# Template of Mid-Term Progress Report

## Water Joint Programming Initiative 2018 Joint Call

## *Closing the water cycle gap - Sustainable management of water resources*

This Template should be used by the Project Coordinator for the reporting of the project.

**This template does not substitute national regulations**

# 2018 Joint Call
# Mid-Term Progress Report
## Closing the water cycle gap - Sustainable management of water resources

### SPy : Sense and Purify

This document must be filled in by the project coordinator with the help of its project partners and must be sent to the WaterWorks2017 Follow-up Secretariat by **Robert Forster** (for Consortium Sense and Purify)**.**

The WaterWorks2017 Follow-Up Secretariat will ensure distribution to the concerned national funding agencies. The project coordinator is responsible for sending a copy of the report to its partners.

## PROJECT TITLE AND ACRONYM

Author of this report (Coordinator): Robert J. Forster
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Date of submission: October 31, 2020
Project Website: https://data-spy.com/
Project code: WaterWorks2017-Spy: Sense and Purify

Duration of project:
Start date: April 1, 2019
End date: March 31, 2022

Period covered by this report: April 1, 2019 to September 30, 2020

1. Publishable Summary

*Maximum 1 page*

The content of this section is intended for communication by the Water JPI on the project, mainly through its website. The style should be adapted to communicate to a wide audience (**non-technical** English) and the quality of the data must enable direct publication.
The authors authorise the publication of information about this project by the Water JPI.

The publishable summary should provide the following information:

- *The project context and objectives;*
- *The main results achieved so far;*
- *The expected final results and their potential impact and use (including the socio-economic impact and the wider societal implications of the project so far); and*
- *The address of the project's public website, if applicable.*
-

**Context and Objectives**. There is a growing recognition that powerful treatments for wastewater are needed that can process diverse biological and synthetic organic compounds and can be implemented at the point of production. Advanced Oxidation Processes (AOPs) are treatment technologies aimed at degrading and mineralizing recalcitrant organic matter from wastewater through reaction with hydroxyl radicals ($^{\bullet}OH$). These technologies can treat emerging contaminants, that are recalcitrant to conventional treatments, especially herbicides, pharmaceuticals and personal care products. ***Sense and Purify*** is a radically new technology that uses electronically conducting diamond particles within an electric field (wireless electrochemistry) to create hydroxyl radicals **throughout the water volume** in a highly efficient way that can then destroy pathogens and decompose the vast majority of organic compounds. The technology will effectively remove these compounds locally and at low cost thus protecting health as well as environmental and economic sustainability. The consortium is led by Dublin City University (Ireland) and has partner labs in Nantes University (France), Universitat Rovira i Virgili (Spain) and the University of the Western Cape (South Africa).

**Main Results Achieved so Far**. The programme has been very successful during the first 18 months. For example, we have developed **new electrochemiluminescent dyes** that generate light when an appropriate potential is applied, and a co-reactant is present. These dyes have been used to create a new antibody based **electrochemiluminescent sensor that can detect as few as 100 E. coli bacteria in one millilitre of water**! Boron Doped Diamond (BDD) electrodes have been explored for the **simultaneous detection and destruction of pharmaceuticals, e.g., antiretrovirals,** that are challenging to remove using conventional approaches. We have made significant progress to optimise the composition of the BDD particles in order to maximise the rate at which the hydroxyl radicals are produced which decompose the pollutants. These systems are **capable of decomposing recalcitrant organic pharmaceuticals, such as the anti-cancer drugs doxorubicin and gemcitabine, within six hours!** We have also developed *in silico* models of the radical generation process that are guiding the design of the reactor.

**Expected Final Results**. The ultimate objective of the programme is to create a reactor with integrated sensors/spectroscopy that measures the pollutants in the incoming water stream, decomposes organics within the water while monitoring the efficiency of the treatment and produces water that can either be reused within the manufacturing process, e.g., pharmaceutical or food production, or discharged.

**Potential Impact.** This programme directly impacts UN SDG **Goal 6: Ensure access to water and sanitation for all**. The ability to locally produce clean water from wastewater for industry or drinking at low capital and operating cost is very significant. To **enhance innovation capacity and integration of new knowledge** prototype reactors will be demonstrated for the treatment of production wastewaters from the food (NU) as well as pharmaceutical industries (DCU). We are also impacting on education through a series of measures including school visits, public outreach articles and social media.

**Website:** https://data-spy.com/

2. Work Performed and the Results achieved during the reporting period

*Maximum 10 pages.*

Please attach any deliverables produced and information on milestones achieved during the reporting period of this report.

### *a. Scientific and technological progress*

*Please describe the work performed and the results obtained during the period concerned, and the conformity of the work progress within the initial schedule.*
*Take into account the following aspects:*

- *Has progress been made towards progressing the project objectives according to the original description and milestones? If not, please, explain the deviation.*
- *Detailed update on methodology & results*
- *How has the progress of the project promoted multi-disciplinary work?*

The Spy programme has made excellent progress during this reporting period achieving the majority of the time relevant objectives and making significant head way on the others. However, the global COVID-19 pandemic has had significant adverse effects including:

- Closure of laboratories for all experimental work for approximately 3.5 months. During this time all the researchers worked remotely analysing data, building *in-silico* models of Spy sensors as well as the wireless reactor for the treatment of wastewater that contains recalcitrant organics molecules.
- Support services, such as ordering in support of remote working activities, e.g., of modelling software, researcher training courses etc., were significantly delayed.
- Additional demands on the PI Partners to provide online teaching and the delivery of modules, course materials and tutorials via online platforms. This was a time-consuming but essential activity that allowed students to complete the taught elements of their courses with a minimum of interruption. Also, the PIs have been deeply involved in creating and monitoring infection control policies, e.g., acting as COVID Coordinators ensuring correct hand sanitising and PPE are being employed.
- Loss of access to real world samples due to industry partners closing or locking down facilities to external people to prevent infection.
- Reduced access to 3rd party suppliers causing delays in sourcing key reagents and other materials.

However, despite these extremely challenging circumstances and the significant number of person months of in laboratory experiments lost, we have made significant accomplishments by working together as an efficient consortium. We remain fully committed to helping to tackle a growing global problem, i.e., the local, efficient and low-cost treatment of waste water that contains organic pollutants that are very challenging to decompose using existing technologies.

**WORK PACKAGE 1: SENSORS FOR WASTE WATER.**

**TASK 1.1 In Reactor Pollutant Sensing. Pathogen Sensing.** The objective of this task is to develop a highly sensitive sensor capable of detecting <100 pathogens per ml within 10 minutes with a short sample to answer time or ideally, for continuous monitoring.
**LEAD: DCU. CONTRIBUTORS: NU, URV.**
**PROGRESS: SENSOR DEVELOPMENT AND REVERSIBLE BINDING OF PATHOGENS TO ENABLE SENSOR REUSE COMPLETED.**

DCU and URV have designed the electrochemiluminescent sensor system for detecting pathogens illustrated in Figure 1. The Consortium has: 1. Created electrodes (UWC) whose surface is modified with immobilised antibodies (URV and DCU). 2. Demonstrated selective capture of E. coli from water samples (DCU). 3. Functionalised secondary antibodies (NU, DCU and URV) with luminescent dyes created by NU (Task 1.3) and allowed them to bind to the captured E. coli bacteria. 4. Generated electrochemiluminescence whose brightness depends on the concentration of E. coli present in the water sample (DCU).

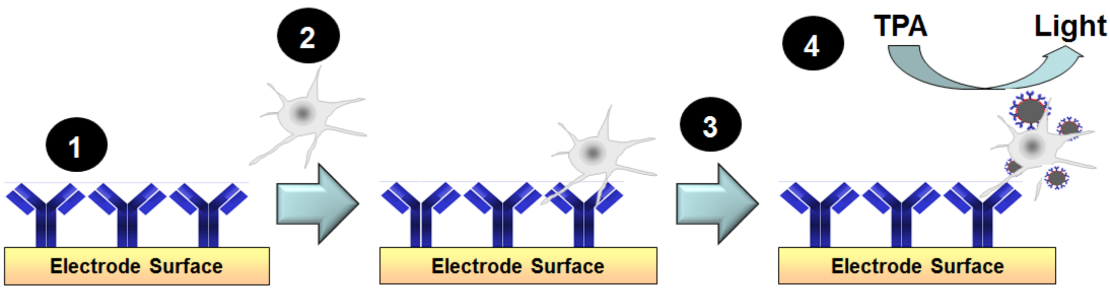



**Figure 1.** Highly sensitive sensor for the detection and quantification of E. coli in water based on the generation of light by applying a voltage- electrochemiluminescence (ECL).

Figure 2 shows the dependence of the ECL intensity on the bacteria concentration, colony forming units per ml, CFU/ml. This figure shows that the sensor response depends linearly on the CFU/ml from approximately 60 CFU/ml to approximately 800 CFU/ml with a limit of detection of approximately 73±6 CFU/ml. **Thus, the core objective of Deliverable 1.1 has been achieved.** The lockdown in both France and South Africa have blocked the collection of samples for testing of the sensor. However, samples that mimic the key components of the French food production waste have been formulated and the sensitivity of the sensor response is only 10% lower than that found in pure water.

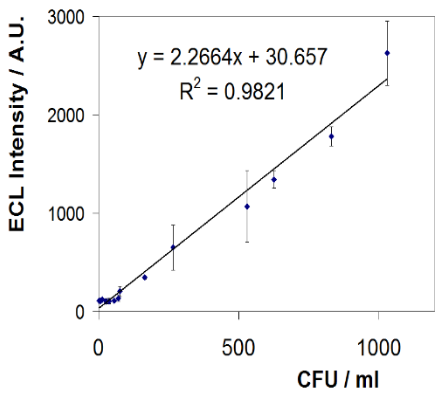



**Figure 2.** Dependence of the ECL intensity on the concentration of E. coli in a water sample.

A second objective of Task 1.1 was to investigate the ability to regenerate the capture surface so that it could be reused by applying a voltage or flowing an electrolyte solution across the capture surface. **This second objective has also been delivered**. Figure 3A shows E. coli captured on an electrode surface (open circuit) that has been functionalised with a film of an electronically conducting polymer, polypyrrole, which contains antibodies for E. coli. Figure 3B shows that the number of captured bacteria decreases by approximately 25% when a potential of 0.5 V is applied. However, applying 1.0 V that oxidises the polypyrrole film triggers complete desorption of the captured bacteria. Figure 3D shows that once the voltage is removed the E. coli can once again be captured on the antibody functionalised electrode. This result demonstrates our objective of reversible bacteria binding using an electrical stimulus.

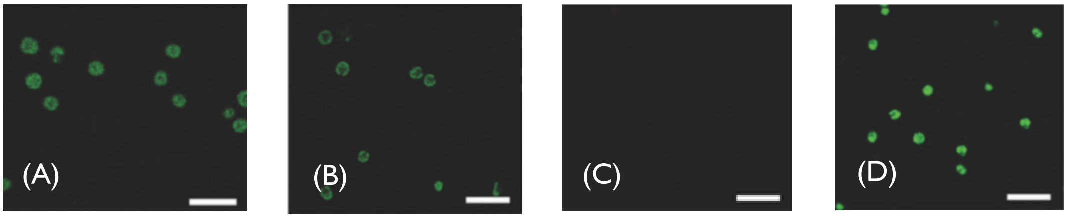



**Figure 3.** (A) E. coli capture on a glassy carbon electrode functionalised with a 550 nm thick polypyrrole film containing E. coli capture antibodies. (B) Captured E. coli when a voltage of 0.5 V is applied. (C) Removal of captured E. coli when a voltage of +1.0 V is applied so as to oxidise the polypyrrole film. (D) Reversible E. coli binding when the electrode is returned to open circuit.

**TASK 1.2 In Reactor Sensing *Organics***. The objective of this task is to develop sensors to measure the "organic load" within the wastewater that will inform the optimisation of the WWT protocol.
**LEAD: UWC. CONTRIBUTORS: DCU, URV.**
**PROGRESS:** Excellent progress has been made on the two approaches, sparingly selective sensors (UWC and URV) and UV-Vis Spectroscopy (DCU and NU).

**i) Sparingly Selective Sensors. Lead: UWC.** Boron Doped Diamond (BDD) electrodes have been characterised and optimised for the determination and electro-decomposition of nevirapine (NVP) and tenofovir (TNF). Cyclic voltammetry (CV) was used to study the amperometric responses for nevirapine and tenofovir drugs in phosphate buffer (PB) and Britton-Robinson (BR) buffer as electrolytes. The process is summarised in Figure 4, which shows the oxidation of nevirapine to a quinonimine which is a two-electron process that produces a current whose magnitude depends on the concentration of the Active Pharmaceutical Ingredient (API) in solution.

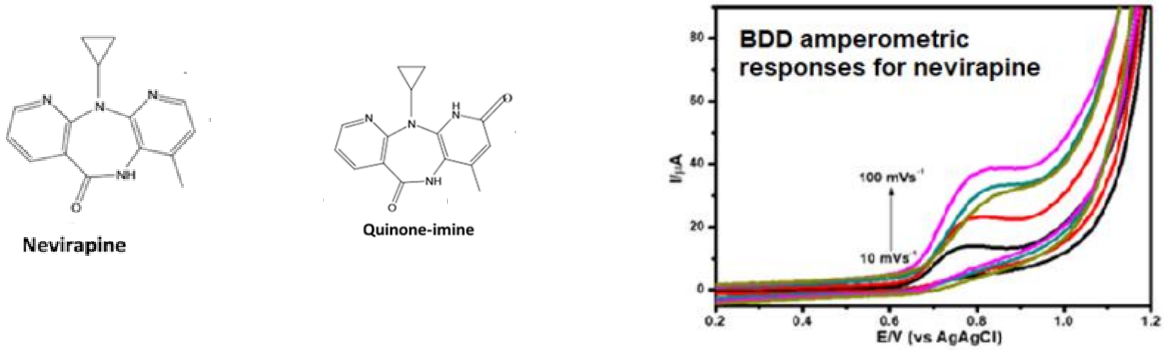



**Figure 4:** A:PIs targeted and cyclic voltammograms for the detection of nevirapine.

The electrooxidation of NVP and TNF were studied in phosphate and Britton-Robinson buffers. The typical voltammogram for the electrooxidation and decomposition of ARV drugs is presented for nevirapine in Figure 5. As part of the analysis of the dc voltammetry results, the following parameters were determined and evaluated: the onset potential for sensing (OPS) and the magnitude of the sensor response (MSS). The data for the sensitivity of the BDD reactor for NVP is presented in Table 1. Significantly, the MSS, OPS and OPM values for NVP are the same for both PB and BR at an alkaline pH of 11.

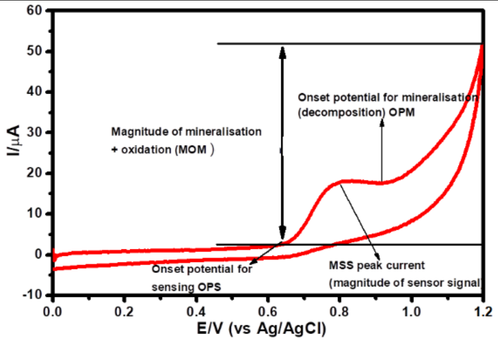



**Figure 5**: Schematics of a typical cyclic voltammogram of an ARV drug response using a BDD electrode. (Onset potential for sensing (OPS), onset potential for mineralisation (OPM), magnitude of sensing signal (MSS) and magnitude of mineralization and oxidation (MOM) are the reactor parameters).

**Table 1:** Electro-oxidation parameters for 4.4 µM NVP at a BDD electrode.

| Reactor Parameter | NVP in 0.1 M PB (pH 11) | NVP in 0.1 M BR (pH 11) |
|---|---|---|
| OPS (V) | 0.652 | 0.6733 |
| OPM (V) | 0.9056 | 0.9069 |
| MSS (µA) | 18.077 | 24.239 |
| MOM (µA) | 49.261 | 238.426 |
| Sensitivity (µA/µM NVP) | 4.10 | 5.51 |

In conclusion, UWC demonstrated that two analytes (nevirapine and tenofovir), which are among the ARV drugs that are highly prescribed in South Africa, can be sensitively detected using a BDD electrode. The ability of this system to decompose the recalcitrant drugs is presented under WP 3 Integrated Reactor.

**ii) UV-Vis Spectroscopy. Partners: DCU, NU**. This task focuses on developing UV-Vis spectroscopy as a cost effective, real time approach to monitoring effective TOC and develop an algorithm to minimise the treatment time. Our objective at the end of Year 1, was to select between sensors and spectroscopy based on its overall analytical performance. The selection criteria are: *1. Limit of Detection 2. Dynamic Range. 3. Broad Applicability*.

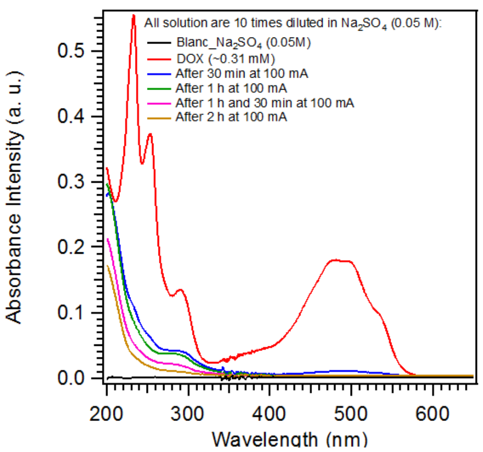


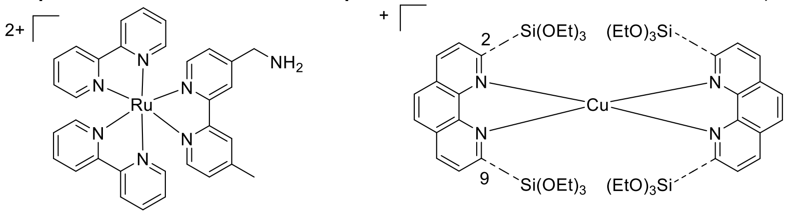

**Figure 6.** UV-Vis spectra of the blank electrolyte solution, the parent drug doxorubicin and during degradation using electrogenerated hydroxyl radicals.

DCU has made significant progress on the use of UV-Vis spectroscopy as a cost effective, real time approach to monitoring the concentration of the parent pharmaceuticals (primarily anti-cancer drugs) and for monitoring their degradation over time. For example, Figure 6 shows the ability of UV-Vis spectroscopy to detect gemcitabine at a concentration of 90 µM while doxorubicin can be detected at 30 µM. Moreover, the degradation of doxorubicin using BDD electrodes and a current of 100 mA in sodium sulphate solution (0.05 M) can be conveniently monitored using UV-Vis spectroscopy. The remaining aspect of this task is to correlate the UV-Vis results with traditional TOC measurements. The collection of the TOC data was prevented by the lockdown but this work is currently in progress. We are also using HPLC to analyse the degradation profile including mineralisation and to strengthen the basis of the TOC UV-Vis correlation.

In conclusion, DCU and NU have made excellent progress on the use of UV-Vis spectroscopy to monitor the decomposition of APIs and correlate those results with HPLC data on sample composition.

**TASK 1.3 High Performance Electrochemiluminescent (ECL) Sensors. Partners:**. This task has two objectives. First, to detect APIs with ultrahigh sensitivity so as to prove they have been adequately removed by the SPy technology. Second, to develop highly sensitive electrochemiluminescent sensors based on sandwich immunoassays, antibodies or aptamers for pollutants of interest.
**LEAD: NU. CONTRIBUTORS: DCU, URV.**
**PROGRESS:** Significant progress has been made on the two approaches, ECL sensors for pathogens (reported under Task 1.1, DCU, URV and NU) and high brightness labels (NU).

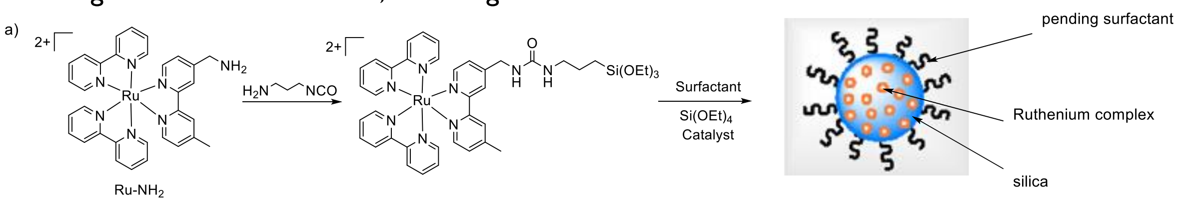
**TASK 1.3 High Performance Electrochemiluminescent (ECL) Sensors. Partners: NU, DCU, URV.** Task 1.1 above reports the DCU, URV and NU collaboration to develop a successful electrochemiluminescent sensor for pathogens. In this task, we present our findings on **i) High Brightness Labels.** NU focused all efforts on the synthesis of the molecular ECL luminophores used in Task 1.1 and especially dye doped silica nanoparticles (DDSN) as luminescent sensors for application in ECL-based assays for targeted pollutants. DDSN have proven to be stable, non-toxic and efficient ECL based probes. The synthetic strategy for DDSN relies on the co-condensation of alkoxysilane bearing dyes with silica precursors in presence of surfactants yielding the desired DDSN. Two types of dyes are investigated: ruthenium(II) and copper(I) complexes (Figure 7). While ruthenium complexes are well documented in the frame of luminescent probes for ECL, there is virtually no reports of ECL generation for homoleptic copper(I) complexes with the general structure given in Figure 7. Monitoring an ECL response from such species is one of the major challenges addressed in SPy.




Ru-$NH_2$ Cu---$Si(OEt)_4$

**Figure 7.** Structures of the dyes used for DDSN preparation. Ruthenium complexes and related DDSN

The ruthenium complex Ru-$NH_2$ has been successfully synthesized in 4 efficient steps. This complex was then easily functionalized by alkoxysilane groups in presence of isocyanato-propyl(triethoxy)silane (TEPI) before being used directly for DDSN synthesis (Figure 8). As mentioned above, DDSN are synthesized by co-condensation of Ru-$Si(OEt)_3$ in presence of tetraethoxysilane (TEOS) and a surfactant acting as a morphological directing agent. Basically, micelles trapping dyes are formed in the first place and a shell of silica is grown around the latter, “freezing” the structure.

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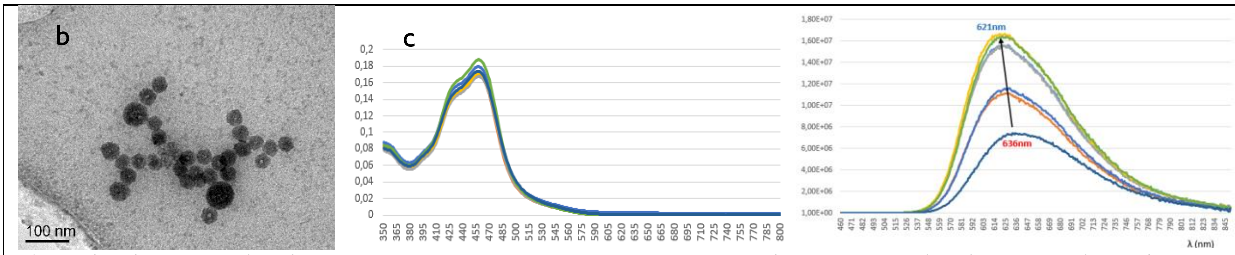


**Figure 8.** a) synthesis of DDSN where the dye is the ruthenium complex Ru-$NH_2$. b) TEM pictures of DDSN obtained from w/o synthesis. c) UV-Vis spectrum of the Ru-Si-2 aqueous suspension. d) Steady state fluorescence spectrum of Ru-Si-2 aqueous suspension.

Two types of micelles were prepared: direct micelles (oil in water emulsions, o/w) and indirect micelles (water in oil emulsions, w/o). For o/w micelles, the used surfactant is famous triblock copolymer Pluronic F127 in an aqueous mixture; for w/o micelles, IGEPAL CO-50 was used in a cyclohexane/water emulsion. In both cases, well-defined nanoparticles were obtained and characterized by dynamic light scattering (DLS) and transmission electron microscopy (figure NU-2b). Stable suspensions of nanoparticles Ru-Si-1 (w/o) and Ru-Si-2 (o/w) were obtained in water and characterized by electronic absorption spectroscopy and fluorescence spectroscopy (Figure 8c and d). The signals obtained for nanoparticles suspensions Ru-Si-1 and Ru-Si-2 are significantly different from those obtained with plain Ru-$NH_2$ dye in the same conditions proving that ruthenium complexes have been successfully included inside $SiO_2$ nanoparticles. Importantly, the emission from the ruthenium complexes doped silica nanoparticles is more intense than the emission from molecular Ru-$NH_2$ alone in the same conditions, showing the relevance of the strategy to obtain highly efficient luminescent probes for ECL.

The strategy NU has focused on is based on the functionalization of positions 2 and 9 of 1,10-phenanthroline by alkoxysilane groups on a pre-formed copper(I) complex. 2 different ligands are sought for, where the length of the alkyl chain between the alkoxysilane group and the phenanthroline is varied from 1 to 5 in order to appreciate the impact of the latter parameter on the overall photophysical behavior of the final DDSN. Ligand L1 has been successfully synthesized. However, ligand L2 is still work in progress. At the moment, only ligand L3 could be isolated.

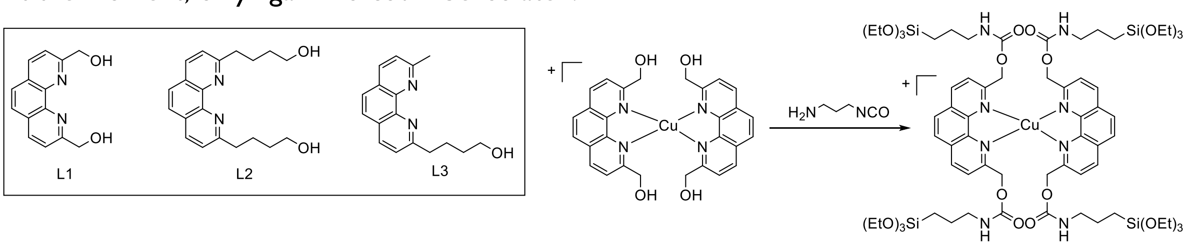


**Figure 9.** Target ligands for the synthesis of Cu complexes, and strategy to design copper complexes bearing alkoxysilane groups.

Complex $Cu(L1)_2^+$ has been synthesized and characterized. Preliminary reactions with TEPI have yielded insoluble materials (likely sesquiloxane polymers, obtained because of the high reactivity of a complex bearing no less than four moisture sensitive alkoxysilane functions). However, new trials have been performed using o/w emulsions and show promising results: a strongly orange, clear aqueous suspension is obtained after purification. Optical characterization is ongoing.

Tethering alkoxysilane groups on $Cu(phen)_2$ complexes is a difficult, but worthy of investigation. In parallel however, we embarked in a simpler strategy in order to bring forth an early proof of concept: we prepared a very hydrophobic copper(I) complex, namely Cu-I (Figure 9) with a $BArF^-$ counter anion, and encapsulated it inside a silica nanoparticle. The dye is only physically trapped inside the silica matrix, not covalently bound to it. Particularly encouraging results have been collected since aqueous suspensions of the nano-objects display intense emission bands in the NIR: this is very promising since molecular copper(I) complexes are usually not luminescent in such strongly coordinating medium.

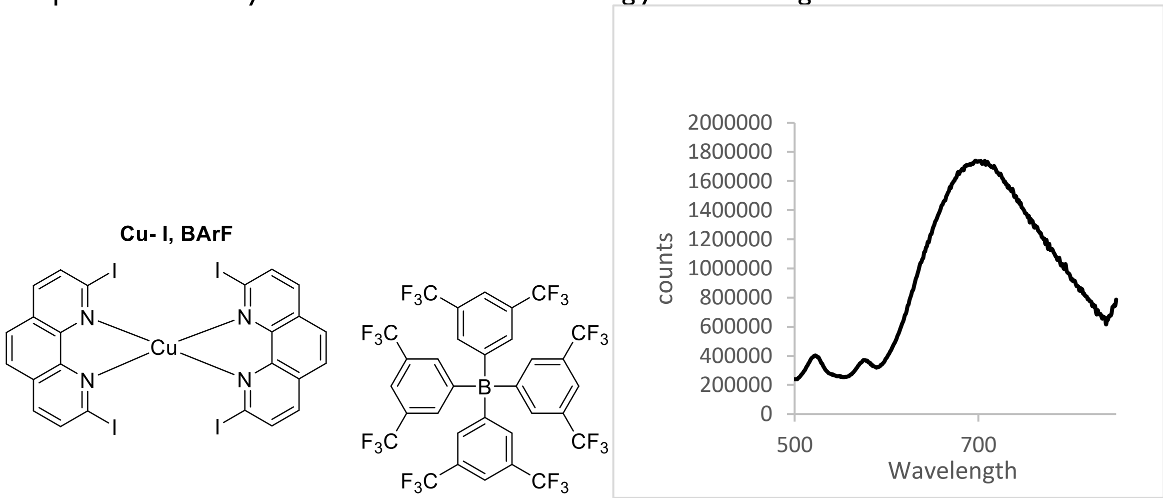


**Figure 10**. Structure of Cu-I complex and emission spectrum of associated DDSN in water suspensions.

**ii) ECL Biosensors. *A) Direct Detection.* As described above,** NU is altering the peripheral ligands to tune the redox potential so as to optimise the light generated in the presence of specific APIs that act as a co-reactant. DCU will continue to screen the ECL luminophores for the direct detection of APIs. ***B) Immunoassays.*** As described in Task 1.1, DCU has already made significant progress on developing an immunoassay for pathogens. This work will continue with URV for the detection of molecular pollutants.

## WORK PACKAGE 2: OPTIMISED PARTICLES FOR WASTEWATER TREATMENT.

**TASK 2.1 Modelling of Electric Field Distribution.** The objective is to understand the potential distribution to identify the optimal conditions (especially electrode size and placement, conducting diamond particle size and composition/conductivity) for optimised hydroxyl generation to decompose pollutants and minimise energy costs.
**LEAD: DCU. CONTRIBUTORS: DCU, UWC.**
**PROGRESS:** Excellent progress has been made and the Task is now complete

DCU has modelled the hydroxyl radical concentration profiles around the BDD particles to identify the optimum concentration of particles in suspension relative to the concentration of the organic pollutant. We have investigated the hydroxyl radical concentration as a function of distance from the particle surface where the contaminant concentration varies from 1.0 µM to 0.25 M. This modelling indicates that even when the pollutant concentration is low, there are essentially no hydroxyl radicals further than about 25 nm from the surface. This situation arises because the radical lifetime is short (2-5 µs) and confirms the absolute need to generate hydroxyl radicals throughout the entire volume of the wastewater sample not just at the surface of a single electrode as has been reported previously in the literature. Additionally, as illustrated in Figure 11, an initial *in silico* COMSOL model of the experimental cell has been developed. This model correctly predicts a more intense electric field close to the feeder electrodes which we have observed experimentally. We have used the predicted electric field distribution through the solution to inform the selection of the optimum BDD particle size.

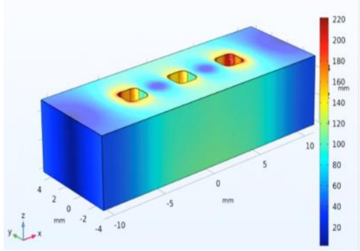

**Figure 11.** Prediction of the electric field distribution through solution using COMSOL

**TASK 2.2. Optimised Particles For Wireless Wastewater Treatment.** The objective is to quantify the electrochemical performance, lifetime and costs of the BDD particles for wastewater treatment/destruction.
**LEAD: DCU. CONTRIBUTORS: DCU, URV.**
**PROGRESS:** Some progress has been made and lead BDD particles have been investigated for the destruction of APIs but significant challenges remain in terms of optimising the composition and size of the BDD particles.

Prior to the COVID lock down, DCU started investigating the optimum conditions for Waste Water Treatment, WWT, using BDD particles with diameters from 50 to 300 μm. However, the loss of approximately 10 person months during this reporting period due to the COVID-19 lockdown means that this work package is **behind schedule**. Beyond the issue of optimising the BDD particles, we are also having difficulties with the **stability of the feeder electrodes** due to the high voltages applied and the highly corrosive nature of the hydroxyl radicals produced. However, DCU has determined that **both the boron doping level and the surface termination** play key roles in dictating the efficiency of hydroxyl radical production. Specifically, hydrogen termination is significantly better than traditional oxide. We are currently using the identified BDD particles in a prototype reactor (described in WP 3) and the performance of these particles will continue to be optimised. However, it is important to note that DCU funding ends in March 2021.

## WORK PACKAGE 3 INTEGRATED REACTOR.

**Task 3.1. Reactor Design.** The objective is to develop and fabricate a WWT reactor with integrated sensors/UV Vis spectroscopy for the destruction of APIs, and food related waste.
**LEAD: DCU. CONTRIBUTORS: DCU, URV, UWC.**
**PROGRESS:** Significant progress has been made with preliminary experiments exploring the capability of BDD electrodes and BDD particles to decompose key APIs carried out.

Initial prototype reactor designs have focused on an electrode stack design. Once sufficient progress has been made on the optimal particle size and composition as well as the electric field strength and distribution the reactor will be modelled and optimised before fabrication. However, the loss of approximately 10 person months due to the COVID lockdown has significantly delayed the collection of the experimental data needed to inform the reactor design and the final reactor may not be fully optimised by the end of the programme.

**Task 3.2. Reactor Fabrication.** The objective is to fabricate a WWT reactor for the wireless destruction of APIs, and food related waste.
**LEAD: DCU. CONTRIBUTORS: DCU, URV, UWC.**

**TASK 3.2 Reactor Fabrication**. Once the reactor design is optimised, DCU will fabricate prototypes using laser cutting and 3D printing. Our immediate plans are to investigate the stability of 3D filament materials (primarily ABS) under wastewater treatment conditions.

UWC has been actively investigating a reactor design based on BDD electrodes under external potential control. Significantly, the magnitude of the mineralisation current (MOM) of the reactor for the API NVP in Briton-Robinson (BR) buffer is about 5 times that of Phosphate Buffer (PB). The Sensitivity (MSS/[NVP]) of the reactor for NVP in PB is slightly lower than that of BR. One can explain this minor difference in sensitivity as being due to the conductivity of the electrolyte which is higher for BR. UWC has investigated the effect of pH on the BDD reactor process and results for TNF are presented in Table 2. Significantly, the treatment of TNF in the BDD reactor does not seem to be affected by pH or the nature of electrolyte. The data in Table 2 indicate close similarity in all the reactor parameters except the magnitude of mineralisation current, which in PB pH 7.2 is about twice the values obtained for TNF in BR pH 1.84. From the data, it appears that the onset potentials for sensing (OPS) and the onset potential for mineralisation (OPM) for NVP are dependent on the pH and independent on other properties of the electrolyte. For TNF, it does appear that differences in the pH and nature of electrolyte have much effect on the values of OPS and OPM. The OPS value of the reactor changed by 0.2 V (200 mV) when the electrolyte was changed from neutral pH of 7.2 PB to a very acidic pH of 1.84 BR. This is not conclusive though, as extensive pH dependence studies will be required to confirm these observations.

**Table 2:** BDD reactor's electro-oxidation parameters for TNF

| Reactor Parameter | TNF in 0.1 M PB (pH 7.2) | TNF in 0.1 M BR (pH 1.84) |
|---|---|---|
| OPS (V) | 1.25 | 1.45 |
| OPM (V) | 1.52 | 1.65 |
| MSS (μA) | 16.04 | 17.22 |
| MOM (μA) | 100.60 | 62.90 |
| Sensitivity (μA/μM NVP) | 0.80 | 0.86 |

In conclusion, UWC has prepared a boron doped diamond electrochemical mineralisation reactor with integrated electrochemical sensing capacity and tested for decomposition of nevirapine and tenofovir in two electrolytes (Britton-Robinson and phosphate buffers). The BDD reactor shows high sensitivity and incineration efficiency for the drugs in both buffers. At high alkaline pH of 11, the mineralisation efficiency of the reactor is much higher in Britton-Robinson buffer. More work is required to optimise the operational parameters of the reactor.

## WORK PACKAGE 4 REAL WORLD WASTEWATER TESTING.

**Task 4.1 Pharmaceutical Production Plant, Dublin, Ireland.** The objective is to test the SPy WWT technology on APIs and other organic molecules used in their production. **LEAD: DCU.**

DCU has engaged with our pharmaceutical manufacturing partner to ensure that the samples used to assess the efficacy of the SPy reactor reflect the commercial samples as closely as possible. However, we have not been able to secure production samples for three reasons: i) Sensitivities surrounding the potential for proprietary manufacturing processes to be reverse engineered based on analysis of production water samples, ii) the COVID-19 lockdown and iii) blocking of third-party access on-site in order to prevent infection after reopening. We are unsure that these issues will be resolved before the DCU funded researchers complete their contracts in March 2021. However, we will continue to refine the composition of the test samples to maximise their industrial relevance.

**Task 4.2 Food Production Facility, Nantes, France..** The objective is to test the SPy WWT technology on food production waste water. **LEAD: NU.**

NU continues to work with our food production partner and is well placed to secure real world samples once the SPy reactor is at a more advanced stage of development.

## b. Collaboration, coordination and mobility

***Is the collaboration between partners effective? Is the contribution of each partner clearly identifiable? Does the project still meet the transnational nature?***

The collaboration has deepened during the Reporting Period and is highly effective at delivering the individual Tasks as well as the overall goal of developing a wireless wastewater reactor with integrated sensors/spectroscopy for the destruction of organic pollutants. It should be noted that the vast majority of these tasks involve at least three of the four partners and the success achieved could not be achieved without the SPy Consortium. For example, in Task 1.1, the initial design of the highly sensitive ECL assay for pathogens was undertaken by DCU and URV, the electrochemical aspects developed by UWC and DCU, the ECL luminophores were synthesised by NU and URV supported the labelling of the antibodies before working with DCU to develop the assay itself. The result of these deep collaborations has been the development of a highly sensitive sensor for pathogens (limit of detection of approximately 73±6 CFU/ml).

The specific partner contributions to each individual task have been clearly identified in Section 2(a).

Despite the challenges posed by the COVID-19 global pandemic, the project remains highly transnational with materials, e.g., ECL luminophores from NU to DCU and URV, antibodies and aptamers between URV and DCU, electrodes between DCU and UWC, and expertise being efficiently transferred between the partners.

***Please, indicate clearly those who performed the work (incl. also in-kind partners).***

The specific partner contributions to each individual task have been clearly identified in Section 2(a). The primary responsibilities remain as described in the original proposal: DCU: development of the wireless WWT technology and testing of pharmaceutical wastewater; URV: sensor development and nanomaterials; NU: ECL luminophore development and testing using food production waste water; UWC: Electrochemistry, sensor and reactor development.

The research teams in each partner location are:

**DCU**: Prof. Robert Forster (Coordinator and Co-PI), Dr. Bacem Zribi (Post-Doctoral Fellow, funded, completed contract in June 2020), Dr. Angelo Fávaro Pipi (Post-Doctoral Fellow, funded)

**UWC**: Prof Emmanuel Iwuoha (Co-PI), Dr Samantha Douman (Postdoctoral Fellow, funded) and Miss Defile Mokwebo (Doctoral student, funded).

**NU:** Dr. Yann Pellegrin (Co-PI), Dr. Clémence Queffélec (Collaborator), Federica Melinato (Doctoral Student, funded)

**URV:** Prof. Ciara O'Sullivan (Co-PI), Dr. Ivan Magriñá Lobato (Post-Doctoral Fellow, unfunded), Dr. Anna Simonova (Post-Doctoral Fellow, unfunded).

***Are the coordination and organisation of the project efficient?***

The Partners PIs have all met in person in Dublin since the programme began – Prof. Emanuel Iwuoha (UWC) and Prof. Robert Forster (DCU, Coordinator) in May 2019 as well as Dr. Pellegrin (NU), Prof.

Ciara O'Sullivan (URV) and Prof. Robert Forster (DCU, Coordinator) in June 2019. Other physical meeting, including a meeting of all partners in Spain in advance of this mid-term report, was planned before the COVID-19 pandemic.

The primary mechanisms of communication and coordination have been email exchanges and discussions by ZOOM that focus on specific tasks (bilateral and trilateral meetings) as well as exchanges to coordinate and focus the individual tasks on the overall goal of a WWT reactor with integrated sensors/spectroscopy.

Overall, the partners communicate effectively and efficiently and this has resulted in significant scientific and technical progress (Section 2a).

The Coordination of the individual Co-PIs with their national funding agencies has been very effective with strong local assessment in place. For example, the Irish Environmental Protection Agency carries out a full review, Technical, Impact and Communications Report as well as an in-person presentation and discussion (half-day) in front of a six person Expert Panel every six months.

***Please, describe the mobility of the researchers within the Consortium.***

Our strategy was to give the researcher recruited under the SPy an opportunity to undergo training and establish expertise in their home laboratory before spending time in a partner laboratory. Unfortunately, the COVID-19 lockdown and subsequent travel restrictions have meant that researchers have not been able to undertake planned research/mobility visits across the Consortium, e.g., the visit of Miss Mokwebo to Dublin City University in March 2020, for training on electrochemiluminescence, or the visit of Dr. Fávaro Pipi from DCU to NU (May 2020) to learn about ECL luminophore synthesis and characterisation in April 2020. Once travel restrictions are lifted, researcher mobility will begin.

***Please indicate coordination with other projects funded in the 2018 Joint Call or national and international projects funded by other instruments.***

We are linking strongly with the **Break Biofilms (https://www.breakbiofilms.com/, Prof. Carmen del Blanco Lopez, Coordinator)** EU funded ITN on the development of sensors for the detection of pathogens.

We also collaborate with **Prof. Gordon Wallace of the Intelligent Polymer Research Institute, Australia** on the development of wireless electrochemical methods for the electrostimulation of biological cells and the development of electroceuticals.

### c. *Impact and knowledge output*

*Are the main impacts achieved?*

1. **UN SDG GOAL 6: ENSURE ACCESS TO WATER AND SANITATION FOR ALL**. The innovative Sense and Purify programme is creating a custom reactor with integrated electrochemical sensors/spectroscopy that is suitable for the local production of clean water for industry or drinking at low capital and operating cost.

We have made outstanding progress on the sensor aspect, demonstrating low limits of detection for pathogenic bacteria (DCU, NU, URV) and the direct detection of APIs (UWC, URV, DCU). Moreover, we have shown that UV-Vis spectroscopy (DCU) can provide direct, real time insights into the decomposition of organic pollutants. Excellent progress has also been made in identifying and optimising the properties of the Boron Doped Diamond electrodes (UWC) and particles (DCU) that will enable the wireless electrochemical destruction of recalcitrant organics.

Soon, we will **enhance innovation capacity and integration of new knowledge** by creating prototype reactors for the treatment of production wastewaters from the food (NU) as well as pharmaceutical industries (DCU). Our results so far have shown that hydroxyl radicals can be produced in significant quantities and have the power to breakdown and even mineralise the most challenging organic molecules found in pharmaceutical production waste water, the pharmaceuticals themselves (the parent compounds and their metabolites can end up in the municipal water supply) as well as food production waste water.

Thus, we are very optimistic about contributing positively to delivering UN SDG Goal 6.

**EDUCATION**. We have delivered a broad range of education impacts from school children (more than eight school visits carried out) to undergraduate and graduate students, as well as industry professionals (pharmaceuticals, food), paying close attention to gender issues.

*Are there any unexpected impacts?*

**Electroceuticals**. The wireless electrochemical approach being developed for the production of hydroxyl radicals to destroy recalcitrant organics is impacting our work with Prof. Wallace of the University of Wollongong, Australia to develop electroceuticals. Electroceuticals, e.g., implanted electrodes for deep brain stimulation in Parkinson's patients for tremor control, are highly successful. However, stimulating multiple sites is very challenging (currently a maximum of 16 electrodes) because of the need to wire each electrode from the head back to a controller located in the chest. Our work on wireless electrochemistry with SPy has inspired a completely new approach in which the voltage of biocompatible particles around biological cells in controlled wirelessly to stimulate the cells to control their function, e.g., random firing in epilepsy, or to control their differentiation.

*Where do the results of the project impact? (e.g. industry, end users, policy, etc.)*

**INDUSTRY:** All partners are continuing to liaise strongly with industry partners, e.g., pharmaceutical manufacturing (DCU and UWC), food production (NU) and sensor manufacturers (URV). These interactions help to ensure that the SPy technology addresses the correct industrial problem, has the performance required and minimises the barriers to adoption once the technology has been appropriately matured.

**POLICY MAKERS**: The study will impact policy makers, as well as water research and water quality management agencies in the partner countries, e.g., the Water Research Commission of South Africa, the Department of Human Settlements, Water and Sanitation (DHWS), the Department of Environment, Forestry and Fisheries (DEFF) and the Environmental Protection Agencies.

*Have the partners identified exploitable results?*

Across the Consortium, it is still too early in the programme's life cycle to identify exploitable results. However, the materials being developed by NU have significant potential for exploitation. The isolation of clear water suspension based on copper complexes doped silica nanoparticles is significant. These nanoparticles show luminescence in a medium where molecular complexes usually do not emit light which paves the way towards many applications, usually covered by ruthenium complexes. The NU DDSN show promising results. In contrast to previous reported copper(I) complexes that are usually fragile and non-luminescent in water, these copper nanoparticles show stable luminescence in water over months).

*Has intellectual property protection been considered?*

Each partner works closely with their university's Technology Transfer Office (TTO) to identify and process any disclosures/results that have IP potential. These periodic reviews cover new materials (NU, URV), detection technologies (DCU, URV, UWC), sensors (DCU, URV, UWC, NU) and the reactor technology itself (DCU).

## 3. Table of Deliverables

Please indicate whether the planned deliverables are completed, delayed or readjusted. Explain any changes/difficulties encountered and solutions adopted. Please add/delete rows, as necessary in the table below.

| Deliverable name | Lead partner (country) | Date of delivery (dd/mm/yyyy) | Changes, difficulties encountered and new solutions adopted |
|---|---|---|---|
| **WP1** | | | |
| D1.1 Device for highly sensitive pathogen detection (<1000 CFU/ml) device in water. | DCU (Ireland) | M18, August 2020 | **COMPLETED**. In collaboration with NU and URV, we have developed a reusable electrochemiluminescent sensor for pathogenic bacteria with a limit of detection of 100 CFU/ml |
| D1.2 100 mg of dye loaded silicate nanoparticles with ECL efficiency >80%. | NU (France) | M24, April 2021 | Ruthenium based DDSN were delivered for gold electrode functionalization. Copper based DDSN are difficult to prepare because of the instability of the complexes but promising results have been obtained and ECL tests are soon to begin. |
| D1.3 ECL based immunoassay for detection of priority pollutant in pharmaceutical wastewater. | DCU and NU (Ireland and France) | M24, March 2021 | NU is currently developing a family of high brightness molecular and nanoparticle electrochemiluminescent dyes. The ability of these dyes to produce light using a range of APIs as co-reactants will be investigated over the next six months. |
| D1.4 Minimum of five public engagement events including school visits, Café Scientifique and debates (see Section 2.2). | ALL (Ireland, France, Spain, South Africa) | March 2022 | Article published in the popularization journal "The Conversation". https://theconversation.com/une-solution-radicale-et-portative-pour-purifier-leau-145120<br><br>Organization of Science fair in Nantes<br><br>School Visits (8 completed) |

| **Deliverable name** | **Lead partner (country)** | **Date of delivery (dd/mm/yyyy)** | **Changes, difficulties encountered and new solutions adopted** |
|---|---|---|---|
| **WP2** | | | |
| D2.1 >100 mg of BDD particles capable of wirelessly mineralising single APIs at an industry relevant rate. | DCU (Ireland) | March 2020 | **COMPLETED** Delivered on time, March 2020 |
| D2.2 In silico model that replicates experimental results on wireless electrochemical incineration of recalcitrant organics. | DCU (Ireland) | March 2020 | **COMPLETED** March 2020. Two models have been developed based on analytical equations and a finite element COMSOL model. The models are fully consistent with the available experimental; data. However, the COVID-19 pandemic prevented the collection of experimental data from March to July. |
| D2.3 Invention Disclosure Form filed on the use of BDD particles for wireless incineration of recalcitrant organics. | DCU (Ireland) | March 2022 | On track, depends on the overall efficiency of the wireless incineration process and its applicability to a broad range of industrial waste waters. |
| D2.4 Following IP protection, minimum of two publications in high impact journals on CDP properties, hydroxyl radical | DCU (Ireland) | March 2022 | A manuscript, "*Sensing and Degradation of Organics Using Hydroxyl Radicals Electrogenerated at Boron Doped Diamond Electrodes*" B, Zribi, R. Forster, is being developed. It will have DCU and UWC co-authors. |
| **WP3** | | | |
| D3.1 In silico model of reactor. | DCU (Ireland) | M18, September 2020 | The COVID-19 pandemic has delayed the development of the reactor. An initial design has been developed based on the electric field modelling. However, developing a complete in silico model (feeder electrodes, mass transfer, sensors/spectroscopy) within the available time (DCU funding ends March 2021) will be challenging. |
| D3.2 Reactor fabricated using rapid prototyping incorporating design features identified by in silico model. | DCU (Ireland) | M30, September 2021 | Expected to be delivered on time. |

| Deliverable name | Lead partner (country) | Date of delivery (dd/mm/yyyy) | Changes, difficulties encountered and new solutions adopted |
|---|---|---|---|
| D3.3 UV-vis sensing system directly coupled to reactor. | DCU and URV(Ireland and Spain) | M30, September 2021 | Expected to be delivered on time. |
| D3.4 (Bio)Chemical sensors integrated into reactor. | URV (Spain) | M30, September 2021 | We are confident the sensors will be developed. However, our current experimental data suggest that the quantity and aggressiveness of the hydroxyl radicals, will mean that the lifetime of the sensors will be short (hours) if integrated into the reactor. It may be that UV-Vis spectroscopy represents a more powerful approach or it may be necessary to sample the reactor content and the analyse using the SPy sensors externally. |
| **WP4** | | | |
| D4.1 Report on performance and use issues surrounding SPy technology in an industrial setting | All (Ireland, France, Spain, South Africa) | M36, March 2022 | Expected to be delivered on time. |
| D4.2 Report on market possibilities for technology and initial assessment of route to market | All (Ireland, France, Spain, South Africa) | M36, March 2022 | Expected to be delivered on time. |
| D4.3 Delivery of minimum of two business focused Master's projects looking at the route to commercialisation. | DCU (Ireland) | M36, March 2022 | Discussions are ongoing with the Business School of Dublin City University to carry out this work in March 2021 |

## 4. Budget review

Please include a budget breakdown here, i.e. how the funding has been used so far.

The funding has been used to cover the salaries/stipend of the Post-Doctoral Fellows/students recruited to work on the agreed programme. Materials/consumables costs and travel represented the other major spend. The budgets are generally on-track with some minor (approximately 20-30%) underspend on materials and travel due to the closure of labs caused by the global pandemic.

## UWC SOUTH AFRICA

| Financial year | *Operational Expenses (ZAR) | Dissemination /Uptake (ZAR) | Total Budget (ZAR) | Expenses (ZAR) | Balance (ZAR) |
|---|---|---|---|---|---|
| **2019/20** | 281250.00 | 90000.00 | 371250.00 | 219293.00 | 151957.00 |
| **2020/21** | 180000.00 | 42750.00 | 222750.00 | 0.00 | 222750.00 |
| **2021/22** | 118500.00 | 30000.00 | 148500.00 | 0.00 | 148500.00 |
| **Total** | 579750.00 | 162750.00 | 742500.00 | 219293.00 | 523207.00 |

*HR costs are included under operation expenses

## DCU IRELAND

| Category | Budget | Spent | Available to Spend |
|---|---|---|---|
| **Salaries** | 158,035 | 140,628 | 17,407 |
| **Research Materials** | 34095 | 16,369 | 17,726 |
| **Travel** | 6555 | 2857 | 3,698 |
| **Access to External Research Facilities** | 5000 | 4890 | 110 |

## NU FRANCE

| Category | Budget | Spent | Available to Spend |
|---|---|---|---|
| **Salaries** | 162,182 | 47094 | 115133 |
| **Research Materials** | 67114 | 10537 | 56577 |

## URV SPAIN

URV does not receive a budget under the programme and is self-funded. This represents a significant leveraged contribution to the SPy programme.

## 5. Consortium Meetings

**Please list below the Consortium meetings which took place during the reporting period, by filling in the table below. Add/delete rows as necessary in the table below.**

Email exchanges have been a significant communication tool (> 150 exchanges since the project began). The following in-person and video meetings also took place.

| N° | Date | Location | Attending partners | Purpose/ main issues/main decisions? |
|---|---|---|---|---|
| 1 | 31/05/2019 | Dublin | R. Forster (DCU), E Iwuoha (UWC) | Strategy planning for overall programme delivery, bilateral collaborations and researcher mobility and the Consortium Agreement. |
| 2 | 11/06/2019 | Dublin | R. Forster (DCU, C. O'Sullivan (URV), Y. Pellegrin (NU) | Strategy planning for overall programme delivery, bi/tri lateral collaborations and researcher mobility and the Consortium Agreement. |
| 3 | 29/06/2019 | Video Conference | R. Forster (DCU), C O'Sullivan (NU), I Magriñá Lobato (URV) | Development of the ECL sensor for pathogenic bacteria, antibody labelling using the NU ECL dyes, cell handling. |
| 4 | 28/08/2019 | Video Conference | R. Forster (DCU), C O'Sullivan (URV), A Simonova (URV) | Strategy and relative performance of whole bacteria antibody assays vs. nucleic acid assays for species identification. |
| 5 | 29/01/2020 | Video conference | R. Forster (DCU), Y. Pellegrin (NU) | Design and synthesis of the ECL probes for the pathogenic bacteria assay |
| 6 | 21/04/2020 | Video Conference | R. Forster (DCU), C O'Sullivan (URV) | Update on ECL assay performance and discussion of direct and antibody-based detection of APIs and breakdown products |

## 6. Stakeholder/Industry Engagement

*Maximum 1 page*

Please indicate how stakeholders/industry were involved in the project during the reporting period:

*Has the project succeeded to engage with stakeholders/industry? If Yes, how? If No – why?*

DCU has engaged with a major pharmaceutical company to understand the nature of their wastewater treatment needs, e.g., total organic load, volume, time profile for generation etc. The provision of actual wastewater samples and the formulation of appropriate test samples has been extensively discussed. The SPy technology has been presented with a view to refining the design and performance and to them becoming an advocate for the technology.

NU has engaged with a leading food manufacturer/processer to understand the composition of their wastewater streams, to discuss accessing real world samples for testing and to raise awareness of the SPy technology. They have been especially helpful in identifying performance criteria with respect to sample volume and throughput rates.

*If applicable, please, describe the provision of data by stakeholders/involvement of industry and dialogue between the project and stakeholders/industry.*

No confidential data has been exchanged between SPy Consortium researchers and industry. From the perspective of industry, there are some concerns that the nature of the analysis we need to carry out, e.g., HPLC, TOC, BOC, spectroscopy, electrochemistry, to characterise the waste water samples could lead to knowledge that would allow synthetic pathways to be reverse engineered, information that is not currently in the public domain.

*Has the cooperation between the Consortium and industry/stakeholder partners influenced the project outcome(s) to date? If Yes, How? If No, why?*

Yes, the industry interactions have influenced the final operational performance needed from the reactor, e.g., outflow composition, flow rates, volumes etc. Moreover, engaging with diverse industries, pharmaceutical manufacturing and food, will help position the technology appropriately to maximise commercial impact. The MBA project students (planned to be recruited in March 2021) will deepen and extend these industry engagements.

*Outline the progress made towards achieving the project expected impacts.*

Excellent progress has been made on the scientific objectives that have been effectively communicated to key target industries, i.e., pharmaceutical manufacturing and food processing/production. We have raised awareness of the technology and sought to reduce the barriers to adoption by ensuring that the technology matches industry needs as closely as possible.

The original Impacts and their timeline are shown below and are on track.

| IMPACT/Year | 1 | 2 | 3 | 4 | 5 | 5-10 Yr |
|---|---|---|---|---|---|---|
| **Scientific:** | | | | | | |
| •Novel wireless electrochemical approach to oxidative electrocatalysis. | | | X | | | |
| •Insights into the rates and mechanism of organic pollutant oxidation | | | | | X | |
| •Novel sensors for rapid and sensitive assessment of water quality. | | | | | | |
| **Economic** | | | | | | |
| •Integrated sense and purify reactor with decreased wastewater treatment costs. | | | | | X | |
| •Enhanced removal of recalcitrant organic pollutants from industrial wastewater streams | | | | | X | |
| **Social** | | | | | | |
| •Enhanced public awareness of water resource issues | | | | X | | |
| **Education and Outreach** | | | | | | |
| •Researchers with the necessary multidisciplinary skills for future industrial, policy, academic and start-up employment | | | X | X | X | X |

*Were there unexpected impacts to date?*

Not at this stage of the programme development.

7. List of Publications produced by the Project - Open Access

- List all presentations, posters, and publications in scientific, peer-reviewed journals derived from this project, separating those in preparation, those in review and those accepted or in press.
- Provide websites and/or electronic copies of the key ones.
- Indicate all the co-authors for each publication.
- Order publications per date (chronologically) and for each year by alphabetical order.

Metadata on all project publications are required to be submitted as part of the final reporting. This will be done via the **Open Data & Open Access platform**, available at: http://opendata.waterjpi.eu/ (also accessible from the bar menu of the Water JPI website).

| | | |
|---|---|---|
| International | Peer-reviewed journals | 1. Electrochemical detection of viruses and antibodies: A mini review, MR de Eguilaz, LR Cumba, RJ Forster, Electrochemistry Communications, 2020, 116, 106762. (https://www.ncbi.nlm.nih.gov/pmc/articles/PMC7247998/)<br>2. *Sensing and Degradation of Organics Using Hydroxyl Radicals Electrogenerated at Boron Doped Diamond Electrodes*" B, Zribi (DCU), R. Forster(DCU), E. Iwuoha (UWC) and S. Douman (UWC) in preparation. |
| | Books or chapters in books | 1.<br>2.<br>3. |

| | | |
|---|---|---|
| | Communications (presentations, posters) | 1.<br>2.<br>3. |
| National (separate lists for each nationality) | Peer-reviewed journals | 1.<br>2.<br>3. |
| | Books or chapters in books | 1.<br>2.<br>3. |
| | Communications (presentations, posters) | 1.<br>2.<br>3. |
| Dissemination initiatives | Popular articles | 1. “The conversation”, « Une solution radicale et portative pour purifier l'eau », https://theconversation.com/une-solution-radicale-et-portative-pour-purifier-leau-145120<br>2.<br>3. |
| | Popular conferences | 1. “Wireless Electrochemistry: From Electroceuticals to Waste Water Treatment”, ARC Centre of Excellence for Electromaterial Science Annual Conference, R. Forster, L Cumba, B. Zribi and A. Fávaro Pipi, May 19, 2020. |
| | Others | 1.<br>2.<br>3. |

8. Knowledge output transfer

For each of the Knowledge Output arising from the project so far, please complete the following table.

| | |
|---|---|
| Short Title<br>*Please provide a short and concise title to describe the Knowledge Output* | |
| Knowledge Output Description<br>*Please only include generated Knowledge Outputs, not those that are expected. Note: Knowledge Outputs can be non-deliverables, milestones or ‘grey knowledge’. Also, multiple Knowledge Outputs could exist within one deliverable, and should be separated.*<br>*Try to give a comprehensive description, making the Knowledge Output fully understandable to a non-expert.*<br>*If relevant please provide detail of where the Knowledge Output differs from its equivalent, e.g. What are the key characteristics of the Knowledge* | |

| | |
|---|---|
| *Output? What research is it adding to and what is innovative about the Knowledge Output? (Max 500 characters).* | |
| Knowledge Type | Please choose one option – delete the rest:<br>* exploitable scientific result<br>* scientific publication<br>* report<br>* book/review<br>* RTD protocol/technical manual<br>* guidelines/standards<br>* training activity/learning module<br>* software/modelling tools<br>* product<br>* prototype<br>* services/tools<br>* multimedia<br>* data<br>* other |
| Link to Knowledge Output<br>*If you can provide a link to the Knowledge Output then please do so, e.g. digital object identifier (DOI), web address, download, research paper.*<br>*If the Knowledge Output is not publicly available currently but will be in the future, please provide details. Also, if it is available but only upon request, please state this.*<br>*If the Knowledge Output is not planned to be publicly available, please state "Not available for public".* | |
| Sectors & Subsectors<br>*Choose as many options as required from the list. Pick those sectors that you think would benefit from the application of this Knowledge Output.* | • Basin Management<br>• Flood Risk Management<br>• Water Scarcity and Droughts<br>• Drinking Water<br>• Bathing Water<br>• Emissions and Water Reuse<br>• Adaptation to Global Change<br>• Others<br>    ○ Other General<br>    ○ Agriculture<br>    ○ Governance<br>    ○ Consumer Health & Welfare<br>    ○ Finance<br>    ○ Modelling & Prediction |

| | |
|---|---|
| | ○ Socio-Economics<br>○ Stakeholder Involvement |
| End User<br>*Choose as many options as required*<br>*Per identified End User, please identify possible applications of the Knowledge Output.* | o Education & Training<br>o Environmental Managers & Monitoring<br>o Industry<br>o Policy Makers / Decision Makers<br>o Scientific Community<br>o Civil Society<br>o Other |
| IPR<br>*Please indicate whether IPR has been applied to this Knowledge Output (applied for a patent, copyright etc), or not.*<br>*Please insert "n/a" if no IPR has been applied.* | |
| Policy-Relevance<br>If the Knowledge Output is relevant to the WFD or any other related Directives, please list and explain why | |
| Status<br>*Please identify whether the Knowledge Output is finalised, is still being generated or whose status/future is unknown. Consider:*<br>*• Is your knowledge conclusive enough that it provides sufficient evidence to make an impact on, or be applied by, an End User?*<br>*• Is there a corroborating body of evidence, or are contradictory results, available?*<br>*• Does your knowledge progress beyond the current state-of-the-art / evidence base?*<br>*• Is more research or demonstration needed to validate the results?* | |

9. Open Data

In relation to Open Data, the funded projects will be requested to submit metadata on all the resources directly generated by the project, as well as additional information on how these data will be exploited, if and how data will be made accessible for verification and re-use, and how it will be curated and preserved. Metadata on all project resources are required to be submitted as part of the final reporting. This will be done via the **Open Data & Open Access platform**, available at: http://opendata.waterjpi.eu/ (also accessible from the bar menu of the Water JPI website).

10. Problems Encountered during Project Implementation

**Please indicate if any problems were encountered during the Project Implementation.**
**Did any of the partners find difficulties related to the grant agreement, the availability of funds at national level or other similar issues not specifically related to the technical part of the project?**

**UWC** The contract between the University of the Western Cape and the Water Research Commission of South Africa was only fully executed (signed by all parties) on 2 September 2019. The project was only approved to commence after that date. Target organic pollutants in the form of E3Ps that have relevance to the South African situation were identified as the ARV drugs used in HAART. Preliminary studies that commenced in September 2019 was suspended in mid-March 2020 when the country went into Covid-19 lockdown. Work on the project will resume in November 2020.

**IMPACT OF COVID-19**

COVID DELAYS DURING THE REPORTING PERIOD:

All laboratory work stopped for the Irish, French and Spanish partners in mid-March and for South Africa in late March 2020. The Irish, French and Spanish labs reopened in July but the South Africa lab will not open until November.

This halted all laboratory experimental work and had the following impacts.

- Support services, such as ordering in support of remote working activities, e.g., of modelling software, researcher training courses etc., were significantly delayed.
- For the PIs, the immediate priority was on the provision of online teaching and the delivery of modules, course materials and tutorials via online platforms. This was a time-consuming but essential activity that allowed students to complete the taught elements of their courses with a minimum of interruption. Moreover, the PI team played central roles in creating policies and procedures for effective infection control to allow a return to work which was very time consuming.
- Loss of access to real world samples due to initial closure of facilities and then exclusion of any third parties from industrial sites in the interests of infection control.
- Reduced access and longer response times by 3rd party suppliers.
- The collection of longitudinal samples from the food production partner was suspended.

**IMPACTS**
- Loss of significant a significant number of person months doing experimental lab work, approximately 30 person months. Moreover, changed work practices, especially infection control measures and the need to coordinate activities strictly avoiding face-to-face interactions, since the return to campus are such that productivity is between 50 and 60% of that achieved previously.

These lock downs have not just limited the collection of experimental data but decimated the number of face-to-face meetings, limited interactions across the Consortium and dramatically decreased the interest and participation of our industrial partners.

Significantly, these delays make it very challenging to complete the programme as planned, i.e., with a fully developed reactor with integrated sensors/spectroscopy that has been field tested in pharmaceutical manufacturing and food processing facilities.

11. Suggestions for improvement regarding project implementation?

1. Remaining compliant with the national and EU award conditions, as well as each partner having to comply with the reporting demands of two organisations is very challenging. This far exceeds those associated with other funding schemes that offer similar levels of funding and submission success rates.

2. The differences between national funding levels and durations poses real challenges for coordinating the individual tasks to be completed by the individual partners. For example, the funding to DCU as Coordinator ends in March 2020 but the overall programme will continue for a further 9 months yet the Coordinator will not have any active funded researcher.

3. The delays in experimental lab work caused by COVID-19 cannot be meaningfully addressed by no cost extensions since the researchers were under contract and had to be paid for the remote working during the lockdown. Hence, beyond some delayed materials costs, the overall impact of the lock downs on spend rates was minimal. In order to recover the lost experimental time fully costed extensions are required.