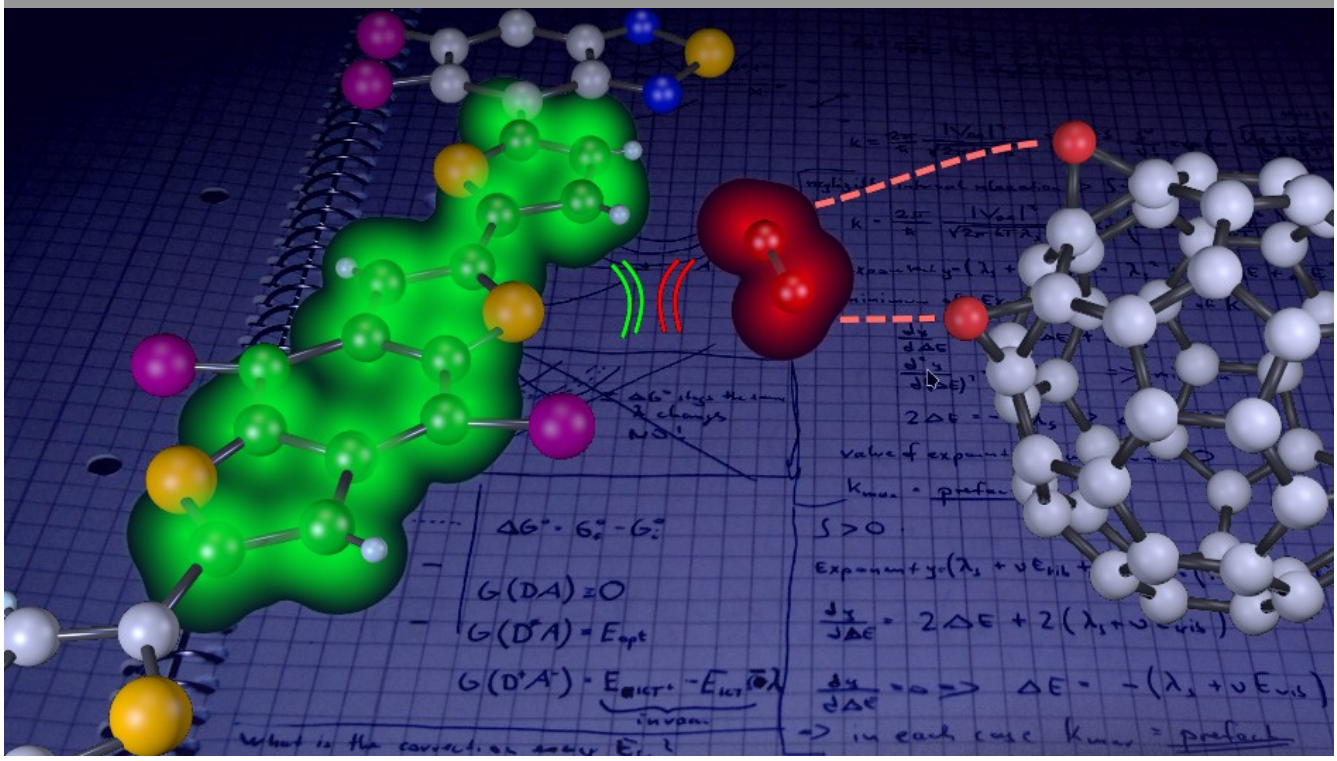
THIRD PHOTOCARBON WORKSHOP
ORGANIC AND HYBRID PHOTOVOLTAICS: SYNTHESIS, PHOTOPHYSICS AND PHOTOCHEMISTRY



Date: 12 September 2017, 10:00 – 15:00
Venue: IMDEA Nanociencia, Sala Hinarejos (next to Main Entrance)
Organizing committee: Larry Luer, Maria Jesus Villa, Jose Luis Casillas, IMDEA Nanociencia

The PhotoCarbon Project invites everybody to join the Third Thematic Workshop. We will share latest results and discuss them in the light of recent developments in the fields of photovoltaics, photophysics, and photochemistry.

– AGENDA --

10:00 – 10:05	Nazario Martín (coordinator) and Larry Luer (local organizer)	Opening

Work Group: Larry Luer, PhD

Laboratory of time-resolved spectroscopy, IMDEA Nanociencia, Madrid

10:05 – 10:40	Larry Luer *IMDEA Nanociencia*	Tutorial: “Design rules for all-small molecule solar cells”

Work Group: Prof. Nazario Martín

Universidad Complutense de Madrid, Departamento de Química Orgánica, Madrid

10:40 – 11:00	Agustin Molina *IMDEA Nanociencia*	Tutorial: “Perovskites”
11:00 – 11:25	Inés García Benito *IMDEA Nanociencia*	"Novel star-shaped hole-transporting materials for perovskite solar cells"
11:25 – 11:50	Rafael Sandoval *IMDEA Nanociencia*	"Design and synthesis of small molecules for organic solar cells"
11:50 – 12:20	Coffee break	
12:20 – 12:35	Javier Urieta Mora *IMDEA Nanociencia*	"Using sulfur-rich polycyclic aromatic compounds as efficient hole-transporting materials for perovskite solar cells"

Work Group: Prof. Manuel Yañez

Universidad Autónoma de Madrid, Departamento de Química, Madrid

12:35 – 13:00	Inés Corral	Competitive cycloreversion and O-O homolysis photo-dynamics in aromatic endoperoxide photosensitizers
13:00 – 13:15	Serra Arslancan	Deciphering the relaxation mechanisms of photoinitiated drugs based on DNA derivatives

Work Group: Prof. Tomas Torres

Departamento de Química Orgánica - Facultad de Ciencias, Madrid

13:15 – 13:40	Giovanni Bottari	Tetracyanobutadiene: A novel electron acceptor for phthalocyanines and subphthalocyanines
13:40 – 14:05	Evelyne van de Winckel	Novel Phthalocyanine-Based Photosensitizers For Photodynamic Therapy

Work Group: Prof. Ibon Alkorta

Instituto de Quimica Medica (CSIC), Madrid

14:05 – 14:30	M. Merced Montero-Campillo	From structure to photochemical properties: A theoretical study of ZnPc(II) derivatives
14:30 – 16:00	Lunch *Cafeteria IMDEA Nanociencia*	

Short Abstracts

Larry Luer, IMDEA Nanociencia, Madrid

Tutorial: Design rules for all-small molecule solar cells

Solution-processable all-small molecule organic solar cells (OSC) have shown an impressive improvement of photovoltaic efficiencies and stability over the last years, now rivalling the best polymer-based OSC. However, details of the elementary steps of free carrier generation, and possible bottlenecks, have not been quantified so far. Here we show that free charge generation in small molecule based OSC is fundamentally different from polymer-based solar cells. Based on Marcus theory, we give guidelines for maximizing open circuit voltage and internal quantum yields.

Inés Corral, Universidad Autónoma de Madrid, Departamento de Química, Madrid

Competitive cycloreversion and O-O homolysis photodynamics in aromatic endoperoxide photosensitizers

Photodynamic Therapy, or the production of cytotoxic singlet oxygen ($^1O_2$, ($^1\Delta_g$)) for the destruction of unwanted tissues following irradiation of nontoxic prodrugs or photosensitizers (PSs), has garnered acceptance in the last years as a treatment option for various cancers and other non-oncologic malignancies. The widespread use of PDT as a medical tool is, however, limited by the chemical constraints of the few administration-approved PSs, triggering the search of alternative dyes with improved properties and more versatile in their application.

A promising family of PSs are oxygen-carrier endoperoxide prodrugs, which are able to release $^1O_2$ in hypoxic areas. The mechanism underlying $^1O_2$ generation in endoperoxides is based on retro-Diels-Alder reactions either at high temperatures or in the presence of light, delivering $^1O_2$.

In this contribution, multiconfigurational *ab initio* calculations supplemented with singlet/triplet semiclassical molecular dynamics simulations on benzene endoperoxide will be presented. These results allow for the understanding of the mechanisms leading to $^1O_2$ in these dyes and their competition with other photochemical or photophysical pathways occurring in manifolds of the same or different multiplicity.

Serra Arslancan, Universidad Autónoma de Madrid, Departamento de Química, Madrid

Deciphering the relaxation mechanisms of photoinitiated drugs based on DNA derivatives

DNA building blocks may be radically affected by minor structural modifications on the substitution pattern of purine or pyrimidine heterocyclic rings, such as carbonyl-by-thiocarbonyl replacement. In the particular case of thiobases, the characteristic topography of their potential energy surface leads to the population to the triplet manifold with high efficiency upon UV light absorption. From their triplet states, these systems are able to generate DNA-damaging reactive oxygen species and other photoproducts which are cytotoxic. Based on this photoreactivity, these prodrugs have been suggested as prototypes for photosensitizers to be used in photodynamic therapy against cancer. In this contribution, we aim to decipher the decay pathways of 2-thiothymine and 2,4-dithiothymine with a combination of static and molecular dynamics study.