



Establis



SUMMER SCHOOL in Computational Approaches to Conjugated Materials

La Cristalera & IMDEA Nanociencia

**16-21
JUNE**
Madrid 2013



Sunday, 16 June

- 14:00 - 18:00 Arrival; Bus transfer from the airport to Miraflores
- 20:00 - 22:00 Welcome Dinner



Monday, 17 June

- 9:00 - 9:30 Welcome and Introduction (Larry Lüer)
- 9:30 - 10:00 School Opening (Roger Hiorns)
- 10:00 - 11:00 Larry Lüer: Photoexcitation dynamics
- 11:00 - 11:30 Coffee break
- 11:30 - 13:00 Larry Lüer: Dynamic modelling: from time-resolved spectra to a photophysical model
- 13:00 - 14:30 Lunch
- 14:30 - 16:00 Larry Lüer: Hands on workshop: analyse time-resolved spectra with state of the art tool on your own laptop
- 16:00 - 16:30 Coffee break
- 20:00 - 22:00 Dinner

Tuesday, 18 June

- 9:00 - 10:30 Begoña Milián-Medina: An Introduction to Quantum-Chemistry
- 10:30 - 11:00 Coffee Break
- 11:00 - 12:30 Begoña Milián-Medina: Calculation of Molecular Properties
- 12:30 - 14:00 Lunch
- 14:00 - 15:30 Johannes Gierschner: Excited States of Conjugated Organic Materials (I)
- 15:30 - 16:00 Coffee Break
- 16:00 - 17:30 Johannes Gierschner: Excited States of Conjugated Organic Materials (II)
- 20:00 - 22:00 Dinner

For more information:

www.project-establis.eu

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instituto
IMDEA
nanociencia

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Wednesday, 19 June

- 9:00 – 10:30 Patrice Bordat: Molecular dynamics simulations: from the classical level to the QM/MD coupling (I)
- 10:30 – 11:00 Coffee break
- 11:00 – 11:45 (Patrice Bordat: Molecular dynamics simulations: from the classical level to the QM/MD coupling (II)
- 11:45 – 12:30 Michael Wykes: Exploring Chemical Reactivity with Computational Chemistry (I)
- 12:30 – 14:00 Lunch
- 14:00 – 14:45 Michael Wykes: Exploring Chemical Reactivity with Computational Chemistry (II)
- 15:30 – 19:00 Mountain Hike / Barbecue

Thursday, 20 June

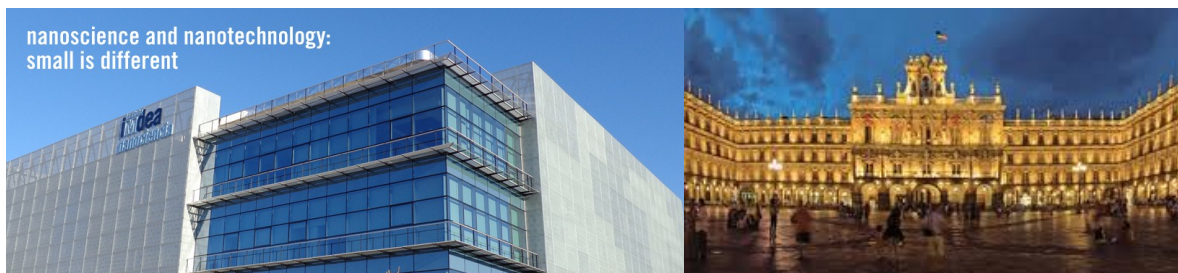
- 9:00 – 10:30 Bus transfer to IMDEA Nanociencia
- 10:30 – 11:00 Coffee break
- 11:00 -13:00 Hands-On Workshop "Quantum-chemical modelling" (Part I)
- 13:00 – 14:30 Lunch
- 14:30 – 17:00 Hands-On Workshop "Quantum-chemical modelling" (Part II)
- 17:00 Check-in at Erasmo Residence

Friday, 21 June

- 9:00 – 10:30 Reinhold Wannemacher: Non-destructive testing of interfacial degradation (I)
- 10:30 – 11:00 Coffee break
- 11:00 – 12:30 Reinhold Wannemacher: Non-destructive testing of interfacial degradation (II)
- 12:30 – 14:30 Lunch
- 14:30 – 16:30 Merck Ltd: Workshop: Use of Chemical Search Databases
- 16:30 - 16:45 Coffee break
- 16:45 - 17:45 David Sayago: Get a life: Funding opportunities for career development
- 18:00 - 22:00 Madrid tour + tapas hopping

Agenda of Establis Meeting

Management Committee



IMDEA Nanociencia
Madrid – Spain
24rd-26th of June 2013

Monday 24th of June

- For Fellows only -

| Time | Min | Speakers |
|----------------------|------------|---|
| 09:00 – 09:30 | 30 | POC meeting: gathering and cheer up before activities Chair Graham |
| 09:30 – 13:00 | 210 | Outreach activities |
| 13:00– 14:30 | 90 | Lunch |
| 14:30 – 15 :00 | 30 | Equipment session : who, how, why? Chair: Dr. Graham Morse |
| 15:00 – 15:15 | 15 | coffee break |
| 15:15 – 16:15 | 60 | Science communication and Writing Paper session : <ul style="list-style-type: none"> • presentation on Science communication by Dr. Larry Lüer • presentation on Paper Writing by Dr. Roger Hiorns |
| 16:15 – 16:30 | 15 | coffee break |
| 16:30 – 17:20 | 50 | Team paper writing and Material Exchange Chair Dr. Stephan Schumann and Dr. Graham Morse |
| 17:20 – 17:30 | 10 | coffee break |
| 17:30 – 18:30 | 60 | Fellow Committee Chair: Dr. Stefan Schumann |
| 19:00 – 23:00 | 180 | Diner - Restaurant to be announced |

Tuesday 25th June

| | | |
|----------------------|------------|--|
| 08:45- 09:30 | | Opening of Management and STC Meeting |
| | | Welcome by Dr. Roger Hiorns, Dr. Larry Lüer and Dr. Paul Topham |
| 09:00 – 09:30 | 30 | <ul style="list-style-type: none"> • Management statement on recent Grant amendment, CA and Scientific Objectives • Presentation STC agenda by Dr. P. Topham • presentation of First Summer School and Workshop by Dr. Larry Lüer |
| 09:30 – 11:25 | | WP4 Presentation – Modelling degradation Chairman : Dr. Larry Lüer |
| 09:30 - 09:35 | 5 | Dr. Larry Lüer – WP4L Presentation of WP4 milestones and objectives |
| 09:35 – 09:55 | 20 | Hugo Santos Silva - ESR1 “Synthesis and modelling of polyfullerenes” |
| 09:55 – 10:15 | 20 | Safakath Haruthedath - ESR4 “Reversible and irreversible oxygen effects on the exciton dynamics in photovoltaic devices: a time domain study” |
| 10:15 – 10:45 | 30 | Coffee Break |
| 10:45 – 11:05 | 20 | Dr. Mike Wykes – IMDEA Postdoc Presentation of SolaRevolution project |
| 11:05 – 11:10 | 5 | WP4 closing and AOB by Dr. Larry Lüer |
| 11:10 – 11:45 | 30 | Establis Finance Situation. Dr. Mélanie Pédeutour |
| 11:45 – 13:00 | 75 | Open Lecture Dr. Hans-Joachim Egelhaaf |
| 13:00– 14h30 | 90 | Lunch |
| 14:30 – 16:00 | | WP2 Presentation – Material Stabilities Chairman : Dr. Agnès Rivaton |
| 14:30 – 14:35 | 5 | Dr. Agnès Rivaton – WP2L Presentation of WP4 milestones and objectives |
| 14:35 – 14:55 | 20 | Isabel Fraga - ESR8 “Identification of the degradation mechanisms of organic materials: active layer and interfacial layers. Chemical and morphological stability” |
| 14:55 – 15:15 | 20 | Ievgeniia Topolniak – ESR9 “Photodegradation and photostabilisation of packaging” |
| 15:15 – 15:35 | 20 | Mamadou Seck- ESR11 “Combining surface and vertical profile studies of organic materials in solar cells”. |
| 15:35 – 15:55 | 20 | Aurélien Tournebize – ESR10 “Electronic structure and degradation of polymer blend materials” |
| 15:55 – 16:00 | 5 | WP2 closing and AOB by Dr. Agnès Rivaton |
| 16:00 – 16:30 | 30 | Tea Break |
| | | Mid term meeting in Pau Chair Dr. Roger Hiorns |
| 16:30 – 17:10 | 40 | <ul style="list-style-type: none"> • presentation of the program Dr. P. Topham • mid-term report Dr. Mélanie Pédeutour |
| 17:10 – 18:00 | 50 | Open Surgery Dr. Mélanie Pédeutour |
| 19:00 – 21:00 | 180 | Social event Down Town Madrid : City Tour |
| 21:00 – 23:00 | 180 | Diner – Restaurant to be announced. |

Wednesday 26th June

| | | |
|-----------------------|------------|--|
| 08:45- 09 :00 | 15 | Opening Dr. Roger Hiorns |
| 09:00 – 09:25 | 25 | FC and POC reports Chair Dr. Roger Hiorns <ul style="list-style-type: none"> • FC report : Dr. Stefan Schumann • POC report: Dr. Graham Morse • OPEN report: Joanna Kolomanska |
| 09:25 – 12:05 | | WP1 Presentation –Synthesis Chairman : Dr. Christine Dagron-Lartigau |
| 09:25 – 09:30 | 5 | Dr. Christine Dagron-Lartigau - WP1L presentation of WP4 milestones and objectives |
| 09:30 – 09:50 | 20 | Hasina Ramanitra- FullInc |
| 09:50 – 10:10 | 20 | Anna Isakova- ESR6 "Synthesis of ligands and polymers for application in organic solar cells" |
| 10:10 – 10:30 | 20 | Joanna Kolomanska – ESR7 "Synthesis of polymers and copolymers for application in organic solar cells" |
| 10:30 – 11:00 | 30 | Coffee Break |
| 11:00 – 11:20 | 20 | Dr. Harikrishna EROTHU - Synabco |
| 11:20 – 11:40 | 20 | ER3 - "Design, synthesis and characterisation of higher stability donor polymers for bulk-heterojunction solar cells" . presentation by Dr. G. Morse |
| 11:40 – 12:00 | 20 | Dr. Stefan Schumann – ER4 "Tailoring PEDOT-dispersions towards their use in organic solar cells" |
| 12:00 – 12:05 | 5 | WP1 closing and AOB Dr. Christine Dagron-Lartigau |
| 12 :05 – 13:00 | 55 | Cotutelle Agreement Dr. Andy Sutherland – Director of Training |
| 13:00 – 14:30 | 90 | Lunch |
| | | Presentation of up coming events |
| 14:30 – 14:55 | 25 | <ul style="list-style-type: none"> • Vilnius workshop – Dr. Kristijonas Genevicius • Summer School in Corsica – Dr. Roger Hiorns |
| 14:55 – 16:55 | | WP3 Presentation – OSC Stability and Performance Chairman : Dr. Hans Joachim Egelhaaf |
| 14:55 – 15:00 | 5 | Dr. Hans Joachim Egelhaaf - WP3L Presentation of miles tones and objectivs |
| 15:00 – 15:20 | 20 | Alberto Gregori – ESR2 "Synthesis and rheological characterisation of (co)polymers for active layers in organic solar cells" |
| 15:20 – 15:40 | 20 | Olena Kozlova - ESR5 "Organic bulk heterojunction solar cells for charge carrier transport and recombination measurements" |
| 15:40 – 16:10 | 30 | Tea break |
| 16:10 – 16:30 | 20 | Meera Stephen – ESR3 "The impact of the design and fabrication of the organic bulk heterojunction solar cells on the charge carrier transport and recombination" |
| 16:30 – 16:50 | 20 | ER1 |
| 16:50 – 16:55 | 5 | WP1 closing and AOB Dr. Hans Joachim Egelhaff |
| 16:55 – 17:55 | 60 | WP Science Breakout <ul style="list-style-type: none"> • Introduction by Dr. Paul Topham • Parallel WP Science Breakout session chair by each WPL |
| 17:55 – 18:00 | 5 | Closure of Meeting - Dr. Roger Hiorns |
| 19:00 – 23:00 | 180 | Diner: Restaurant - La Venta del Gordo |

Appendix 1 – List of attendees

| Partner Name | Name | Role | E-mail addresses |
|----------------------------------|-------------------------------|-----------------------|--|
| UPPA (P1) | Dr Roger Hiorns | Coordinator, PL1 | roger.hiorns@univ-pau.fr |
| | Dr Mélanie Pédeutour | Project manager | melanie.pedeutour@univ-pau.fr |
| | Dr. Christine Dagron Lartigau | Supervisor, WP1L | christine.dagron-lartigau@univ-pau.fr |
| | Dr. Didier Bégué | Supervisor | didier-begue@univ-pau.fr |
| | Hugo Santos Silva | ESR1 | hsansilva@gmail.com |
| | Alberto Gregori | ESR2 | gregori.alberto@gmail.com |
| | Hasina Ramanitra | Fullinc PhD | hbarhasy@gmail.com |
| Konarka (P2) | Dr. Hans Joachim Egelhaaf | PhD fellow | adistler@konarka-technologies.de |
| Vilnius (P3) | Dr. Kristijonas Genevicius | co-supervisors | kristijonas.genevicius@ff.vu.lt |
| | Meera Stephen | ESR3 | meera.stephen@ff.vu.lt |
| MERCK (P4) | Dr Steve Tierney | PL4 | steven.tierney@merckgroup.com |
| | Dr Nicolas Blouin | Supervisor | nicolas.blouin@merckgroup.com |
| | Dr. Graham Morse | ER3 | Graham.Morse@merckgroup.com |
| IMDEA (P5) | Dr Larry Lüer | PL5 | larry.luer@imdea.org |
| | Dr. Juan Cabanillas Gonzalez | supervisor | juan.cabanillas@imdea.org |
| | Dr Reinhold Wannemacher | supervisor | Reinhold.Wannemacher@imdea.org |
| | Dr. Begona Medina | supervisor | begona.milian@imdea.org |
| | Dr. Marta Mroz | supervisor | |
| | Safakath Karuthedath | ESR4 | k.safakath@imdea.org |
| HERAEUS (P6) | Dr. Andreas Elschner | PL6 | andreas.elschner@heraeus.com |
| | Dr. Stefan Schumann | ER4 | stefan.schumann@heraeus.com |
| Linz Universität | Dr. Reinhard Schwödiauer | supervisor | Reinhard.Schwoediauer@jku.at |
| | Olena Kozlova | ESR5 | olena.kozlova@jku.at |
| Aston University (P8) | Dr. Andrew Sutherland | Dir. Of training | a.j.sutherland@aston.ac.uk |
| | Dr. Paul D. Topham | Vice-coordinator, PL8 | P.D.TOPHAM@aston.ac.uk |
| | Anna Isakova | ESR6 | isakovaa@aston.ac.uk |
| | Joanna Kolomanska | ESR7 | joanna.kolomanska@gmail.com |
| | Dr. Harikrishna Erothu | Synabco postdoc | h.erothu@aston.ac.uk |
| CNRS-LPMM (P9) | Dr Agnès Rivaton | PL9, WPL2 | agnes.rivaton@univ-bpclermont.fr |
| | Prof. Luc Gardette | supervisor | luc.gardette@univ-bpclermont.fr |
| | Dr Sandrine Theiras | supervisor | Sandrine.THERIAS@univ-bpclermont.fr |
| | Isabel Fraga | ESR8 | Isabel.Fraga_Dominguez@etudiant.univ-bpclermont.fr |
| | Ievgenia Topolniak | ESR9 | levgeniia.Topolniak@etudiant.univ-bpclermont.fr |
| E.K. Univ. Tübingen (P10) | Thomas Chassé | PL10 | thomas.chasse@uni-tuebingen.de |
| | Aurélien Tournebize | ESR10 | aurelien.tournebize@tuebingen.de |
| International Laser Center (P11) | Alexander Satka | supervisor | satka@ilc.sk |
| | Dr Andrej Vincze | supervisor | vincze@ilc.sk |
| | Dr. Daniel Hasko | supervisor | hasko@ilc.sk |
| | Mamadou Seck | ESR11 | mamadou@ilc.sk |

Appendix 2 – How to get There

How to get there

..from the Airport "Madrid Barajas"

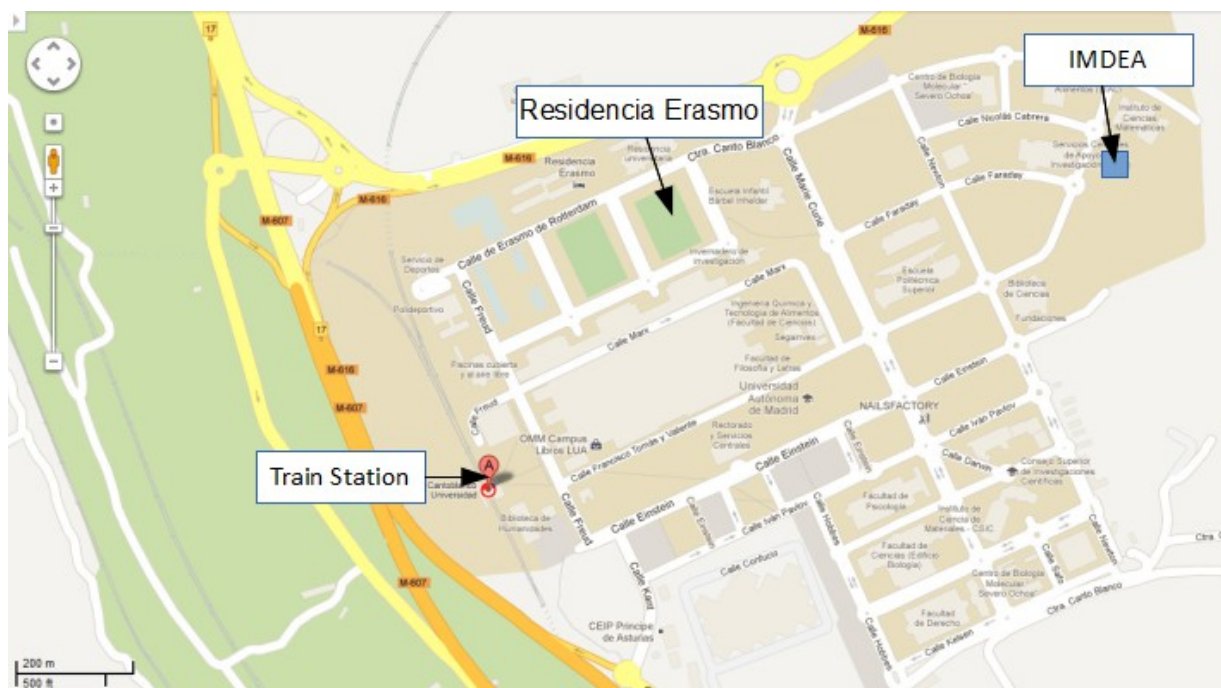
If you arrive at terminal T4, there is a new "Cercanías" train line C-1, which brings you to "Chamartin" in just 11 mins and further proceeding to "Atocha". To get to "Sol" you switch in "Chamartin" or "Nuevos Ministerios" to line C-3 or C-4.

If you arrive at Terminal T1, 2 or 3: You can take the (free) shuttle bus to T4 and proceed as previously described. Alternatively, there is a Metro (no. 8) which brings you to "Nuevos Ministerios" (ca. 20-25 from T1-3). To get downtown (Sol, Atocha) from there, proceed with metro (lines 6 and 1) or by Cercanías.

•...to the Campus: Take the "Cercanías" train line C-4 in the direction "Colmenar Viejo" or "Alcobendas/San Sebastian de los Reyes" and stop at "Cantoblanco Universidad" (approx. 1/2h from "Atocha").

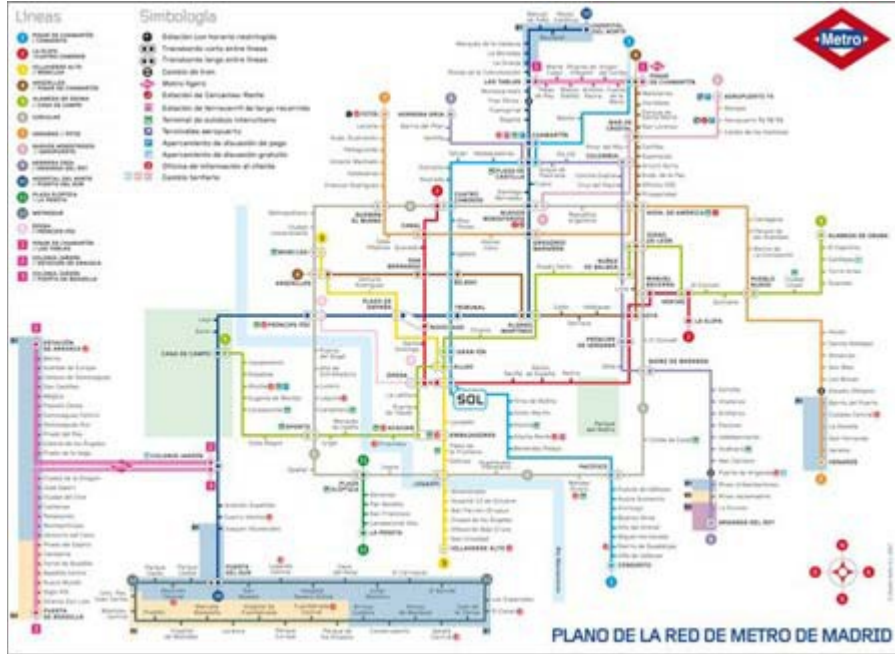
http://www.renfe.com/EN/viajeros/cercanias/madrid/mapa_zonas_madrid.html

To get from the train station to IMDEA Nanoscience, go straight to the pedestrian road "Avenida Tomás y Valiente" and follow it to the third roundabout (ca. 1000 m), turn right and you stand right in front of the institute. My office is B27 in the ground floor.



Appendix 2 – How to get There

Metro map



Train map



Appendix 3 – Addresses

IMDEA Nanociencia

Calle Faraday 9,
Ciudad Universitaria de Cantoblanco
28049, Madrid (Cantoblanco)
SPAIN



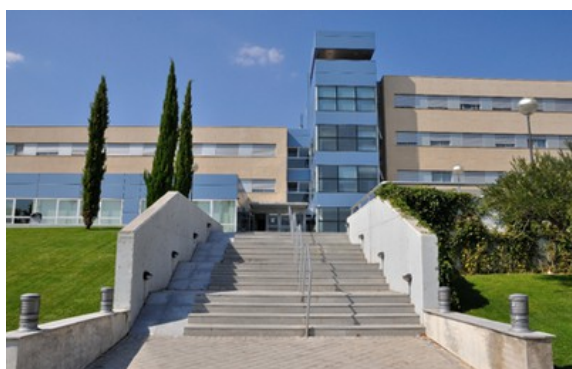
Dr. Larry Lüer

Tel.: +34 91 2998 782 (office), + 34 91 2998 776 (lab)

Dr. Johannes Gierschner: Mobile: +34 652 224335 Institute: +34 91 299 8783

Residencia Erasmo

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E-mail: erasmo2@resa.es



Restaurante la Venta del Gordo

Av de los Labradores, 3, 28760 Tres Cantos, Madrid, Espagne
+34 918 03 72 21

Recommendation regarding weather conditions: the climate in June in the Madrid region is usually hot and dry, with temperatures going up to 35 °C. Avoid direct sunlight exposure around 14:00, when the sun is nearly at vertical incidence. Please bring a sunscreen, a hat and/or an umbrella to protect against photodegradation, and drink lots of water against dehydration. In the mountains, occasional thunderstorms might occur; avoid longer excursions without shelter if weather conditions seem unstable.