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## Ultra-high Charge Carrier Mobility to Elucidate Transport Mechanisms in Molecular Semiconductors

Type of action: MSCA-ITN-ETN

Call identifier: H2020-MSCA-ITN-2018

### D6.3 – Annual report on training, including school

Project funded by the European Commission within the H2020 Programme (2014-2020)			
<b>EC Grant Agreement n°</b>	811284		
<b>Start date/ Duration</b>	01 May 2019 / 48 months		
<b>Deliverable leader</b>	M. Mas-Torrent (CSIC)		
<b>Deliverable contributor(s)</b>	All partners		
<b>Deliverable reviewer(s)</b>	All partners		
<b>Due date (DoA)</b>	30/04/2021	<b>Submission date</b>	30/04/2021

Type		
R	Document, report excluding the periodic and final reports	X
DEC	Websites, patents filing, press & media actions, videos, etc.	
ETHICS	Ethics requirement	
ORDP	Open Research Data Pilot	
Dissemination level		
PU	PUBLIC, fully open, no embargo e.g. web	
CO	CONFIDENTIAL, only for members of the consortium (including the Commission Services)	X

Release	Date	Reason for change	Status	Distribution
R0.1	29/01/2021	Template initiated	Draft	Deliverable Leader
R0.2	30/03/2021	Update of Section 3	Draft	Coordinator & Deliverable leader
R1.0	30/04/2021	Final Release	Final	EU

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## 1 Executive summary

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The present report provides an overview of the training that the ESRs have pursued during this second period including the technical training delivered by Prof. R. Resel (TUGraz) during the last progress meeting.

Finally, this report also describes the training School that is being organised and that will take place next May-June 2021, where all the ESRs will participate.

## 2 Introduction

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During this period, all ESRs have been trained in different technical aspects in order to be able to carry out their research. In addition, ESRs have also had the chance to perform complementary courses, to attend lectures, to participate in some conferences and even to learn some language skills. Finally, ESRs also attended the training course in X-ray characterisation that was organised by Prof. R. Resel (TU-Graz) in conjunction with the last progress meeting.

The ESRs will also attend the training school that UHMob is organising, as it will be described below.

## 3 ESRs Training

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### 3.1 Training during the UHMob progress meeting

During the UHMob Month 18 meeting (9-10/11/2020) a scientific training on the topic: **X-ray based techniques for organic thin film studies** was organised.

This training course on X-ray methods to characterize thin films and surfaces was organized in a remote way by Roland Resel, Graz University of Technology on 9th November 2020.

The course was divided into two parts: X-ray reflectivity (XRR) and X-ray diffraction (XRD). For each of these two sections short introductory videos (40 minutes + 31 minutes) were prepared. Based on the videos, individual problems had to be solved by the ESRs. For this purpose, the ESRs were divided in groups of two. This had to be done in advance to the training.

During the course the ESRs presented the solutions of their individual problems. Additionally, two short presentations on recent research work of the two school topics (XRR, XRD) were given by the organizer.

### 3.2 Other ESRs training activities

During the second project year, ESRs have jointly followed the following trainings:

- Soft skills: Improving presentation skills and defining research and progress. – Training performed in advance for the M12 remote meeting. All ESRs participated except for ESR5, who had not yet started at the time.
- Lecture on “Light-matter strong coupling” by Prof. T. Ebbesen held remotely on 24/06/2020. This lecture provided a better understanding of some of the scientific concepts that are included in the project.
- Lecture on “Molecular Semiconductors for logic operations: Dead End or Bright Future” by Prof. Y. Geerts held remotely on 22/01/2021. This lecture provided a better understanding of the project and the need to pursue research in the area.

Table 1 summarises all the training activities that the ESRs have carried out in the last twelve months.

ESR N°	ESR Name	Training and Courses
1	Martina Volpi (ULB)	<ul style="list-style-type: none"> <li>- Soft skills: seminars within the research group to help the improving of her presentation skills and in defending her research and progress.</li> <li>- Training in instruments useful for characterization of the synthesised products synthesis: DSC, TGA, polarized optical microscope (with hot stage), HPLC.</li> <li>- Language: French classes held by ULB.</li> </ul>
2	Rahul Meena (ULB)	<ul style="list-style-type: none"> <li>- Soft skills: seminars within the research group to help the improving of his presentation skills and in defending her research and progress.</li> <li>- Training in organic synthesis and instruments (TGA, DSC and Powder-XRD).</li> <li>- Language: free online French lectures.</li> </ul>
3	Nemo McIntosh (UMons)	<ul style="list-style-type: none"> <li>- Master class in theoretical photophysics at University of Tubingen by Pr. Giershner.</li> <li>- Webinar : "Frontiers in nanochemistry on surfaces" by Pr. De Feyter.</li> </ul>
4	Marco Bardini (UMons)	<ul style="list-style-type: none"> <li>- Training in coding: enrolled in online Python classes offered by the University of Michigan on the Coursera platform, training in writing .bash scripts and rudimentary fortran and C.</li> <li>- Lectures on the photophysics of small molecules in solution (2020) and in the solid state (2021) given by Prof. Johannes Gierschner.</li> <li>- Languages: French classes offered by UMons three times a week.</li> </ul>
5	Mindaugas Gicevicius (UCAM)	<ul style="list-style-type: none"> <li>- Introductory, graduate level lecture series on the basic physics of organic semiconductors organised by the Optoelectronics Group at the Cavendish Laboratory.</li> <li>- Participated in various training events organized by University of Cambridge Researcher Development Programme (RDP) on: 1) Scientific writing and publishing, 2) Time management, remote work, and stress management &amp; resilience.</li> </ul>
6	Kripa M. Joseph (UNISTRA)	<ul style="list-style-type: none"> <li>- Several seminars and conferences organized by doctoral school related to the basic and advanced concepts that are beneficial for his research topic.</li> <li>- Training on techniques required for the fabrication and characterization of Plasmonic structures and Fabry-Perot cavity to achieve light-matter strong coupling: 1) Focused Ion Beam and Scanning Electron, 2) Microscope (FIB/SEM), 3) Photolithography and 4) Fourier Transform IR and UV Vis absorption spectroscopy.</li> <li>- Basic courses on Python programming language and Matlab through the application Coursera during lockdown days.</li> <li>- Language course: French course organised by university.</li> </ul>
7	Nicholas Turetta (UNISTRA)	<ul style="list-style-type: none"> <li>- Training in the following techniques: 1) Photoemission Yield Spectroscopy, 2) Kelvin Probe Force microscopy, 3) Conductive AFM Bernauer–Emmett–Teller (BET) surface area analysis, 4) Probe station in air with use of a humidity/nitrogen controlled chamber for electrical characterization of devices, 5) Scanning Electron Microscopy (SEM), 6)</li> </ul>

ESR N°	ESR Name	Training and Courses
		<p>Contact angle and wettability of surfaces, 7) Fabrication of thin films of small organic molecules via spin coating.</p> <ul style="list-style-type: none"> <li>- Participation in a series of lectures including topics such as: carbon capture, catalysis, ultrafast spectroscopy, mechanochemistry, non equilibrium assembly and self-assembly, organic transistors, cellulose nanocrystal, biological systems, 2D materials, integrity in research, etc.</li> <li>- Language: French courses.</li> </ul>
8	Ann Maria James (TUGraz)	<ul style="list-style-type: none"> <li>- Introduction to laboratory safety (chemical preparation laboratory, X-ray laboratory).</li> <li>- Training in: experimental determination of surface energy, thin film preparation by solution processing (drop casting, spin coating, dip coating), thin film annealing procedures (temperature, solvent vapor), microscopies (atomic force microscopy, optical microscopy).</li> <li>- Training in X-ray methods by using laboratory machines (X-ray reflectivity, specular X-ray diffraction, grazing incidence X-ray diffraction). <ul style="list-style-type: none"> <li>- Training in grazing incidence X-ray diffraction by using synchrotron radiation (beamtime).</li> </ul> </li> </ul>
9	Christos Gatsios (UBER)	<ul style="list-style-type: none"> <li>- Training in Photoelectron spectroscopy on organic semiconductors (X-ray photoelectron spectroscopy (XPS), Ultraviolet photoelectron spectroscopy (UPS), Inverse photoelectron spectroscopy (IPES), Angle-resolved photoelectron spectroscopy (ARPES), Angle-resolved time-of-flight photoelectron spectroscopy (ArTOF)).</li> <li>- Training in UV-vis absorption spectroscopy (of thin-films and solutions of organic molecules).</li> <li>- Training in low energy electron diffraction (LEED) on organic monolayers deposited on crystalline metal surfaces.</li> <li>- Training in Atomic force microscopy (AFM) on organic thin films.</li> <li>- Training in DFT calculations on organic molecules (Orca 4.2.0 – Quantum chemistry program package).</li> </ul>
10	Lucia Di Virgilio (MPI-P)	<ul style="list-style-type: none"> <li>- Laser labs: laser lab safety instructions before starting to use laser labs.</li> <li>- Technical training: how to use FTIR and UV-Vis spectrometer, spin-coating method and Stylus Profilometer from KLA Tencor.</li> <li>- Lecture Cycle: "Advanced Spectroscopy" in August 2020</li> <li>- Lecture Cycle: "Spectroscopy and Optics" offered by Bonn group in Max Planck Institute for Polymer Research ( 16.11.2020 - 8.3.2021).</li> <li>- Language: German classes offered by Max Planck Institute for Polymer Research in Mainz two times per week.</li> </ul>
11	Alessandro Greco (MPI-P)	<ul style="list-style-type: none"> <li>- Training in improving presentation skills.</li> <li>- Laser safety instructions.</li> <li>- Course: "X-ray based techniques for organic thin-film studies".</li> <li>- Lecture cycle "Spectroscopy and Optics".</li> <li>- Lecture cycle "Advanced Spectroscopy".</li> <li>- German language course.</li> </ul>
12	Lamiaa Fijahi (CSIC)	<ul style="list-style-type: none"> <li>- Training in a variety of techniques at CSIC: 1) IRRAS (Infrared Reflection-Absorption Spectroscopy, 2). Photolithography training at ICMAB.</li> </ul>

ESR N°	ESR Name	Training and Courses
		<ul style="list-style-type: none"> <li>- Course “Academic writing skills” offered by The Doctorate Program in Materials Science (UAB) devoted to the writing of scientific texts (16 hours).</li> <li>- Group seminars to improve her presentation skills.</li> </ul>
13	Priya Pandey (PCL, UNIBO)	<ul style="list-style-type: none"> <li>- Webinars in: X-ray, luminescent coordination polymers, crystallisation, nanomechanics.</li> <li>- Course “Basics and Analysis of Mechanochemical Reaction Using MS/FT-IR Coupled Simultaneous Thermal Analysis and X-Ray Sub-micro-tomography”.</li> <li>- Soft skills training: 1) From IP management to technology transfer for business, 2) Learn: How to Write an Effective Research, 3) How to Submit a Journal Article and Get it Published, 4) Case Study Methodology, 5) From information science to technology, 6) Sustainable business in renewable energy sector, 7) Introduction to industrial property: Patents, designs and trademarks, 8) Working in Multidisciplinary teams, 9) Higher education for sustainable development course.</li> </ul>
14	Inês Martins (PCL, UNIBO)	<ul style="list-style-type: none"> <li>- Webinars in: polymorphism, X-ray, luminescent coordination polymers, crystallisation, computer simulation for organic crystal structures.</li> <li>- Course “Basics and Analysis of Mechanochemical Reaction Using MS/FT-IR Coupled Simultaneous Thermal Analysis and X-Ray Sub-micro-tomography”.</li> <li>- Soft skills training: 1) From IP management to technology transfer for business, 2) Learn: How to Write an Effective Research, 3) How to Submit a Journal Article and Get it Published, 4) Case Study Methodology, 5) From information science to technology, 6) Personal risk reduction in insecure contexts, 7) Working in Multidisciplinary teams, 8) Higher education for sustainable development course.</li> </ul>
15	Federico Modesti (BASF)	<ul style="list-style-type: none"> <li>- Disciplinary training in a variety of techniques and processes such as: Raman spectroscopy, X-ray, material engineering and processing, visual data, DSC and TGA, etc.</li> <li>- Transversal training: Information protection, how to be successful interviews, leadership, German language, etc.</li> </ul>

**Table 1: Training carried out by ESRs.**

Some ESRs have registered during this time to some conferences that were cancelled or postponed due to the COVID-19 situation. Other ESRs managed to participate in some conferences, mostly online. In Table 2, the conferences where some of the ESRs participated are summarised.

ESR N°	ESR Name	Conferences
1	Martina Volpi (ULB)	She should have participated to the ICSM 2020 Glasgow conference that for covid reasons will be held in 2022.
2	Rahul Meena (ULB)	In the last year, he registered for a few conferences but due to Covid situation they were cancelled or postponed. He plans to participate to the postponed ICSM 2020 Conference (Glasgow, summer 2022).

ESR N°	ESR Name	Conferences
4	Marco Bardini (UMons)	<ul style="list-style-type: none"> <li>- Journée Rencontre des Jeunes Chimistes, University of Namur. Symposium with other PhD students active in Belgium.</li> <li>- MSSC2020 Summer School, Online. School organized by the University of Turin and University College London to illustrate the latest developments in solid-state ab-initio simulation, especially concerning the Crystal17 software.</li> </ul>
5	Mindaugas Gicevicius (UCAM)	<ul style="list-style-type: none"> <li>- Online conference on Innovations in Large Area Electronics – innoLAE 2021 <a href="http://www.innoLAE.org">http://www.innoLAE.org</a>, 23-25 Feb, 2021.</li> </ul>
9	Christos Gatsios (UBER)	<ul style="list-style-type: none"> <li>- Online HIOS symposium, Berlin Germany (poster), 10.09. – 11.09.2020</li> <li>- Young researcher workshop, Berlin Germany, 18.11. – 19.11.2020.</li> <li>- Virtual MRS Spring/Fall meeting, November 27 – December 4, 2020.</li> </ul>
10	Lucia Di Virgilio (MPI-P)	<ul style="list-style-type: none"> <li>- Woche Vortragsreihe "Halbleiter zum Frühstück" / 3rd week lecture series "semiconductors for breakfast":</li> <li>- On Line Working Meeting: Quantum Materials in Cavities offered from Max Planck Center.</li> </ul>
12	Lamiaa Fijahi (CSIC)	<ul style="list-style-type: none"> <li>- JPhD 2020 conference: 5th Scientific Meeting of PhD Students of the UAB Campus, 17th-18th September 2020.</li> </ul>
13	Priya Pandey (PCL, UNIBO)	<ul style="list-style-type: none"> <li>- Two days international virtual seminar CEFMC2020 (Crystal engineering: From molecule to crystal), 19th-20th June 2020.</li> <li>- Poster Presentation in GCI@Home by Associazione italiana di Crystallografia, 28/9/2020.</li> </ul>
14	Ines Martins (PCL, UNIBO)	<ul style="list-style-type: none"> <li>- Two days international virtual seminar CEFMC2020 (Crystal engineering: From molecule to crystal), 19th-20th June 2020.</li> <li>- Poster Presentation in GCI@Home by Associazione italiana di Crystallografia, 28/9/2020.</li> </ul>

**Table 2: Conference attendance of ESRs.**

## 4 UHMob School

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The UHMob training school is going to be organised as part of a series of training schools of the *International School in Crystallography*. In particular, the topic of this school will be “**Molecular Crystal Engineering**” and will be held online between 31st May - 4th June 2021 (<https://crystallalice.org/2021/>).

The programme will highlight the relevance of this discipline from both, academic and industrial perspectives. Prominent scientists in the field will illustrate theoretical and practical aspects of crystal engineering in lectures, workshops and hands-on trainings. Additionally, the significance of crystal forms in different areas of chemical industry will be discussed, with particular emphasis on synthetic strategies and the design of desired material properties.

All the ESRs will participate in the Summer school and they are also encouraged to present a poster. Further, some of the principal investigators of UHMob will also be involved giving lectures.

## 5 Conclusions

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The ESR training is progressing well. All the ESRs have received the suitable technical training to carry out their research as well as other complementary courses which will be useful during their research work and future scientific careers. Further, they have also performed the X-ray training course that was provided by the University of Graz in the 18 month progress meeting.

The UHMob School in “*Molecular Crystal Engineering*” is being organised and will be held online between 31st May - 4th June 2021. All ESRs will participate in the School and also some of the principal investigators (PI) will give lectures.

Some of the ESRs could not participate in some conferences since the events were either cancelled or postponed due to the COVID-19 situation.