



# LASERLAB-EUROPE

# The Integrated Initiative of European Laser Research Infrastructures III

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Intermediate report on human resources development activities

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PP = Restricted to other programme participants (incl. the Commission Services)				
RE = Restricted to a group specified by the consortium (incl. the Commission				
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CO = Confidential, only for members of the consortium (incl. the Commission				
Services)				

# 1 Introduction and objectives

This workpackage deals with the coordination of Human Resources (HR) Development for Laserlab-Europe. It includes a wide spectrum of activities, focused to enhance the efficient use of the facilities in the Transnational Access programme by attracting new users, to develop the user community, and to reach new scientific sub-communities. The target groups of these activities are namely i) younger scientists at the doctoral or post-doctoral level, and ii) new research groups, e.g. from new members states within the EU or groups from other scientific disciplines such as biology and medicine.

The main Laserlab training objectives are:

- Developing and training of new user communities with no or little past experience in laser research, addressed by Task 1;
- Attracting and training of new users from new scientific communities (e.g. life sciences) in a multi-disciplinary perspective, addressed predominantly in Task 2;
- Coordinating externally funded activities, particularly education activities, for the development of human resources in close collaboration with other organisations, addressed by Tasks 3 and 4.

# 2 Short summary

- Within Task 1, the first Thematic User Training School on Biophotonics was held in Kosice, Slovakia, which was delivered according to the planned schedule in June 2013. The upcoming next event is a General Training School to be held in Riga, Latvia in April 2014.
- Four training visits under the scheme of Task 2: User Training in Lasers and Photonics for Biology and Health, took place between August 2013 and November 2013.
- An International School on Lasers in Materials Science SLIMS, July 2012, Venice, Italy was supported in Task 3: Cooperation with existing training programmes. A call for further proposals closed on 15 September 2013 and two new events have been selected and approved for support in 2014.
- Laserlab partners participate in a new FP7 project "GoPhoton! Photonics for everyone", recently launched in collaboration with the ECOP Alliance under the scheme of Laserlab HR issues related to external projects and organisations (Task 4). Collaboration of Laserlab Europe with the FP7 project CELIM helped to develop the biophotonics community in Slovakia and resulted in closer involvement of Laserlab partners in the EuroBioImaging ESFRI initiative.

# 3 Task 1: User Training Schools

# Task leader: ILC

The User Training Schools in Laserlab III are organised at two levels: as General Training Schools on the Pan-European scale, and smaller (regional) Thematic Training Schools focused towards potential user groups from selected scientific disciplines. While the General Training Schools will be organised at multi-national level and thus will involve a larger number of participants from the broader community, the Thematic Schools will be held more frequently and will be oriented to a smaller number of participants with extended hands-on training and an intensified learning phase in the specific theme.

Within the first reporting period, one Thematic Training School dedicated to Biophotonics has been organised in Kosice, Slovakia by ILC in June 2013. The first General Training School is under preparation and will be held in accordance with the WP5 timeplan in April 2014 in Riga, Latvia.

# User Training Workshop on Biophotonics, Kosice, Slovakia, 17-30 June 2013

The concept of thematic schools builds on the previous experience with Laserlab II training events, blended with the successful training school concept VINO-STELLA. These advanced schools deal with specific topics in laser physics where training in experimental techniques is delivered directly on research equipment in a real laboratory and with the goal of resulting in real projects and/or journal publications. Based on these foundations, we delivered a thematic workshop focused on Biophotonics in June 2013 in Košice, Slovakia. The school, organized at the premises of Pavol Jozef Safarik University (UPJS) in Košice in collaboration of ILC, UPJS and Université P. et M. Curie, Paris (UPMC), served to improve the theoretical and practical knowledge of doctoral students in advanced methods of biophotonics. One of the aims of the thematic school was to provide participants a personal contact with leading-edge laser and photonics instrumentation producers, which was ensured by close collaboration with our industrial partners as the school was supported by Becker & Hickl, GmbH, Berlin and Carl Zeiss, Slovakia.

Attended by 17 PhD students and young researchers from 5 countries, the lectures and practical trainings were imparted by 14 internationally recognized experts in the field. An upgraded concept for Laserlab user training workshops provided students with a 10-day set of lectures on recent advances in biophotonic research, supplemented by practical demonstrations of the respective experimental techniques (spectroscopy, microscopy, time-resolved techniques). In addition, dedicated lectures on safety and good laboratory practice, as well as on ethical issues in biophotonics were included in the programme. Interdisciplinary teams (each of 3-4 students) were formed, which had to select and develop their own individual projects that were publicly defended and evaluated during the last day of the school. Prices were awarded for the best student contributions. Monitoring the outcome of the workshop was implemented by User Questionnaires, mapping the post-school comments gathered from all school attendees.

The budget of Laserlab Europe III dedicated to this meeting accounts only for about 50% of the total cost of the event and was realized by means of an agreement between ILC and UPJS in Kosice.

# User Training Workshop, Riga, Latvia, 9-12 April 2014, in preparation

In contrast to Thematic Training Schools, General Training Schools will be organised with a larger number of participants from the broader community. They aim to introduce some of the basic know-how for laser users together with blocks dedicated to hands-on training and to introduce research-related soft skills, including know-how on writing a project proposal, academic writing skills, etc.

The forthcoming Regional Baltic / Northern Europe Training School For Potential Users "Laser Applications in Spectroscopy, Industry and Medicine" is set to take place on April 9-12, 2014, Riga, Latvia. The scientific directions of the school will comprise:

- An applied laser science module with a list of topics from which the users will select their practical training (Laser physics and spectroscopy, Biophotonics, Optical materials and phenomena).
- A user support / interdisciplinary module targeted at the Laserlab-Europe access programme; where all interested potential users will find the relevant organisations with which they would like to cooperate within the Laserlab network and will initiate work toward the preparation of their application for access.

The meeting is now in the final phase of preparation; for dissemination among potential users the networks of Laserlab-Europe, as well as SPIE, OSA and further academic and scientific cooperation networks will be used.

#### Other training activities

As a complementary activity under WP5, we continue our efforts in developing the online (web-based) course, which allows to provide information related to the user training activities to anybody anytime (available in testing regime at http://www.ilc.sk/training/courses). In the forthcoming period we plan to further optimise the design of the e-learning framework, as well as to add new chapters mapping the Laserlab III activities and the user training events which were held up to now. In this respect, R. Hozak has been subcontracted by ILC for audiovisual content creation for the web-based training.

# 4 Task 2: User Training in Lasers and Photonics for Biology and Health (BIOPTICHAL)

Task 2 is organised through subcontracting to CLL Coimbra, Portugal. Task leader: 14 FVB

Specific short-term training visits are designed to increase the experience of potential European users and to provide special experimental skills and competencies in the scientific area related to the JRA BIOPTICHAL. Support for short-term training visits is granted on the basis of applications for research projects, which are evaluated by an external committee of experts.

#### Selection procedure

During the reported period a call for applications for short-term training visits was opened. The call ended on the 3rd of June 2013 and was published on the Laserlab-Europe and the Coimbra Laser Lab web pages.

http://www.laserlab-europe.eu/networking/user-community-training/user-training-cll

http://www.uc.pt/en/uid/laserlab/projects/call

The selection procedure is an independent process, led by Professor Wolfgang Demtroeder (University of Kaiserslautern, Germany) as chairman of the selection panel. Each project was evaluated by two expert reviewers and projects with average score higher than 80% were proposed to be implemented.

The Laserlab-Europe online submission tool for user training applications was used for the first time for the Coimbra Laser Lab activities. The integration of the call into the electronic Laserlab-Europe proposal management system greatly improved the administrative process of the selection procedure leading to a very satisfactory time for evaluation and selection.

Four visits within six selected training projects were already performed in the period of the present report. For the total period of the project, ending 2015, a total of about 10 visits are planned.

# User training activity

During the period reported four visits were performed, two of them were led by post-graduate female researchers (PhD students) and two by more experienced researchers (one male and one female). The researchers came from four countries: Turkey, Germany, Poland and Slovakia. The four projects were carried out using all three laser facilities at CLL. Experiments were done at the Transient Absorption and Photoacoustic Lab (projects 3 and 4), the Lifetimes Lab (projects 2 and 3) and the Low Temperature Molecular Spectroscopy Lab (project 1).

The duration of the training visits was from 15 days to 29 days. The table below gives details about the duration of each visit.

Visit number	Duration	Travel days	Week days	Weekend days	Laser days
1	29	2	20	9	15
2	20	2	15	5	11
3	15	2	11	4	7
4	18	2	12	6	8

For all visits the laser facilities use was intense. On average 75% of the usable week days during the visit were laser experiment time. The remaining 25% of visit time was spent in experimental sample preparation (wet lab), experimental design and results discussion. During this period we performed 41 full experimental laser days during the four visits (of the 100 for the total Laserlab III contract).

Number of visits	Week days present in the lab	Full laser days
4	55	41

# Scientific output of the users at the facilities

The four training visits took place between August 2013 and November 2013, and although all visiting researchers expressed the intention to publish the results obtained and judged the results as publishable, the visits are too recent to yield publications already at this time.

# List of Projects and Users

# Project 1

Title: FTIR Spectroscopic and Theoretical Study of Matrix-Isolated Ionic Liquids

Visiting researcher: Nihal Kuş, nationality: Turkey, status: experienced researcher

Home institution: Anadolu University, Eskişehir, Turkey

#### Objectives:

lonic liquids (ILs) have been attracting much attention during the last decade and started to receive industrial use. It is nowadays well-known that the initial belief that ionic liquids exert no measurable vapor pressure was wrong, since many ionic liquids could already been distilled at low pressure without deterioration. Though there are now strong indications that when aprotic ionic liquids vaporize under reduced-pressure distillation the gas phase is composed of discrete anion-cation pairs, whereas protic ionic liquids seem to exist as separated neutral molecules in the gas phase, the nature of the species that are present in the gaseous phase are still controversial. To investigate this problem, we propose here to use matrix-isolation spectroscopy together with quantum chemical calculations and in situ laser-photochemistry as an alternative methodology to the general approaches previously used, which have been mostly focused on variants of mass spectrometry.

#### Achievements:

In this mission, the molecular structures and vibrational signatures of isolated 1-ethyl-3methyl and 1,3-dimethylimidazolium cations and of this species in the presence of CI- and methylsulfate anions were investigated using quantum chemistry theoretical methods and FTIR spectroscopy. The studied ionic liquids were found to exhibit local environments in both the liquid and crystalline phases which are very similar. In both environments, the dominant forces were found as being of Coulomb type, between the ions. This is reflected in the fact that the IR spectra obtained for the compounds in the liquid and crystalline phases as a function of temperature practically do not change in the whole temperature range studied (room temperature up to 150 C). Nevertheless, in agreement with the non-negligible contribution to the intermolecular interactions in the studied systems of the hydrogen bond like interactions between the C(2)-H moiety of the imidazolium ring and the anion, some spectral changes could be observed upon changing temperature in the spectral features associated with this fragment (in particular in the vC(2)-H stretching band). For the isolated species, the observed spectra were in consonance with the presence in the cryogenic matrices of the isolated ions, with jbands of the anions dominating the spectra. Assignment of the spectra and normal coordinate analyses to characterize the vibrations in both DMIM-MS and EMIM-CI were undertaken. The calculations also indicated that the imidazolium cation possesses a modest degree of  $\pi$ -resonance, measured in terms of the aromaticity index HOMA (Harmonic Oscillator Measure of Aromaticity, defined by Kruszewski and Krygowski), similar to those found for the  $\alpha$ -pyrone ring of coumarin. UV-irradiation of the matrices proof that, under the used experimental conditions, the isolated species are photostable within the 230-370 nm range.

# Project 2

Title: Excited state dynamics of indigo-fluorene-copolymers

Visiting researcher: Anika Eckert, nationality: Germany, status: post-graduate researcher (Ph D student)

Home institution: Wuppertal University, Wuppertal, Germany

Objectives:

Characterization of the excited states in indigo-fluorene-copolymers in solution and thin films at different temperatures.

#### Achievements:

During my stay in the Coimbra Laser Lab a comprehensive investigation of the excited state characteristics of four indigo-fluorene-copolymers with different chain length (degrees of polymerization, DP: 3, 5, 8 and 11) and a didodecylfluorene-dibromoindigo model compound together with the dibromo-didodecylfluorene and dibromoindigo counterparts was undertaken in solution at room temperature and as a function of temperature. The study comprised absorption, fluorescence and phosphorescence emission and triplet-singlet difference spectra, together with quantitative measurements of fluorescence, phosphorescence and triplet decay times.

# Project 3

Title: Study of physicochemical properties of NADH and its binding dynamics to enzymes.

Visiting researcher: Júlia Horilová, nationality: Slovakia, status: post-graduate researcher (Ph D student)

Home institution: Pavol Jozef Šafárik University, Košice, Slovakia and International Laser Centre Bratislava, Slovakia

Objectives:

Endogenous fluorescence of NADH is a useful tool in monitoring mitochondrial metabolic oxidative state in living cells and tissues. Time-resolved approach provides additional information about this molecule; however precise physicochemical properties of NADH and mechanisms of its binding to dehydrogenases are still largely unknown.

Achievements:

Time-resolved data of NADH fluorescence in vitro were obtained for the first time with picosecond time resolution. Higher time-resolution of data gathered with ps TCSPC set-up revealed ultrafast NADH fluorescence decay component. Moreover, valuable information was obtained on management of the instrument response function. In addition, binding of NADH to its dehydrogenase was tested: treatment with specific inhibitor rotenone prior to addition of NADH modestly decreased the fluorescence lifetimes of NADH indicating possible alteration of pre-inhibited enzyme affinity to NADH. However, experiments mimicking changes in molecular environment showed that fluorescence lifetimes are more likely to be caused by the environment than by its chemical binding. Gathered results also pointed to the possibility that the NAD(P)H fluorescence is predominantly caused by the adenine moiety of this fluorophore.

# Project 4

Title: Early events in the interaction between photosensitizers and small molecules

Visiting researcher: Janusz M. Dabrowski, nationality: Poland, status: experienced researcher

Home institution: Jagiellonian University, Krakow, Poland

#### Objectives:

Electron and/or energy transfer between small molecules and porphyrin-based compounds are among the most important types of reactions occurring in biological systems. They are key stages of many biochemical processes, take responsibility for activation or deactivation of biologically relevant compounds. They also play a considerable role in the photocatalysis and photodynamic therapy. Despite the broad-scale studies and a number of reports on the courses of these reactions, many of them still await in-depth mechanistic explanation. It particularly concerns the reactions that may take place in the excitation of ground-state complexes that occur in the femto and picosecond timescales.

The nature of the reactive oxygen species generated by photosensitizers, namely singlet oxygen, superoxide ion and hydroxyl radical may depend on the extent of the charge transfer interactions in the encounter complex between the photosensitizer and the small molecules such as O2 and probably also NO. A good understanding of the mechanisms of energy and electron transfer taking place in the ultrafast regime may contribute to improve the success of the photosensitizers in photodynamic therapy and photocatalysis.

The charge transfer interactions in complexes between the photosensitizers and the small molecules, the tendency of these sensitizers to associate with serum albumin and the ability of such formed complexes sensitizer-albumin to induce ROS/RNS will be investigated using the picosecond time-correlated single photon counting and femtosecond transient absorption spectroscopy.

# Achievements:

The "early events in the interaction between photosensitizers and small molecules" were studied in Coimbra LaserLab with picosecond time-correlated single photon counting and femtosecond transient absorption spectroscopy, using 5,10,15,20-tetrakis(2,6-difluorophenyl-3-N-methylsulfamoylphenyl)bacteriochlorin as prototype photosensitizer. In particular this bacteriochlorin was investigated with excitation at 370 nm (S3 band), 750 nm (S1 band) and 1480 nm (2-photon absorption). In the latter case, a first analysis of the data did not support the relevance of 2-photon absorption for this specific bacteriochlorin. On the other hand, the excitation at 370 nm revealed the existence of a 770 fs intermediate in the decay to a 3.3 ns intermediate, that was identified using fluorescence techniques as the S1 state. The data collected on this and other systems will be further analyzed and will hopefully lead to a better

understanding of the early events taking place in bacteriochlorins used for the photodynamic therapy of cancer.

# 5 Task 3: Cooperation with existing training programmes

Task leader: ILC

Laserlab-Europe embraces existing specific training efforts organised and funded by leading European institutions and organisations in laser science. The aim is to gain coherence between Laserlab's user training goals and external periodic initiatives, training schools and workshops. Not only will Laserlab-Europe users benefit from such existing external training programs, but such interaction will help to promote the Laserlab-Europe access opportunities at distinguished training sites. Within the first reporting period, one external event has been supported and two have been selected for support in 2014.

# 3rd International School on Lasers in Materials Science – SLIMS, July 2012, Venice, Italy

The Venice International School on Lasers in Materials Science (SLIMS) was held in Isola di San Servolo, Venice, Italy from 8th to 15th of July, 2012. It was organised in the framework of the activities of the Venice International University (VIU) and continued the tradition of the first two editions of the school that took place in the same location in 2008 and 2010. The main purpose of SLIMS is to provide PhD students and young research scientists, working in the field of laser-materials interactions, with robust fundamental knowledge that is often lacking in their training, so that they may benefit from interaction with colleagues working in areas neighbouring their own research field. While a number of well-established international conferences regularly bring together researchers working in the field of laser-materials interactions, along with bringing students up to date with the current state of the art in laser materials processing.

The 2012 school targeted mostly the level of PhD students, however advanced undergraduate and Master students as well as post-doctoral researchers joined in this edition as well. Lectures were given by 17 international experts in the field of laser-materials interaction. A total number of 35 students from 13 countries attended the school, with 25 students coming from EU countries. Participation of students was articulated through posters and brief oral contributions, followed by dedicated sessions of structured discussions. Prices were awarded in a closing ceremony for the best student contributions. Dissemination of Laserlab-Europe took place in a 20-minutes presentation given by Marta Castillejo, one of the School Directors and Chair of the Committee of User Representatives in Laserlab-Europe III. Opportunities for Access and User Training Events were advertised and a round of questions and discussions about Laserlab-Europe took place afterwards.

# Selection of further external events

In the beginning of 2013 a new scheme of selecting external events to be supported had been proposed and agreed upon by the Laserlab-Europe Networking Board. Accordingly, a call for applications for cooperation with international training and summer schools was published on the Laserlab-Europe web page during the summer of 2013 (http://www.laserlab-europe.eu/networking/user-community-training/first-call-training-events). The call was closed on 15 September 2013 and evaluated. Five proposals for training events were received, out of which two have been approved by the Laserlab Networking Board and will be co-funded by Laserlab in 2014, namely:

- The Advanced X-ray spatial and temporal metrology training school (with COST action MP1203), Dubrovnik, Croatia, August 2014

- LA3NET 3rd School on Laser Applications, Salamanca, Spain, 22-26 September 2014

# 6 Task 4: Coordination of HR issues related to external projects and organisations

Task leader: LU

The planned investment of nearly a billion Euros of structural funds in the set-up of new research infrastructures in three new Member States (ELI) requires substantial efforts to cope with the impending need in human resources both for these new RIs and for the already existing laser infrastructures. Laserlab-Europe should help developing such human resources through available measures within and beyond the IA instrument. The aim of this task is to build closer links and collaboration with major EU laser and photonics initiatives, professional organisations like EOS, SPIE, Photonics21 and other potential external partners of Laserlab-Europe.

# Interaction with other FP7 and ESFRI projects

The achievements, knowledge and experience obtained within the Laserlab network allow the teams built by Dr. D. Chorvat (ILC) and Prof. P. Miskovsky (University of P.J. Safarik in Kosice) to start a fruitful collaboration between Laserlab III and the FP7 project CELIM -Fostering Excellence in Multiscale Cell Imaging, coordinated by the Department of Biophysics, Faculty of Natural Sciences, University of P.J. Safarik in Kosice. The aim of this project is to develop an excellent interdisciplinary research group in cell bioimaging and improve the conditions for a participation in prestigious international projects. Based on this mutual collaboration, interlinked with the support of Structural Funds, Slovakia has recently joined the EuroBioImaging (EuBI) initiative, a project on the ESFRI roadmap, where Dr. Chorvat has become a deputy of the Ministry of Education, Science, Research and Sport of the Slovak republic in the Inter-Governmental working group of EuBI. We hope that these initiatives together will help us to consolidate the biophotonics community in Slovakia and beyond, as the EuBI initiative includes also other partners of Laserlab-Europe (e.g. ICFO, LENS).

For future outreach activities in photonics a new FP7 project GoPhoton! - Photonics for everyone was submitted to ICT Call 11, FP7-ICT-2013-11 under the lead of ICFO, with several members of the consortium belonging to the Laserlab-Europe network. The project was evaluated with a high score and is starting in January 2014, aiming to increase awareness within the EU member states about the importance of photonics for the economy, society and career opportunities. The project is based on the framework of the Alliance of European Centres for Outreach in Photonics (ECOP), which is committed to create long-term partnerships for enhanced engagement in photonics outreach. ECOP's goal is to promote the importance, potential, pervasiveness and ubiquity of optics and photonics - "The Science and Technology of Light". Its long-term mission is to impact all levels of European society, from students and teachers, industry, entrepreneurs, citizens of all ages to multidisciplinary institutions at large, and raise awareness of the importance of photonics in a sustained way.

The ECOP Alliance connects nodes in European countries by building a network of photonics research groups and outreach teams that aim to strengthen links with their local communities. This is accomplished by developing tailor-made programmes and activities to address schools, universities, museums, media, industry, hospitals, etc. to communicate the impact of photonics, the latest scientific research, discoveries, and innovations. Overall, the initiative offers a place for substantial broadening of educational and outreach activities in photonics in the EU and opens new possibilities for collaborations related to Laserlab-Europe's HR-related tasks and issues.

The Laserlab-Europe National Contact Points (NCPs, see WP8) have, during this first reporting period, played an important role in interacting with relevant initiatives of the ELI

project towards building and consolidating the communities of researchers in Eastern European member countries. They also interact with other Networking Activities involved in User Training and the development of human resources for the future needs of the European research infrastructure. In particular, PALS organized the first ELI-Beamlines International Summer School in June 2013.

# Collaboration with the International Laser Centre SPIE Student Chapter

The ILC SPIE student chapter was inaugurated during the 5th Slovak Biophysics Symposium, which took place in Bratislava on 19-21 March 2012. Chapter advisor Dr. Chorvatova is a core member of the Laserlab III team, thus close cooperation between SPIE chapter events and Laserlab presence is maintained and highly appreciated since the beginning of the Laserlab III operation.