

Brussels, 12 May 2023

COST 041/23

#### DECISION

Subject: Memorandum of Understanding for the implementation of the COST Action "Supramolecular LUminescent Chemosensors for Environmental Security" (LUCES) CA22131

The COST Member Countries will find attached the Memorandum of Understanding for the COST Action Supramolecular LUminescent Chemosensors for Environmental Security approved by the Committee of Senior Officials through written procedure on 12 May 2023.





#### MEMORANDUM OF UNDERSTANDING

For the implementation of a COST Action designated as

#### COST Action CA22131 SUPRAMOLECULAR LUMINESCENT CHEMOSENSORS FOR ENVIRONMENTAL SECURITY (LUCES)

The COST Members through the present Memorandum of Understanding (MoU) wish to undertake joint activities of mutual interest and declare their common intention to participate in the COST Action, referred to above and described in the Technical Annex of this MoU.

The Action will be carried out in accordance with the set of COST Implementation Rules approved by the Committee of Senior Officials (CSO), or any document amending or replacing them.

The main aim and objective of the Action is to create a scientific and technological platform working towards the development of luminescent sensors used to help resolve environmental security problems. A multidisciplinary team of experts from academy and industry will strongly cooperate for the success of this goal. This will be achieved through the specific objectives detailed in the Technical Annex.

The present MoU enters into force on the date of the approval of the COST Action by the CSO.



#### OVERVIEW

#### Summary

The main goal of LUCES is the creation of a multidisciplinary network, comprised of researchers with complementary expertise from academia, technological centers and industry, working towards the development of luminescent sensors to be used to help resolve environmental security problems. The luminescent signaling unit will confer a high sensitivity to the sensor and be activated following the molecular recognition event. The Action will gather the leading research groups in the field of supramolecular chemistry, chemical sensors, (nano)materials, electronics, theoretical calculations as well as experts in different analytical techniques, researchers from industry and interested stakeholders, in order to be able to fulfil all the requirements to arrive to bridge the gap between fundamental research and the market. This multidisciplinary group will be strongly committed to promote a competitive European network in which the participation of Young Career Innovators and Inclusiveness Target Country will be highly valued. In this way, LUCES is expected to become an international reference network that can be contacted by any researcher and/or company looking for specific solutions in this topic. Transfer of knowledge will be also carried out through conferences, annual meetings, workshops, training schools and STSMs. Mobility of young researchers between different centers (academic and industry) will reinforce the existing contacts and ease the success of the Action. Dissemination of results will raise awareness about what science, in particular supramolecular luminescent chemosensors, can do for society, promoting the active collaboration between academic and non-academic researchers.

Areas of Expertise Relevant for the Action	Keywords
<ul> <li>Chemical sciences: Supramolecular chemistry</li> </ul>	chemosensors
Chemical sciences: Molecular architecture and structure	<ul> <li>supramolecular chemistry</li> </ul>
	<ul> <li>detection of contaminants</li> </ul>
	Iuminescence
	<ul> <li>prototypes and devices</li> </ul>

#### **Specific Objectives**

To achieve the main objective described in this MoU, the following specific objectives shall be accomplished:

#### Research Coordination

• Establishing a reference European network on the development of sensing devices to respond to all the scientific demands of the scientific community and stakeholders on the topic of the project and become a reference at the European level for researchers inside and outside the Action.

• Coordination of complementary expertise and facilities, and identification of protocols for the development of applied sensors.

• Establishing new protocols for the design and development of new sensors and sensing devices with a potential high success rate.

• Contribution to the development of technological devices. This will be uniquely achieved thanks to the international coordination of the different Action members including industrial.

• Communication and dissemination of the research objectives, challenges, results, activities and good scientific practices. This will be relevant for the exchange of knowledge and promotion of the results that might be of industrial interests, as well as European policies and to identify new industrial partners potentially interested in the Action.



#### Capacity Building

• Fostering knowledge exchange and the development of a joint research agenda around a topic of scientific and socio-economic relevance.

• Fostering knowledge exchange and the development of at least one final device to be used for the detection and sensing of contaminants with very low LoD under real-life conditions.

• Training students in supramolecular methodologies and providing them with skills and knowledge to apply in the construction of materials and devices for chemosensing applications.

• Acting as a stakeholder platform or trans-national practice community by reinforcing socio-economic applications of supramolecular LCs in the area of environmental monitoring and human safety.

• Supporting a high proportion of YRIs, ITCs and assure gender balance in the Action.

### TECHNICAL ANNEX

#### 1. S&T EXCELLENCE

#### 1.1. SOUNDNESS OF THE CHALLENGE

#### 1.1.1. DESCRIPTION OF THE STATE OF THE ART

Environmental security, which can be understood as "the absence of risk or threat to the environment that communities depend on and live in", is of major concern for all living organisms. The consumer culture in "prosperous" countries, high-yield agriculture but also war and military operations, affect the safety of ecosystems. Quality of life, public health and sustainable human activities are all at stake and solutions are needed to mitigate the negative impact of industrial and technological activities on air, water and soil. In order to help develop corrective measures to ensure a safe and healthy environment, **affordable and ubiquitous sensors for the detection of contaminants and hazardous chemicals** are needed. In this context, luminescence based chemosensors are of particular interest due to their high sensitivity enabling the detection of very low levels of contaminants (*Coord. Chem. Rev.* 2020, *420*, 213425; *Chem. Rev.* 2019, *119*, 322).

Environmental security is concerned not only with direct and indirect threats to human survival but also with environmental degradation and environmental (global) change in general. Population growth, extensive land-use, resource exploitation, pollution patterns, economic interdependency (globalization), and other social and political factors all affect our environment. The COVID-19 pandemic has recently shown us why the monitoring of a safe environment is so relevant. The detection of contaminants in the environment (water, soil, air) is without any doubt of great importance.

Supramolecular Chemistry and Nanochemistry are particularly well-suited frameworks for the design of tailored made chemosensors. These fields are now mature enough to apply the acquired fundamental knowledge to develop **functional devices equipped with sensing units** for the selective detection of **contaminants**, such as common organic materials found in sewage soaps, residues from industrial activities and agricultural effluents, most of them identified by the European Environment Agency. Recent relevant efforts in the field are the development of supramolecular optical sensor arrays for onsite analytical devices (*J. Photochem. Photobiol. C :Photochem. Rev.* **2022**, *51*, 100475) and the supramolecular systems for the detection of biologically relevant compounds, such as heparin (*J. Med. Chem.* **2022**, *65*, 4865).

With luminescent chemosensors (LCs) it would be possible to achieve higher sensitivity and improved limits of detection (LoD) compared to current detection methods. LCs would also enable fast and direct detection without preliminary treatment, as needed in the case of chromatographic techniques. This has been categorically proven by the successful application of Photoinduced Electron Transfer (PET) sensors, originally developed by A.P. de Silva using supramolecular design principles, for the detection of various targets, both at the laboratory scale and in environmental conditions (Chem. Soc. Rev., 2015, 44, 4203). Commercial systems based on this principle have been developed for the detection of Na<sup>+</sup> or K<sup>+</sup> in blood (OPTITM cassettes distributed by Optimedical). LCs for environmental monitoring are still the object of fundamental research and adequate and general procedures for their implementation into devices for real-life applications are still needed. The conversion of smart molecules and nanomaterials into robust sensors and the delivery of a final device to the market for general use, requires the collaborative effort of researchers with complementary expertise (supramolecular, analytical and computational chemists, material scientists, photophysicists, engineers, electrotechnicians, ...) from academia and from industry. The collaboration is mandatory in order to bridge the gap between laboratory scale research and the technology needed for the development of a sensing device (product). The design and development of specific signalling units in academic laboratories must be combined with the know-how of more technological units in order to produce final prototypes that respond to the needs of the market and those related to environmental concerns. The principles applied for the successful implementation of the optical sensor arrays and OPTITM cassettes, are of great relevance for this Action and will carefully be analysed and taken into consideration.

# LUCES emerges as a European platform where the know-how of academic and industrial researchers with complementary expertise, from fundamental to more applied research areas, are brought together to design and develop LCs for real-life environmental applications.

LUCES considers that the direct involvement of industry is key for its success. All researchers will work together to ensure that LUCES becomes a European reference for the design and development of highly sensitive sensing devices based on supramolecular luminescent signalling units and high-affinity binding molecular scaffolds.



The Action includes researchers with strong expertise in the development of sensors, particularly LCs, using (supra)molecular systems and (nano)materials. A fluid transfer of information between all Action members, both academic and industrial, will be ensured during the in-person general meetings of the Action, as well as in regular on-line meetings of the researchers involved in each working group. PhD students and post-doctoral researchers will perform short scientific missions in the laboratories of the academic and industrial partners. The network comprises, already at the time of submission, top level researchers working on cutting-edge investigations of molecular sensors and devices applying state-ofthe-art, as well as emerging technologies, and having at their disposal well equipped facilities. Some of the Action members have recognised expertise in the design and synthesis of chemosensors for the detection of several analytes that are relevant to this Action; others have the required skills in electronics, electrochemistry and engineering to develop devices based on the molecular sensors. There are 7 industries participants that will provide expertise in the manufacturing of sensing devices and, as important stakeholders, will help define the special needs for the detection of contaminants in air, soil and/or water. The equal involvement and participation of the academic and industrial partners in the Action will give rise to a constructive co-creation and co-design environment that will enhance the transfer of knowledge and scientific results into the construction of sensing devices for real-life applications and their commercialization. Well-defined communication and dissemination plans of the Action' progress, results and activities, will encourage the involvement of additional partners and industries. This will have an important impact on the success of the Action. Our strategy to develop sensing prototypes and devices, together with a strong communication within the Action and strong dissemination to the society, is unprecedented in the European community. Supramolecular chemistry and Nanochemistry (chemical nanotechnology) are already well-established research areas that have had a reduced success in the development of molecular sensors and devices. The Action believes that this is mainly due to a lack of interaction between groups working in the different aspects and steps required for the development of a molecular sensing device. Hence, the development of sensing prototypes and devices will be pursued during the whole network's life span by combining the knowledge and skills provided by the Action members for the different necessary steps. That is, from the synthesis of molecules or nanostructures, anchoring them to solid materials, development of small prototypes and achieving the final goal of producing sensing devices. A key difference of LUCES with respect to previous existing networks resides in combining the complementary efforts, knowledge, skills and expertise of researchers (academic and industrial) working together towards a common goal. In this sense, the combination of basic science and applied research will provide an ideal platform to achieve the long-term goal of the Action.

#### 1.1.2. DESCRIPTION OF THE CHALLENGE (MAIN AIM)

The LUCES Action will create and establish a scientific and technological platform to gather, under a unique umbrella, a critical mass of European research groups able to develop high affinity and sensitivity chemosensors for the detection of different analytes of concern for human environmental security. Luminescent signalling units represent a clear advantage with respect to other detection methods due to their extreme sensitivity, which can be as low as a few ppb, for specific analytes. Using supramolecular approaches chemists are able to design molecular sensors featuring high affinity and selectivity. Thus, the use of supramolecular LCs opens the possibility for extremely sensitive and selective detection of analytes, that is difficult to achieve using other methodologies. Additionally, their extreme LoD mean that low quantities are required, and this eliminates the need to concentrate samples through complex processes. The successful incorporation of the LCs into portable devices however still needs substantial efforts.

The initial Action members are an excellent starting point for the creation of the network. This initial team is based on experts in the different disciplines and aspects required for the development of LCs in devices as final products. Most of the researchers involved in the application have not been working together but joined enthusiastically this project since the Action believes in the possibility of achieving together this goal. It demands an in-depth knowledge on how to develop a real sensing device. That is, starting from the proof of concept and the understanding of the intermolecular interactions established between the sensor and the analytes of interest (molecular recognition) to their implementation in the functional devices. The inclusion of additional participants to the Action and the diffusion of the results to other researchers will further help us achieve our goal. The Action aims at **becoming a reference network in Europe for researchers, both from academia and industry, wishing to develop sensors for specific analytes in response to the needs of final users.** The strengthening of international research with a view to harvest all the advantages that derive from the exchange of expertise and knowledge between the research groups, represents one of the benefits of promoting the Action. Collaborative efforts will take advantage of the networking opportunities to address our



# S&T challenge and to promote participation of Young Researchers and Innovators (YRI) and Inclusiveness Target Countries (ITC).

The transfer of knowledge between fundamental research and real-life applications, and the training of early-stage researchers working in this cutting-edge research field, will be pursued. The Action believes that COST is the perfect framework to achieve these goals. The involvement of the industrial stakeholders offering their perspectives on the topic and highlighting their needs will be highly beneficial to align the research programmes of the academic partners. The results of the research emanating from the Action will be spread, not only to the scientific community, but also to the society in general that represents the main beneficiary of the transfer of knowledge pursued by the Action. In addition, the Action's members will disseminate the results highlighting its importance in relation to the development of sensing devices for environmental monitoring and their application in ensuring compliance with laws and regulations to mitigate risks of harmful effects to the natural environment and human health. The training of YRI is potentiated when carried out within the framework of a European network offering many competences and facilities, accessible through short-term missions (STSM) and training schools. The Action will also integrate YRI in the management of the project as co-leaders of the WGs. LUCES will certainly represent the most concrete chance to tackle key problems regarding environmental safety/security sensing and will: i) Create and establish a unique European network of researchers able to design and develop sensors, acting as a S&T resource for researchers and industrial stakeholders; ii) Create a virtual laboratory with unique facilities and technological equipment available to all participating research groups; iii) Constitute a real platform where academics and industry researchers can exchange ideas and expertise in the research field; iv) Optimize scientific methods and data treatment procedures for the study of molecular recognition in complex systems and nanomaterials regarding environmental sciences and safety and doing it with short times response; v) Develop LCs, specifically designed to sense analytes of environmental concern in water, soil or present in the air; vi) Establish and update reports regarding molecular sensing of analytes causing environmental problems. All these points will be coordinated by the Core Group (CG) that will also be in charge of directing the match-making and pushing forward specific collaborations, to ensure the achievement of planned deliverables and milestones.

#### 1.2. PROGRESS BEYOND THE STATE-OF-THE-ART

# 1.2.1. APPROACH TO THE CHALLENGE AND PROGRESS BEYOND THE STATE OF THE ART

The aim of all Action participants is the translation of the building principles of supramolecular LCs into flexible and scalable prototypes and devices able to tackle the monitoring of chemical threats to human health and environmental safety. The industrial stakeholders that are the endusers of the developed technology, will be an important part of the Action. Three industries, with specific needs for the detection of a series of analytes, are already members of this Action and other end-users are expected to be identified during the implementation of the Action. Four other companies, also members of the consortium, have expertise in manufacturing sensing devices, where one of them is also an active policy maker with respect to definition of the legal limits of the manufactured sensors.

The essence of LUCES will be moving one step further in the field of LCs, already well established at the fundamental level, with the goal to connect academic researchers with those working in industry. LUCES aims to be an active platform suitable to provide solutions to the industrial stakeholders for the sensing of harmful environmental analytes. This scientific platform will be unique in Europe thanks to the multidisciplinarity of the participants, the involvement of companies and stakeholders and the wide variety of available approaches for the design of the final sensors. The collaborative efforts of the researchers together with their complementary expertise will rapidly boost the knowledge in the field beyond the state-of-the-art.

There is a current need for sensitive, rapid, and selective sensors/devices to detect and screen pollutants to manage effective environmental monitoring and bioremediation processes. This will be achieved using Supramolecular Chemistry principles, which are based on molecular interactions and their function at the molecular scale. Complementary molecular interactions can be used to recognise an analyte by a synthetic host, assemble them in a supramolecular complex with high affinity and selectivity. Supramolecular scale to the macroscopic scale is key to developing sensing systems displaying unprecedented functionalities. This strategy represents the main difference between LUCES and other existing networks based on changes of the macroscopic properties (resistance, conductivity etc.) of materials following nonspecific binding.



The research in the field of Supramolecular Chemistry has significantly advanced in the last two decades and is mature enough to enable to exploit molecular recognition processes to address real-life problems. The expected scientific results will be in the form of: i) the development of different type of sensors with desired properties and functions for specific targeting; ii) the establishment of new collaborations at the European level between groups working with complementary and specific techniques that will allow the development of the final devices; iii) the development of portable prototypes and devices (from bench to market-final products). It is a complex approach that is only possible thanks to the multidisciplinary background from the partners taking part in LUCES, which are experts in synthesis, multi-technique characterization, molecular and nanomaterials chemistry, engineering, analytical chemistry, theoretical chemistry, and electronics. Very importantly, LUCES will also ensure an excellent level in training. It will provide the working force involved in the network with an outstanding level of competences and knowledge in the field of supramolecular sensors and its real-life applications on environmental security. This approach will also confer to the socioeconomic impact of the Action a significant role in improving the quality of life of the population by delivering concrete and valuable results, as well as technological innovations. To fulfil these goals, the Action will actively work in the following areas:

- **Stimuli-responsive systems for sensing**. The Action will develop new and reliable methods for the rapid screening of the binding of small molecules and ions to synthetic molecular sensors. The developed sensors will feature low LoD and high specificity. The binding event will be translated into changes of the luminescence properties of the sensors.

- **Prototypes and Devices for industrial applications**. In recent years, groups involved in this Action have synthesized receptors that bind among others biogenic amines, cyanides and volatile organic compounds selectively. These molecular scaffolds are useful for the development of molecular sensors for quality control in food and environmental contaminants, as well as for medical diagnosis. Within the frame of the Action expertise will merge and afford useful and simple prototypes and devices based on these molecular sensors, which will be used in real-life sensing experiments and tested by the industrial partners.

- **Training.** The only way to advance in obtaining high-quality results is by training early-stage researchers to high levels of excellence in research. In addition, good laboratory practices must be promoted, and experimental results should be backed-up by theoretical calculations. Only very well-trained researchers can apply their knowledge and outstanding skills to produce significant advancements in any subject in academia, research centres, industries and/or other institutions.

- **Communication and Dissemination.** Sharing of knowledge, scientific background and results between research groups will be ensured throughout the implementation of the Action by holding yearly meetings for all members and regular "on-line" discussions by those involved in the different working groups. The dissemination of the results will also be guaranteed by inviting representative of other academic institutions, enterprises, governments, and other stakeholders interested on safety-environmental security and sensing to attend and participate in the general yearly meeting of the Action.

The Action is convinced that the establishment of LUCES will help this research field to grow stronger. It will also increase the awareness of the importance of molecular sensing to the general public by providing real-life applications. Synergies with other Actions (COST, Marie Curie RISE, European and National networks) will also be promoted by contacting researchers involved in Actions with scientific proximity to LUCES and inviting them to any of the annual or WG meetings. The participation in EU programmes (e.g. Researchers' Night) and the engagement of Action's members in joint applications to obtain funding from European Projects (e.g. DN, ERC Synergy, Pathfinder) will be also promoted. These activities will evidence the important role played by LUCES in scientific networking at an international (European) level.

#### 1.2.2. OBJECTIVES

#### 1.2.2.1. Research Coordination Objectives

LUCES will be strongly committed to reach tangible and high-level scientific objectives. To achieve this goal, the networking between the different experts of the Action will be stimulated and reinforced promoting the exchange of knowledge within, and between, WGs. The resulting activities will ensure the growth and exchange of expertise and facilities/technology between countries. All this is crucial to achieve success in the following defined Research Coordination Objectives:

i) *Establishing a reference European network on the development of sensing devices.* The global scientific background present in the Action will allow to respond to all the scientific demands of the scientific community and stakeholders on the topic of the project and become a reference at the European level for researchers inside and outside the Action.



ii) Coordination of complementary expertise and facilities, and identification of protocols for the development of applied sensors. The WG coordinators will report on the progress of the different WGs to the Core Group on a regular (trimestral) basis. The Core Group will thus be able to ensure that the different researchers of the Action are able to access the adequate equipment/expertise to move from fundamental to more applied studies.

iii) Establishing new protocols for the design and development of new sensors and sensing devices with a potential high success rate.

iv) Contribution to the development of technological devices. This will be uniquely achieved thanks to the internal coordination of the Action members. The more promising sensors will be delivered by the members that are specialists in the design of devices. For example, material chemists will consider the coupling of the supramolecular receptors to the adequate (nano)materials and analyse the sensing response; computational chemists will suggest chemical modifications in order to boost the sensing/recognition capacities of the systems for a specific analyte; the industries, who at the start will have defined their specific needs and requirements, will test the final devices; the good operation of each sensor (individual electronics) will be checked and characterized under specific environmental conditions to have a quality control of the developed prototypes.

Intellectual property rights (IPR) will be carefully considered. One of the fundamental goals of the Action is to protect the most relevant findings with patents. The consortium will produce regulation concerning the handling of IPR. This will consider the following: 1) all previous scientific knowledge made available for the execution of the Action remains the exclusive intellectual property of the party holding it prior to the beginning of the Action; 2) any results resulting directly and exclusively from the activities developed under this agreement that can be protected by IPR shall be owned by the party that contributed for such results. In case it isn't possible to separate such contributions, then results shall be owned by both parties; 3) the parties agree to negotiate the terms of the shared results in a separate agreement until 3 months after the end of the Project; 4) The Action partners reserve the right to carry out education, research and development (R&D) activities based on the project results.

v) Communication and dissemination of the research objectives, challenges, results, activities, and good scientific practices. The communication, dissemination and sharing of knowledge within the network and with the general public, and stakeholders is basic to the progress of science and will be strongly and closely followed in all the networking activities of LUCES. This will also be relevant for the promotion of the results that might be of industrial interests, as well as European policies and to identify new industrial partners potentially interested in the Action. A particular WG will be mainly dedicated to this task (WG4) since it is of great importance for the success of the Action.

#### 1.2.2.2. Capacity-building Objectives

LUCES is focused on the main capacity-building objective of creating a solid and recognized network, working on developing tools to help mitigate environmental contamination and human-health security problems. To this end, LUCES brings together leading researchers with complementary expertise and different scientific and technological backgrounds. The general public, research centres, industries and academia will be made aware of the importance of the research field. This main goal will be achieved through different capacity-building objectives, such as:

i) Fostering knowledge exchange and the development of a joint research agenda around a topic of scientific and socio-economic relevance. Short term scientific missions (STSMs) will be encouraged and will enable Action members to access different laboratories with different expertise (more specifically addressed to the students, YRIs and ITCs). LUCES will also use project management software packages to ensure efficient communication and collaboration between team members such as an intranet to post monthly results. Thus, each researcher will be kept up to date and quickly informed about the issues as they arise. Research profiles will be accessible to all Action members facilitating the emergence of collaborations among partners. Communication within the network will create a frontier-less area where resources and knowledge are shared and used to the full. Newly established research groups and YRIs will be provided with networking opportunities and participation, to form future leaders in science, policy and management.

ii) Fostering knowledge exchange and the development of at least one final device to be used for the detection and sensing of contaminants with very low LoD under real-life conditions.

iii) *Training of young researchers in supramolecular methodologies.* This objective is clearly of great importance and could underpin the emergence of the next generation of European researchers working both in academia and industry having a wide range of expertise in molecular sensing. The Action will



provide them with skills and knowledge for chemosensing applications. They will be responsible of translating the breakthroughs of supramolecular LCs revolution into real-life applications. The attendance to programmed Training schools will be extensively promoted and encouraged for all young researchers involved in the Action.

iv) Acting as a stakeholder platform or trans-national practice community by reinforcing socio-economic applications of supramolecular LCs in the areas of environmental monitoring and human safety. This will ensure the formation of a broad network and highly competitive consortium. LUCES will work on building the capacity to create, enhance and develop participants' ability beyond national level, as well in assisting them to provide solutions to important scientific challenges related to molecular sensors.

v) Supporting a high proportion of YRIs and ITCs participants and ensure gender balance in the Action. LUCES will ensure the involvement of YRIs, ITCs and female researchers to actively take part in leading and managing the Action. They will be actively involved in the organisation of the different activities and decision making of the Action. For YRIs, this will be an important step for their career development.

**This platform is perfectly aligned to the Horizon Europe issues** (Pillar 2 clusters – Global Challenges and Industrial Competitiveness: Health; Digital & Industry; Climate, Energy & Mobility) and the Agenda 2030 for Sustainable Development (e.g. Goal 3: Ensure healthy lives and promote wellbeing for all at all ages; Goal 6: Ensure availability and sustainable management of water and sanitation for all; Goal 11: Make cities and human settlements inclusive, safe, resilient and sustainable; Goal 13: Take urgent action to combat climate change and its impacts; Goal 14: Conserve and sustainably use the oceans, seas and marine resources for sustainable development; and Goal 15: Protect, restore and promote sustainable use of terrestrial ecosystems, sustainably manage forests, combat desertification, and halt and reverse land degradation and halt biodiversity loss).

#### 2. NETWORKING EXCELLENCE

#### 2.1. ADDED VALUE OF NETWORKING IN S&T EXCELLENCE

2.1.1. ADDED VALUE IN RELATION TO EXISTING EFFORTS AT EUROPEAN AND/OR INTERNATIONAL LEVEL

LUCES represents a relevant added value in comparison to some existing (running or ended) collaborative projects in Europe. To the best of our knowledge, there is no large network currently active (neither at the European nor international level) dedicated to merge the knowledge and possibilities that LUCES offers. Individual collaborations between research groups already exist. but this cannot substitute the real advantages that will emanate from the possibility to create this large network. The topics addressed by the Action are highly challenging and multidisciplinary but, at the same time, they share a common goal: chemosensing for environmental security. Supramolecular Chemistry and Environmental Research are fields of broad interest. Other research programs addressing some related aspects of these fields have been funded in the past. However, none of them is based on the integrated approach of LUCES. Focusing on COST Actions the following can be cited, for example: D31 (Organising Non-Covalent Chemical Systems with Selected Functions, 2004-2009), CM1005 (Supramolecular Chemistry in Water, 2011-2015), CM1105 (Functional metal complexes that bind to biomolecules, 2012-2016), CA 18202 (Network for Equilibria and Chemical Thermodynamics Advanced Research, 2019-2023) dedicated to supramolecular chemistry and weak interactions; CM1304 (Emergence and Evolution of Complex Chemical Systems, 2013-2017), CM1402 (From molecules to crystal; Crystallize; 2014-2018) covering some aspects of (nano)materials chemistry; ES1202 (Conceiving Wastewater Treatment in 2020 Water\_2020; 2012-2016), TD1407 (Network on Technology-Critical Elements: From Environmental Processes to Human Health, NOTICE, 2015-2019); CA18125 (Advanced Engineering and Research of aeroGels for Environment and Life Sciences, 2019-2023), dedicated to environmental issues and chemical engineering. None of these Actions covers our main goal of bridging the established know-how and possibilities of research groups working on the development of LCs (using supramolecular chemistry and molecular recognition) with the know-how of technological centres, engineers, electrochemists and companies in designing and producing prototypes and devices for environmental monitoring of chemical threats to safety and human health.

The relevance of Supramolecular Chemistry and Environmental research is also reflected in different **International Conferences**. These include the Conference held in 2018 in Gregynog, Wales (52<sup>nd</sup> ESBOC-European Symposium on Biological and Organic Chemistry Symposium) focused on "Biological applications of Supramolecular Chemistry"; the cycle of Gordon Conferences on "Self-Assembly & Supramolecular Chemistry" started in 1977 taking place every two years; the annual



International Symposium on Macrocyclic and Supramolecular Chemistry Challenges in Organic Materials & Supramolecular Chemistry (ISMSC, 15<sup>th</sup> Edition in 2022; more than 700 participants in the last years); the International Symposium on SupraBiomolecular Systems (SupraBio) (Spain, 2019); the International Conference on Multifunctional Hybrid and Nanomaterials (6<sup>th</sup> Edition, Spain, 2019); the biannual PhotoIUPAC Conference (27<sup>th</sup> Edition, Ireland, 2018); the International Conference on Climate Change Adaptation (virtual format, September 03-04, 2020); and the International Conference on Environment, Ecology, Energy and Biotechnology (virtual format, September 16-17, 2020). Additionally, Action's participants will be strongly encouraged to join other conferences addressing more specifically the topic of Molecular Sensing and focusing on applications and technology transfer, such as IEEE Sensors (Dallas, October 30-November 2, 2022), Sensors (Athens, October 26-28, 2022), International Conference and Expo on Sensors and Sensing Technology (Barcelona, June 6-7, 2023). These avenues will provide direct opportunities for the dissemination of our results and the Action, and will allow us to contact new stakeholders both from academia and industry and increase the membership of the Action.

The presence of the LUCES participants in the next editions of these Conferences will be encouraged and will be used to disseminate the results and progress of the Action. These events, however, do not offer the opportunity to achieve high level applied objectives that are only possible by bringing together the expertise of different research groups working in a common trans/inter/multi-disciplinary project. The organization of an *International Symposium on Optical Sensing and Devices* will be carried out at the end of the Action in order to join under a common roof, researchers that until this point have been working separately on the two disciplines. **Taking together all the above, LUCES will offer an added and really positive value in the field of the Action compared to the current existing efforts at the <b>European and/or international levels**.

#### 2.2. ADDED VALUE OF NETWORKING IN IMPACT

# 2.2.1. SECURING THE CRITICAL MASS, EXPERTISE AND GEOGRAPHICAL BALANCE WITHIN THE COST MEMBERS AND BEYOND

This COST Action is currently formed (supported) by 41 interdisciplinary scientists with broad expertise in Supramolecular Chemistry, Photophysics, Sensing, Molecular modelling, Engineering, Materials, Nanotechnology and Electronics. The group is composed by Institutions of 20 COST member countries that are adequately distributed geographically. It also contains a 55 % of COST Inclusiveness target countries (ITCs) and one International Partner Country (IPC). 13 of the members (32 %) are YRIs with very strong scientific backgrounds. Gender balance is also accomplished (51 % women). The network comprises researchers from universities, research and technological centres and industries ensuring the feasibility of the different steps of the objectives, from the design of molecular sensors to their implementation into prototypes, and the production of technological end products. Efforts will be made in the Communication and Dissemination process to attract more international companies interested in bringing to this scientific community the points of views for issues that remain to be solved in this field.

The large number of scientists involved in this network, having complementary and multidisciplinary background, secures the required critical mass and expertise to successfully develop the main goals. It also demonstrates the interest of the research topic in Europe ensuring the necessary resources and facilities to achieve a successful outcome of the Action. The high-quality track records ensure the required capacity to obtain high level scientific results. The network will be open throughout its implementation, in order to promote the continuous evolvement of complementary expertise required for the success of the Action. The appropriate funds for research will be guaranteed by the numerous ongoing national and international financed projects, in which the associated members of the Action are involved. The participants are widely distributed geographically, and it is expected that they will increase and activate new collaborations in all Europe. The Action will be important for the careers and international recognition of YRIs and ITCs. STSMs will be performed within research groups with complementary expertise, ensuring the training of the scientists of the future.

#### 2.2.2. INVOLVEMENT OF STAKEHOLDERS

This Action identifies stakeholders ranging from individuals to industries and policy makers. Internal stakeholders are the core principal investigators and representatives of the industrial partners of the Action, and the external stakeholders are potential investors, policy makers, press agencies and researchers outside the Action. The success of the Action will allow the development of new methods to monitor the impact of contaminants on the environment with a socio-economic dimension thanks to the development of prototypes and devices for real-time detection of contaminants and also the



development of a portfolio of supramolecular systems, databases, decision support tools, capacity building actions and policy recommendations related to the prevention and mitigation of contaminants. The involvement of stakeholders in LUCES will be carried out through different mechanisms:

- Direct participation in the Action. The Action starts with the direct participation of 7 companies that will at the beginning of the Action identify a series of analytes that are key to their interests. Molecular sensors and devices for the identified analytes will be developed during the progress of the Action. The different research groups will be in charge to design and develop the molecular sensors using fundamental steps. The participation of non-academic and academic members committed to the main goal of the Action will be managed through the Core Group (CG) with final acceptance by the Management Committee (MC).

- Potential investors, end-users and the public in general will be invited to attend conferences and meetings organized by the Action. These events will serve to stimulate the dialogue and common activities with the aim to increase the awareness of the research performed within LUCES. Special efforts will be made to contact potential investors from the public and private sector. This will be done by dissemination of the Action but also through direct contact with companies that may benefit from being partners of this interdisciplinary European team.

- Action members will be encouraged to *contact additional stakeholders* interested in finding answers to their specific needs regarding the aim of the Action. Additionally, the attendance of the Action members in specific conferences, their participation in the dissemination sessions dedicated to industrial activities in the LUCES research topic, the organization of LUCES meetings to share experiences and ideas with researchers working in industries, and, the realization of STSMs with industry, will all be highly beneficial to find stakeholders and partners interested in joining the network.

#### 3. IMPACT

# 3.1. IMPACT TO SCIENCE, SOCIETY AND COMPETITIVENESS, AND POTENTIAL FOR INNOVATION/BREAK-THROUGHS

# 3.1.1. SCIENTIFIC, TECHNOLOGICAL, AND/OR SOCIOECONOMIC IMPACTS (INCLUDING POTENTIAL INNOVATIONS AND/OR BREAKTHROUGHS)

LUCES Action has a strong potential to make a timely and cutting-edge impact on science and society in terms of innovation and breakthroughs in the field of LCs. Moreover, it is expected to have a significant socioeconomic impact. The Action foresees the scientific, technological and socioeconomic innovation impact as follows:

- Scientific: Combining research expertise of the Action members, to be able to develop models, prototypes and devices for selective molecular recognition of analytes responsible for environmental security issues. The achievement of this goal will benefit and have a tremendous influence on society. For example, by improving water quality through monitoring and keeping under control and regulation the limits of pollution. In turn, and through a cascade effect, this main benefit will also positively affect the quality of marine waters. Concerning air pollution, high levels of substances like CO<sub>2</sub>, NO<sub>2</sub>, O<sub>3</sub>, CO<sub>x</sub> are noxious to human health and may harm the environment. The sensing of these analytes has been realized using supramolecular materials like modified carbon nanotubes within polymer matrices and excellent sensitivity has been demonstrated for the specific cases of CO and CO2. Supramolecular receptors and containers have been designed for sensing and fixation of NO<sub>x</sub> gases, and specifically target NO<sub>2</sub>/N<sub>2</sub>O<sub>4</sub>. There is significant room to improve the properties of these receptors. All the sensing systems briefly mentioned above are already available in the Action members' labs and can be adapted/modified to support the development of new technologies. Synthesis of new receptors will be performed with the aim to detect and improve the sensing and quantification of specific analytes. The direct interaction and the exchange of knowledge between the members of the Action (within and between the different WGs) will be extremely relevant for the development of the first models and prototypes.

- <u>Technological</u>: The presence of members that belong to well recognized research and technological institutions, as well as companies will ensure the development of the final devices and its accurate testing before moving to commercialization. Additionally, the combined facilities of the different members of the Action surpass those commonly present in a single laboratory. This is the ideal environment for the development of new technologies, protocols and devices.

- <u>Socio-economical</u>: The development of prototypes and devices for a fast and reliable monitoring of important contaminants covering the gap "from bench to market" will represent, without any doubt, the



most relevant socio-economic impact of LUCES. In this sense, all the Action members will protect their relevant results with patents either alone or in collaboration with the industrial partners involved in the commercialization and development of the final devices. The society as a whole will benefit these devices and the industries producing them will increase their market share and the number of employees in different sections (sales, engineering, etc).

There is a low risk and a high reward in this research, since the Action members already have the necessary expertise for the development of the proposed sensing systems (molecules and devices). For this reason, the impact on science and society of the Action is guaranteed owing to the know-how and expertise of the network members.

#### 3.2. MEASURES TO MAXIMISE IMPACT

### 3.2.1. KNOWLEDGE CREATION, TRANSFER OF KNOWLEDGE AND CAREER DEVELOPMENT

Knowledge creation and transfer of knowledge for the development of sensors, that is going from the first steps of the design and understanding of the detection process to the final implementation of the molecular sensors in the development of the devices, will emerge from a dynamic networking within and between the different WGs of LUCES. Additional networking activities will take place during the Action meetings, workshops, STSMs, Training Schools, and lectures delivered at the different Institutions (academic and industry) where Action members, stakeholders and general public, will exchange their ideas and results. All the members will be invited and encouraged to frequently discuss scientific results, problems, share new ideas, concepts and techniques to create strong collaborating working groups. This will be a key point for knowledge creation and transfer of knowledge. In particular, the methods for enhancing and promoting knowledge creation and transfer of knowledge in LUCES are:

- The CG will evaluate twice a year the degree of networking and cooperation between the different members of the WGs and between the different WGs. This evaluation will be discussed with the MC and shared with all the Action members at the annual Action meetings;

- The research opportunities of the ITCs will be reinforced mainly by finding adequate partners possessing facilities/expertise required for assuring the positive outcome of the high-quality research collaborations;

- The intellectual property of the best prototypes will be protected through patents and managed as specified above in Section 1.2.2.1;

- LUCES will allow the development of new approaches and policy recommendations with the main goal of mitigating the effects of contaminants in Europe and beyond. Key Performance Indicators (KPIs) will be identified at the first CG meeting and approved by the MC. They will be defined as the minimum number of publications/year, oral communications at International Conferences, dissemination activities, and STSMs, prototypes for the self-evaluation of the successful implementation and development of the network activities. KPIs will also be useful in gauging the increase in the capacity building and stakeholder involvement on environmental issues and detection of contaminants, as well as the alignment of the Action with the United Nation objectives according to the Sustainable Development Goals;

- Adhering to the recommendations of the EU in the Guidelines on FAIR Data Management in Horizon Europe, LUCES will collect and make available the data via the Action intranet to support the credibility and raise the quality of the scientific publications based on those data. This will allow the follow-up of projects and that new students can continue the work, building up new results upon existing data sets, validate previous results and document the improvement of materials and production techniques in a verifiable manner.

Regarding Career Development:

- The broad network created by this Action will be a direct opportunity for YRIs to: establish their own collaborations in Europe, develop their future research activities, achieve higher visibility, gain access to new job opportunities and be directly involved in knowledge transfer and project management. YRIs will be involved in key projects of the Action, such as the organization of meetings, events for communication of results to the society and dissemination activities and will act as co-leaders of the different WGs;

- Individual training will be also carried out for the young researchers belonging to the different participants' labs of the Action. This will create an even more expanded network of "researchers of the



future" with unique opportunities to gain a real multidisciplinary knowledge, not only by attending theory classes but also by performing practical STSMs at both academic and industry research laboratories. Interactions with researchers from companies will provide ideal opportunities for future employment. Virtual training sessions will be also organized for young researchers to gain key scientific knowledge on the design, development and design of prototypes and sensors for real-life applications and on the transfer of knowledge and IPR. These virtual meetings will be scheduled at the kick-off meeting.

# 3.2.2. PLAN FOR DISSEMINATION AND/OR EXPLOITATION AND DIALOGUE WITH THE GENERAL PUBLIC OR POLICY

This Action will disseminate its results to promote the leadership of the European supramolecular community, in particular to those interested in sensing. The Action will also raise awareness about what science can do for society and the environment. Dialogue co-creation and co-design with the public is vital to realizing the great potential of LUCES. For this reason, and in order to involve European citizens more closely, exhaustive lines of communication will be open.

The Action believes strongly in the role played by dissemination and its broad relevance. For this reason, it is fully integrated into each of the general objectives addressed by this project and a special WG will be dedicated to it. Involving European citizens more closely with science requires having extensive lines of communication. For this, different strategies to disseminate LUCES' activities and scientific results will be developed:

- A **website** (and logo) dedicated to the Action will be created. The website will introduce the Action and report on its aims and general organization. A list of the people involved, news and announcements for the members of the Action, as well as for the general public, concerning the upcoming public events, scientific meetings and initiatives, will also be posted. All this information will be constantly updated. Videos/pictures and links to scientific talks or news of interest to the public will also be announced. Additionally, **professional social networks** like Youtube, Facebook, Twitter (@LUCES\_COSTAction) and Instagram will be used to involve and engage scientists and the general public. Dissemination issues, progress and future plans, will be in the agenda of all meetings of the Action.

- **Collaborative joint publications** in leading scientific journals will be promoted (at least 5 articles/ year). The mission of dissemination will be accomplished through **open access publication** and so that data are freely available to the largest possible audience. Major scientific journals will be contacted to plan themed issues dedicated to LUCES research;

- The results of the work carried out in LUCES will also reach the research community by established **scientific communication channels**, i.e. oral and poster presentations at conferences, seminars, video tutorials, etc. Public outreach articles (at least 1 per year) will be a powerful tool to come in contact with citizens, policy makers at the national and European level, public authorities, media, industries, civil society organisations;

- The network will also share their research with the general public by active participation in science open-days, such as the **European Researchers' Night**. The **organization of diffusion conferences at the different institutions** will be promoted. Additionally, Action members will contact their Institutions (Universities) to try to include at least one laboratory experiment for the Degree students about simple designed reactions based on Supramolecular Sensing approaches;

- International experts on Supramolecular Chemistry, Chemosensing and Technological development of prototypes and devices, whether they are part of the Action or not, will be invited to the Action's summer schools and master/PhD-level courses at academic institutions in order to increase visibility and attract other recognised researchers on the topic;

- The Action also wants to fight against the platitude that "many good ideas never make it to market" through the strong collaboration between academic and non-academic participants. All results with potential to give rise to IPRs will be protected by patenting and licensing in accordance with the IPR policy (see section 1.2.2.1). As a rule, the partners involved in the research activities working on the development of exploitable results will own the intellectual property. Any potential conflict or issue will be discussed by the Core Group and the necessary help sought so as to solve the problem;

- Dissemination events will be organized (at least 3/year) in the different Institutions and international conferences (mainly in the last years) to show how interdisciplinary and collaborative work has been translated into final sensing processes and devices with real-life applications;

- The members of this Action are encouraged to maximize their participation in trade-fairs, industry exhibitions and forums, in particular with the aim of communicating and disseminating new methods and technology developed within LUCES;



- Other companies, professional associations and European clusters will be contacted in order to invite them to participate in the Action, to give valuable feedback for successful final products;

- News regarding final products for real-life applications and marketplaces will be disseminated through communications in newspapers, scientific magazines, websites of the different Institutions and via Institutional and public TV channels.

A success of the dissemination of the Action will be quantified by the number of visits at the different social networks, scientific communication channels, conferences' attendees and number of new research groups and industries interested to join the Action.

#### 4. IMPLEMENTATION

#### 4.1. COHERENCE AND EFFECTIVENESS OF THE WORK PLAN

#### 4.1.1. DESCRIPTION OF WORKING GROUPS, TASKS AND ACTIVITIES

The LUCES Action will be divided into four WGs. The participants of the WGs will possess different knowledge and skills in order to promote interdisciplinary working environments. This will be of pivotal importance for the exchange of knowledge within, and outside, the academic community, as well as for the direct interaction of academic partners with those from industry. Two of the WGs will be oriented towards the fundamental development of signalling units adequate for the detection of specific analytes, (WG1 and WG2). WG3 will be oriented to the development of models (functionalized materials), prototypes and devices. Different specific applications will be possible thanks to the expertise of the non-academic participants in dissimilar topics including the design of automated analytical solutions to control water, biofluids, soil, food and others and detect very low-limit contaminants; development of modified screen-printed electrodes with nanomaterials for optical and/or electrochemical detection of designed systems; use an own methodology to calibrate light information collected in digital cameras, to perform optical measurements with easily available tools like smartphones. Finally, WG4 will be strongly committed to the Dissemination of the news, results and ongoing highlights of the Action, and their exploitation. This organization of the WGs will ensure a high efficiency in the project development from the start with constant communication and exchange of information between them. Tight interconnection between the WGs scientific programs will be pursued on transversal objectives such as systems under investigation, procedures or computational approaches. Participation in more than one WG will be promoted. Good communication between academic and non-academic partners will be pivotal. The WGs will envisage short term objectives that will be progressively fulfilled in the timeframe of the Action. Information on the progress of achieving these objectives will be delivered twice a year to the CG by the WG coordinators. The CG will monitor all the provided data and results in biannual faceto-face or virtual meetings. Extra meetings may be carried out, if needed, to discuss relevant information or problems with the development of the main goals in any particular WG. The main (but not limited) objectives and milestones within single WGs are presented below.

#### \* Working Group 1: (Supra)molecular systems as sensors.

*Objectives*: O1.1) Design and synthesis of molecular and supramolecular systems (host-guest and related indicator displacement systems) with specific signalling units suitable for the detection of gases, ionic contaminants and residual drugs in aqueous environments, soil or food; O1.2) Study of the suitability of the systems to detect the selected contaminants; O1.3) Use of *in silico* studies to support rational and dynamic combinatorial strategies, for the design of new sensing systems for the selective recognition of targeted analytes.

Functionalized nanocavitands, calixpyrroles, metal-sal(oph)en, organometallics, (metallo)cages, cyclopeptides and different type of scavenger molecules containing a signalling unit will be synthesized. Special attention will be paid on the functionalization of these systems by the introduction of alkyl chains ended by specific connecting groups (such as -OH, -COOH or -SH) for the interaction with the nanomaterials and the development of prototypes and final sensing devices.

*Milestones*: M1.1) Synthetic protocols for the development of (supra)molecular sensors containing luminescent signalling units; M1.2) Strategy for molecular recognition and sensing in these systems; M1.3) Development of theoretical models; M1.4) Identification of the best candidates as models for final sensing devices.

\* Working Group 2: Supramolecular assemblies and (nano)materials as sensors.



*Objectives:* O2.1) The design and development of complex molecular assemblies for sensing, such as supramolecular aggregates, vesicles, lipid layer, nanoparticles and other nanomaterials and thin films; O2.2) Initial tests of their use in the detection of selected contaminants; O2.3) Studies on the interaction between the sensor and the detected species through theoretical models, photophysical and physico-chemical approaches.

A direct connection with WG1 will be established aiming at anchoring some of the simple (supra)molecular systems developed there on nanomaterials employed by WG2. All nanosystems will share the incorporation of a common motif: an optical (luminescent) signalling unit. Electrochemical signalling units will also be considered in cases of weak luminescence. Complementary characterization techniques will be used for the understanding of the interaction taking place between the small analytes and the (nano)materials.

*Milestones*: M2.1) Library of new LCs in the range of nanomaterials and complex assemblies; M2.2) Strategy for molecular recognition and sensing in these systems; M2.3) Understanding the interaction of small analytes with more complex systems and surfaces; M2.4) Identification of the best candidates to be analysed as models for final sensing devices.

# \* <u>Working Group 3:</u> Models, prototypes and devices. Technology transfer and research valorisation.

*Objectives:* O3.1) The development of functionalized materials as models, prototypes and devices based on sensor arrays; O3.2) Development of a toolkit of technological solutions and small equipment; O3.3) Development of electronic devices, thin films, and other materials based on optical signalling units; O3.4) Definition of a "bench-to-market" development plan and the creation of products to solve problems identified by stakeholders from industry, society and policy makers.

The achievement of the suggested objectives will be possible thanks to the close collaboration between academic and non-academic participants with noted expertise in different applied fields related to sensing. Their expertise include the development of supported micro and nanodevices, nanogenerators, light-matter materials, microhotplates, modified screen-printed or ink-jet printed sensors or electrodes with nanomaterials, electrochemical sensors and small equipment for sensing applications and to the presence of high-level academic and research centre facilities. Microarrays of optical sensors for simultaneous multiplexed analysis of more than one species will also be investigated. Artificial intelligence, machine learning, and Digital Technology are key aspects that will be considered in the development of prototypes and devices based on differential sensing.

*Milestones*: M3.1) Protocols with the experimental conditions to support the (supra)molecular systems and (nano)materials on models or prototypes; M3.2) Development of the first models and first devices prototypes with the adequate conditions and technologies to develop the final products; M3.3) Database with the adequate conditions for the development of the different types of final sensors prototypes and devices; M3.4) Development of sensors for market interest.

#### \* <u>Working Group 4:</u> Dissemination and Exploitation.

*Objectives:* O4.1) Ensuring the Action members share news relevant for the Action on the website and social media; O4.2) Organization of activities for the dissemination of the Action; O4.3) Evaluation of different potential exploitation of the results as patents.

This WG will be devoted to the dissemination of the Action's results to the scientific community and general public, both at the European and non-European level. Special efforts will be focused on the dissemination of the Action's news on social media and web pages. The WG will be committed to provide help to the Action members with applications for competitive European funds and other innovation grants. The contact between the participants and stakeholders and general public will also be promoted through the organization of specific meetings and round tables. WG4 will also be responsible for the monitoring of the potential IPR.

*Milestones:* M4.1) Dissemination of the news on the website and social media; M4.2) Conferences, round tables, lectures and meetings involving participants, stakeholders and general public for the dissemination of the Action; M4.3) Evaluation of different potential exploitation of the results as patents at the earliest possible stage.

**WGs Common Milestones:** 1) Complete analysis of the molecular interaction and sensing process; 2) Validation of data through interlaboratory and blind round-robin experiments to check reliability and consistency of results obtained; 3) Core Group and Management Committee meetings.

WGs Common Activities. WG meetings will be carefully prepared by the WG leaders and specific discussion/sharing of common and complementary interests will be programmed. Cooperation between



different groups will be promoted in these sessions and, in particular of YRIs. Gender balance will be also taken into consideration. We aim to have both genders equally represented in all decision-making within the whole project.

Continuous evaluation of the progress will be carried out in collaboration between the WG leaders and the CG. The CG will help find other laboratories who can join the Action to solve specific problems.

A database/platform containing the different outputs and the resulting standardized protocols for the evaluation of the sensors from individual groups and from cooperative efforts will be created and shared between all members of the Action to ease exchange of information and cooperation between different WGs. A "wish-list" of the different partners will be also incorporated in the platform to ease the collaboration and possible resolution of lack of infrastructure/possibilities in individual groups. To monitor the correct progress of the project, the CG will analyse these data twice a year and the conclusions will be also shared and discussed with the management committee members at the annual meetings.

The organization of an *International Symposium on Optical Sensing and Devices* will be programmed in the Concluding Action Meeting. STSM participants will be encouraged to be involved in this organization with the support of the Core Group members.

#### 4.1.2. DESCRIPTION OF DELIVERABLES AND TIMEFRAME

The general deliverables of the Action, together with the WG responsible for them and the expected timeframe are shown in the table below. The number indicated in some cases between parenthesis corresponds to the minimum number considered for a successful item:

Deliverable	WGs	Year 1	Year 2	Year 3	Year 4
Creation and updated contents of website, instagram, facebook and Twitter accounts.	WG4				
Portfolio of the available systems.	WGs1, 2				
Publications (20), themed journals' issues (1).	All				
Portfolio of 1) new (supra)molecular systems functionalized to be anchored to surfaces for models' development and the best practices identified and 2) new supramolecular assemblies and (nano)materials as sensors and best practices identified	WG1, 2				
Final developed models (10), prototypes (5) and devices (2).	WG3				
Final report of the best practices identified to develop the new models, prototypes and devices.	WG3				
Selected best 2 systems to be tested as potential candidates for "from bench to market".	All				
Final report on Awareness and Dissemination activities conducted.	WG4				
Videos about the obtained Action's achievements (5).	All				
Invited lectures or seminars by Action participants at high level Conferences and different Institutions (10).	All				
Created content for workshops (3) and Training Schools (3).	All				

#### 4.1.3. RISK ANALYSIS AND CONTINGENCY PLANS

It is common knowledge that highly innovative projects can be risky. Considering the vitality and the rich expertise present in the scientific community involved in LUCES, risk should be limited. Interdisciplinary



collaboration will be at the core of this project, and this will without doubt increase success chances. Despite this, unexpected problems may arise during the course of the Action. If such situations arise, several actions would be immediately taken, mainly by the MC, which has the responsibility of assessing the progress of the Action regularly and taking corrective and incentive measures to ensure the success of LUCES network. Additionally, the MC will undertake reviews of the network activities (see Gantt Diagram below) to ensure that no problems arise or that they are resolved in a timely fashion. The identified potential risks of LUCES and the possible mitigation actions are presented in the table below.

Risk Nº	Description of Risk	WGs	Level	Contingency Plans
R1	Research Progress / Possible delay in the achievement of the scientific deadlines.	WG1-3	Medium	Progress in science is not always as fast as desired. In case of delays, the WG coordinator will contact the MC to find the best possible solution.
R2	The designed sensors do not exhibit the desired change in luminescence upon recognition of specific analytes.	WG1-2	Medium	New molecules will be designed, and their properties tested. WG leader (in collaboration with Core Group) will help find the adequate Action participants to help solve this problem.
R3	Failure in "bench" to market process.	WG3	High	The industrial members of this Action will provide important feedback about the best ways to test the best systems for preliminary market process.
R4	Lack of success of dissemination activities.	WG4	Low	The MC will consider alternative plans for diffusion of the activities.
R5	Lack of success of workshops and Training Schools.	All	Low	The MC will make great efforts for disseminating the interest of these activities in their countries
R6	Difficulties in involving more industries in the Action.	All	Medium	The CG will organize new dissemination actions that will be coordinated by WG4. The international offices form the different institutions will be involved to contact other companies.
R7	Difficulties in the organization of meetings and STSM due to world heathy problems (covid-19)	All	Low	The CG, in collaboration with the WG leaders, will organize virtual meetings in the expected periods for the global participation and exchange of scientific information with all the participants.

4.1. <mark>4</mark> .	GANTT DIAGRAM	Year 1			Year 2			Year 3				Year 4					
	LUCES	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
	Ad	tion Act	ivitie	5											_		
	Meetings (CG: Core Group; MC: Management Committe; WG: Working Groups)	Kick-Off		CG	MC/WG		CG v			vc /wo		CG		MC /WG		CG	мс
	STSM (S) / Articles (A) (both expected along all the period highlighted in yellow)																
	Reports (R)/Patents(P)/Videos(V)				R				R				P/R				V/P/R
Ann	ual Action Conference (C) /Workshop (W) / Training School (TS) / International Symposium (IS)						TS	с	w	С			R	С	TS	W-IS	R
	Working Group Objectives (left), expected duration of the objective (colored cells in t	he right)	and	expect	ed locali	zatio	n of th	ne ider	ntified	milesto	ones i	n the c	orresp	ondingp	eriod	(right)	)
	WG 1: (Supra)molecular systems as sensors.																
	O1.1. Design and synthesis of functionalized (supra)molecular systems									M1.4							M1.1
	O1.2. Detection of gases, anionic and cationic contaminants, pesticides, residual drugs												M1.2				
	O1.3. Exploring strategies for new systems, supported by in silico studies									M1.3				M1.3			
	WG2: Supramolecular assemblies and (nano)materials as sensors.																
02.	1. The design and development of assemblies, nanoparticles, nanomaterials and thin films										M2.4						M2.1
	O2.2. Detection of gases, anionic and cationic contaminants, pesticides, residual drugs									M2.2				M2.2			
	O2.3. Understanding the interaction small analytes - more complex systems/surfaces												M2.3			M2.3	
	WG3: Models, prototypes and devices. Technology transfer and research valorization.																
	O3.1. Development of supported micro and nanodevices								M3.1								
	O3.2. Development of toolkit of technological solutions and small equipment											M3.2					
0	3.3.Development of electronic devices, thin films, or other materials with optical signaling units													M3.3			
03	3.4.Definition of bench-to-market plan development and creation of products to solve problems															M3.4	
	WG4: Comunication, Dissemination and Exploitation.																
	O4.1. Creation, management and update of website and social media	M4.1 (f	rom t	he beg	ggining a	nd ald	ong th	e Actio	on)								
	O4.2. Organization of activities for the dissemination of the Action				M4.2				M4.2				M4.2			M4.2	
	O4.3. Evaluation of different potential exploitation of the results as patents												M5.3			M5.3	3
	All WGs																
	Complete analysis of the interaction and sensing process									M1					M1		
	Validation of data through interlaboratory and blind round-robin experiments													M2			