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# Discussion Meeting 2020

## Progress in Organic Optoelectronics and Energy Conversion

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Coodinators:

Dr. Johannes Gierschner  
Dr. Begoña Milián Medina

The Organization Team:

Liangxuan Wang  
Juan Carlos Roldao  
Siyang Feng  
Javier Enrique Sebastian Alonso  
Emilio López Díaz



Thursday, 17.12.2020

Session 1 Chair: M. Carmen Ruiz Delgado

9:00-9:20 Welcome & Introduction

Johannes Gierschner, Begoña Milián Medina

09:20-09:40 Johannes Gierschner (IMDEA)

Charge Transfer States in Optoelectronics and Energy Conversion

9:40-9:50 Lucía Velasco (IMDEA)

Structure and Excited-State Dynamics of Dimeric Copper(I) photosensitizers Investigated by Time-resolved X-ray and Optical Transient Absorption Spectroscopy [shot]

9:50-10:10 Emilio M. Pérez (IMDEA)

Encapsulation of Active Molecules in SWNTs for Organic Electronics and Spintronics

10:10-10:30 Javier Carmona García (University of Valencia)

On the Computation of Photolysis Rates with Multiconfigurational Quantum Chemistry

10:30-10:50 Miriam Navarrete Miguel (University of Valencia)

Inverting the Paternò-Büchi Reaction by UV and Photo-oxidation/reduction

10:50-11:30 Virtual Coffee Break

Session 2 Chair: Juan Aragón

11:30-11:50 Juan Cabanillas González (IMDEA)

Effect of Phenyl-fluorene Backbone Intercalation in the Stimulated Emission Properties of Fluorene-based Polymer Blends

11:50-12:10 Chen Sun (Lund University)

Influence of  $\beta$ -Phase Content on Photophysics and Light Amplifying Properties of Polydiarylfuorene

12:10-12:30 Jorge González Sierra (IMDEA)

Conjugated Polymer Based Microcavities for Lasing and Sensing

12:30-12:50 Raquel Rubert Albiol (University of Valencia)

*Ab Initio* Modelling of Dicyanomethylene-Based  $\pi$ -Conjugated Compounds with Diradical Character

12:50-13:10 Azahara Doncel Giménez (University of Valencia)

Structure-mechanism Relationship in N-annulated Perylene Bisimides

13:10-13:30 Ricardo Ortiz (University of Alicante)

Frustrated Magnetism in a Cyclacene Crystal

Friday, 18.12.2020

Session 3 Chair: Johannes Gierschner

9:00-9:20 Alexandra Harbuzaru (University of Málaga)

Understanding Charge Transport Mechanisms of Ladder-type Heteroarenes in OFETs

9:20-9:40 Irene Badía-Domínguez (University of Málaga)

Controlling the Extent of Diradical Character in Indolocarbazole Isomers

9:40-10:00 Sergio Gámez-Valenzuela (University of Málaga)

In silico Design of Truxene-based 2D Polymers

10:00-10:10 Sara Fernández-Palacios (University of Málaga)

Evaluating the Role of Intermolecular Interactions in Piezochromic Materials by Raman Spectroscopy [shot]

10:10-10:30 Juan Carlos Roldao (IMDEA)

Excited state absorption of  $\pi$ -conjugated compounds: How reliable is the “single excitation” model?

10:30-10:50 Liangxuan Wang (IMDEA)

Stereochemistry & Direct Observation of Tautomerization of Single Hypericin Molecules

10:50-11:10 Conclusion

Johannes Gierschner



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