

# Institutul Național de Cercetare-Dezvoltare pentru Tehnologii Izotopice și Moleculare INCDTIM



## Procedure for differentiating wines through the corroboration of spectroscopic data with machine learning methods

Ariana Raluca Hațegan, Dana Alina Măgdaș, Ana Camelia Groșan

### 1 MOTIVATION

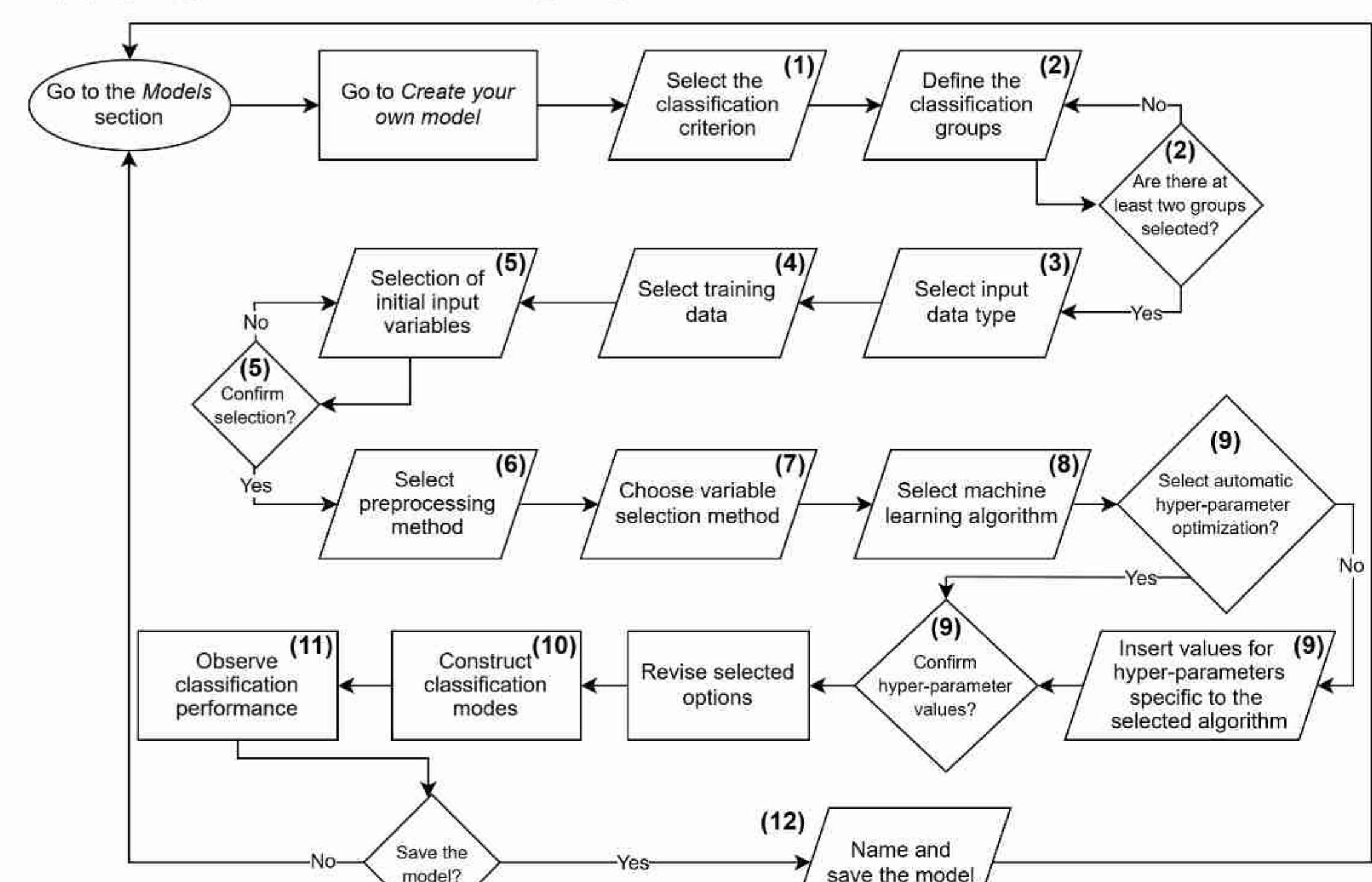
**Rapid product evaluation** and **fraud detection** represent a growing necessity at both national and international levels. Given the structural complexity of wines and the numerous factors influencing their composition, the evaluation of wine quality must consider various elements, including the variety, geographical origin, vintage, producer, and storage conditions.

**Wine authentication** techniques predominantly employ analytical methods that analyze organic or inorganic compounds, as well as the ratios of light stable isotopes inherent in their composition [1]. While effective and globally acknowledged, these methods entail significant costs and a high degree of expertise.

The development of **faster approaches** that use reduced solvent levels and allow the identification of wine fingerprints has recently engaged researchers' attention. This, coupled with the rapid advancement of **spectroscopic portable equipments**, has facilitated their application in the authentication of various product categories [2].

### 2 RESULTS

The invention proposes an **efficient sequence of steps for processing** experimental Raman or  $^1\text{H}$  NMR data, integrated into a **computer system** with a user-friendly interface that allows non-computer experts to create and utilize **advanced models** for recognizing the variety, geographical origin, and vintage of wine by applying machine learning algorithms.



Proposed sequence of steps for processing Raman or  $^1\text{H}$  NMR experimental data, integrated into a computer system with a user-friendly interface that enables non-experts to create and apply wine recognition models based on machine learning algorithms.

### HIGHLIGHTS

- Assessment of **wine authenticity** in an **efficient and rapid** manner;
- Possibility to use **several experimental data types** for wine origin recognition;
- Application and development of wine origin prediction models based on **advanced data processing methods** under an **intuitive and user-friendly** interface;
- Development of efficient wine differentiation models, depending on the **user's options** for input data, spectral domain, classification criteria or machine learning algorithms;
- **Automatic** recognition model optimization;
- **Efficient management** of experimental data;

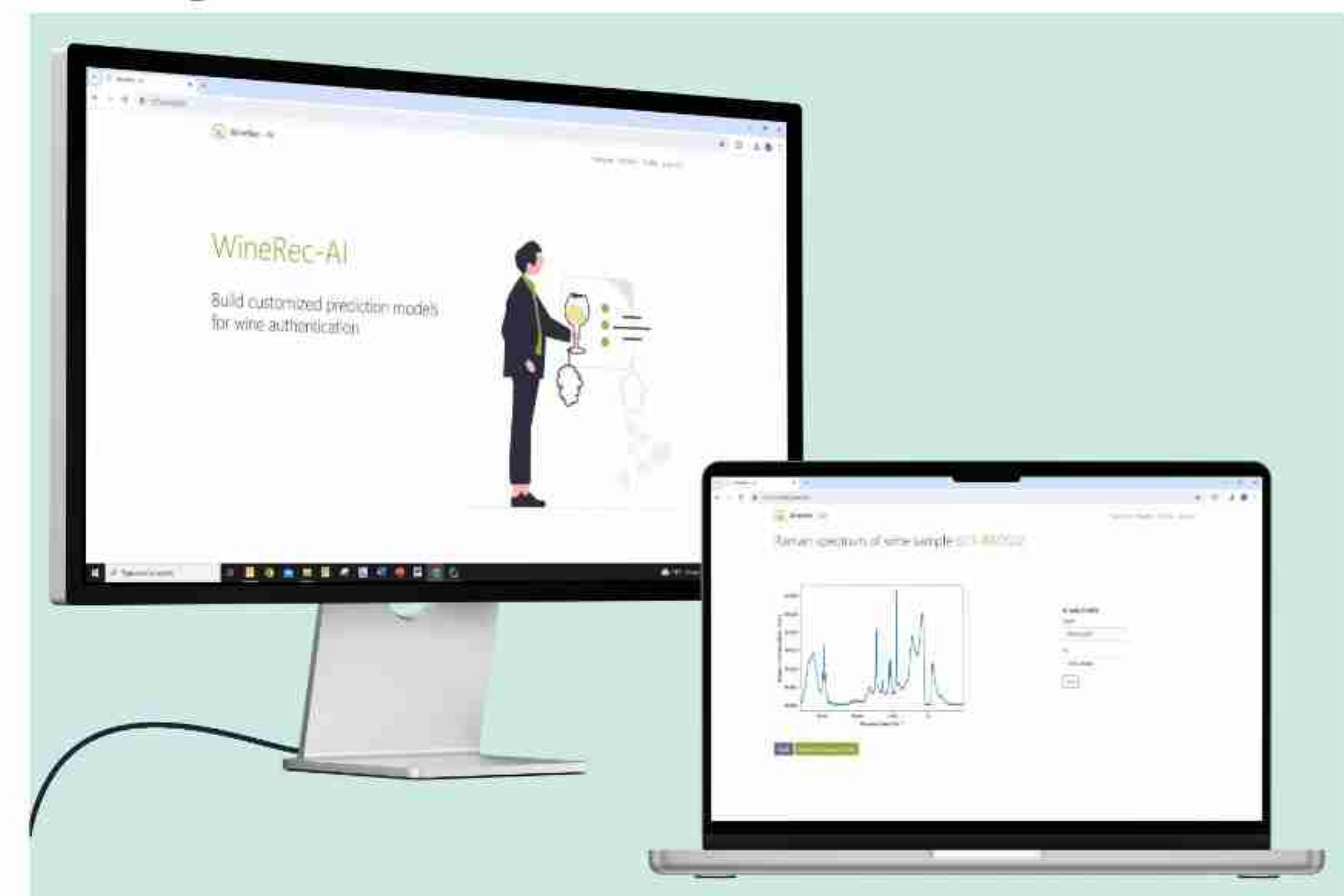
### 3 APPLICATION

The present invention offers a **practical and robust solution** for the authentication and classification of wines based on grape variety, geographical origin, and vintage year.

By integrating Raman or  $^1\text{H}$  NMR spectroscopic data with machine learning algorithms, the proposed solution allows **effective predictive modeling**.

The **intuitive interface** and **automated processes** allow users without specialized expertise in data processing to build wine recognition tools.

As a result, the proposed solution is particularly well-suited for applications in **quality control, certification, fraud detection, and research** within the wine industry and the broader field of alcoholic beverage authentication.



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- Danezis, G. P., Tsagkaris, A. S., Brusic, V., & Georgiou, C. A. (2016). Food authentication: state of the art and prospects. *Curr. Opin. Food Sci.* 10, 22-31.

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## Method and device for storing free atoms, molecules and ions in a contact-less, albeit well-defined near surface arrangement Patent no US12041864B2/16.07.2024

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Luiza Buimaga-Iarinca and Cristian Morari

### 1 MOTIVATION

We present a new approach and a device to stably hold atoms, molecules, clusters and also ions in contact-less, low interacting state with spatial resolution in the fractions of a nanometer or even down to the nm range.

This is achieved by confining them within the single quantum cells of the quantum well structure or the quantum well arrays implemented at the solid surface substrates.

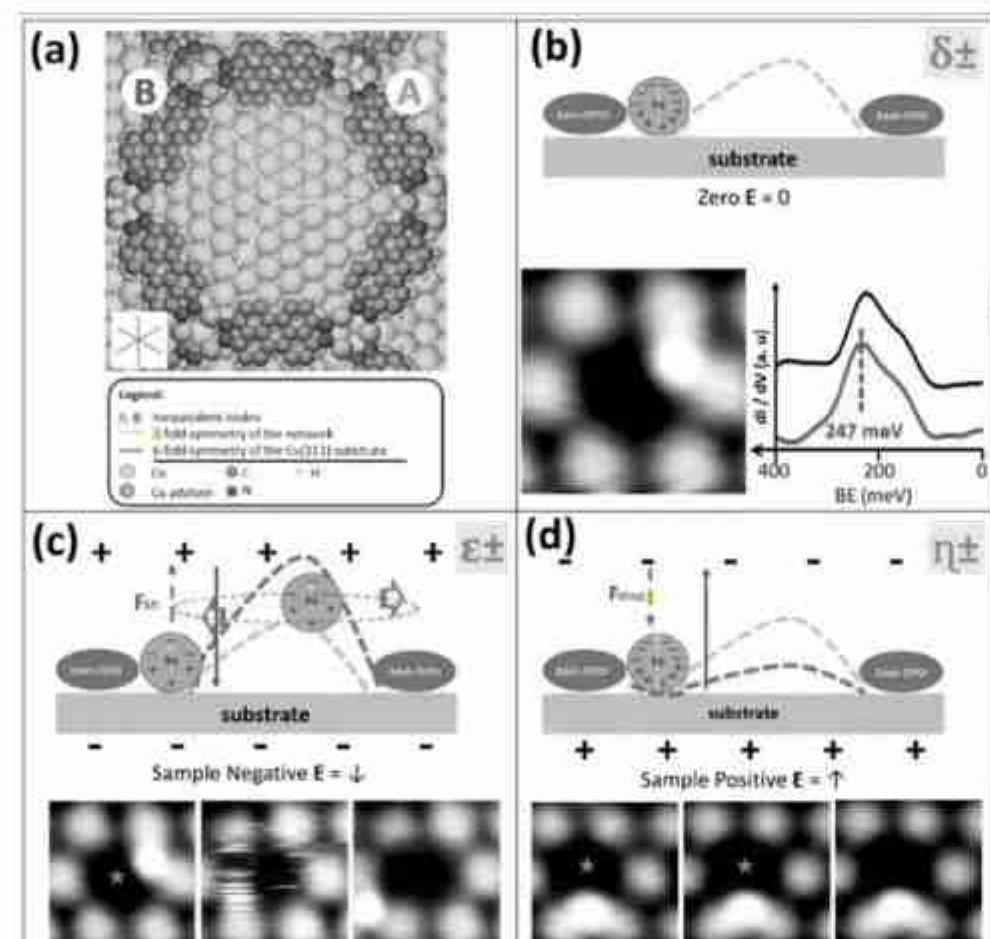


FIG. 1 schematically shows a local field induced phase transition in quantum wells.

### 2 RESULTS

The present invention demonstrates that surface supported quantum wells comprising a confined surface state capture and stably confine neutral atoms and molecules in a nanometer precise environment. Depending on the physico-chemical conditions in the capturing process and/or the degree of occupancy and/or the temperature of the solid substrate and/or the history of external stimuli like electromagnetic field pulses, these atoms, molecules, clusters and ions assume unique configurations which have not been observed outside of the gas or plasma state. The present invention reveals that these atoms or molecules are able to remain coupled to the quantum-well specific electronic state in the confinement and as such exhibit local and delocalized quantum entanglement (see fig 2)

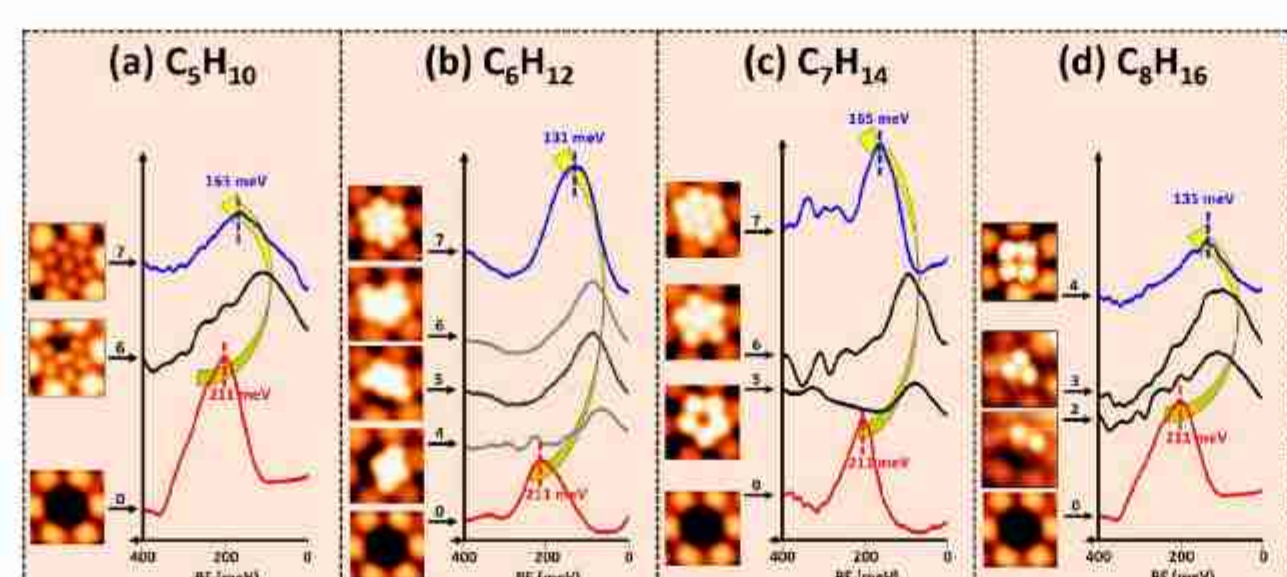


FIG. 2 Is a schematic view evidencing contact-less states at higher occupancy from the back-shifting of the quantum well state

### HIGHLIGHTS

The device at hand offers:

- well defined quantum mechanical contact-less interaction between the hosting quantum well state and the captured atoms / molecules / clusters / ions
- unprecedented addressability, sub-nm precision and long-range periodicity in 1 or 2 dimensions of the quantum well structure
- local control and access for single atom / ion / molecule / cluster experiments
- the potentials are of stronger local character with considerable binding energies but still soft enough to allow for long relaxation times and to hold complex clusters and complexes
- the spatial locality of the atoms / molecules / clusters / ions is well specified by the quantum well state(s).

### 3 APPLICATION

The ability to trap atoms, clusters (i.e., groups of cohesively interacting atoms), molecules and ions in a combination of DC and AC electric fields emitted by electric leads or electromagnetic waveguides has been a key enabler for atomic, molecular and plasma physics and has been driving innovations ranging, by way of example, from plasma science, fusion energy research to physical and bio-physical chemistry by the ability to detect very small interatomic and molecular forces with optical tweezers.

Recently, these activities further gained importance for their demonstrated potential towards the development of quantum devices and quantum computing.

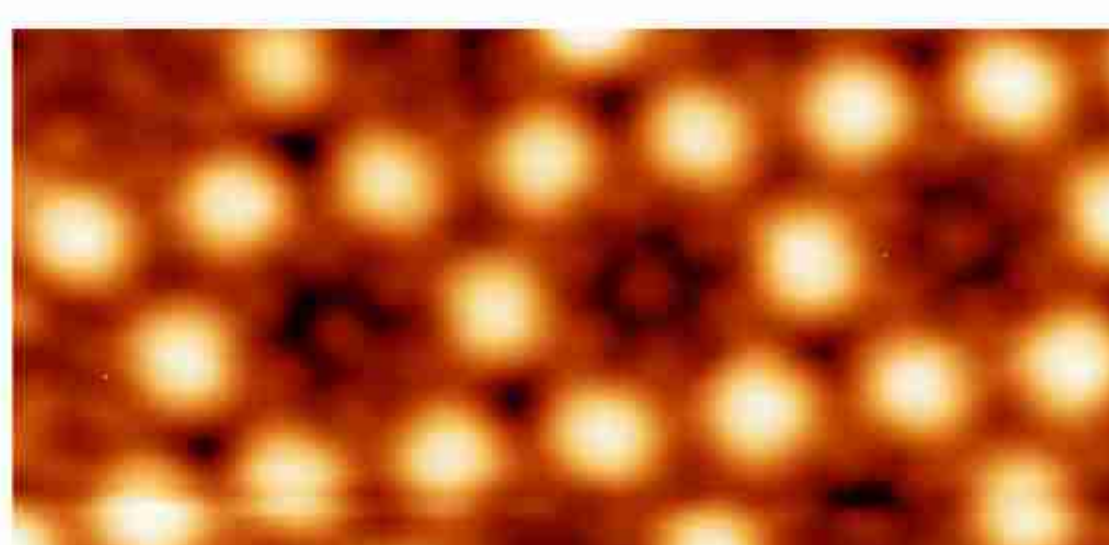


FIG. 3 Is a STM measurement of C5H10 molecules filling the quantum wells

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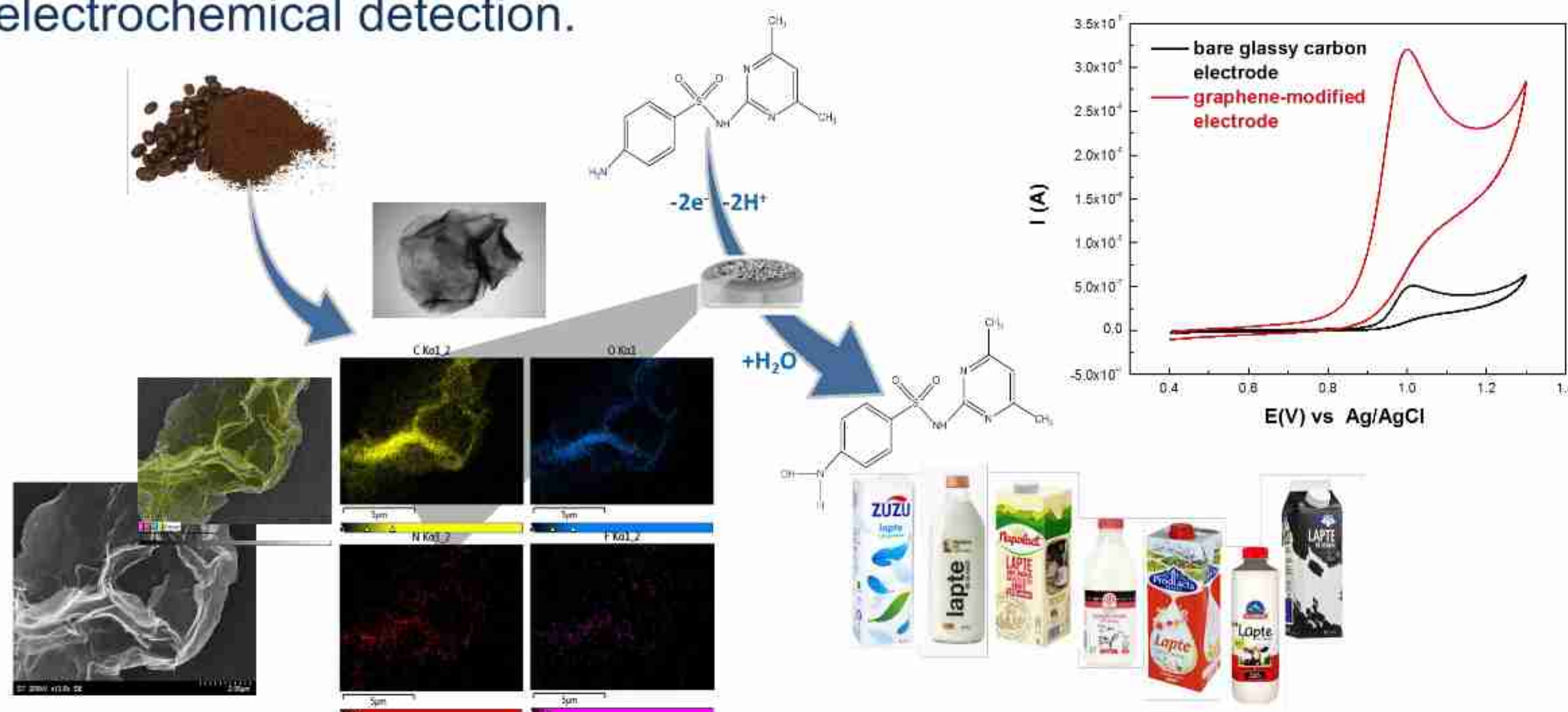
## Ecological procedure for obtaining nitrogen/fluoride co-doped graphenes applicable in the sulfamethazine detection

Patent application No. A0031/06.06.2024

Lidia Măgerușan, Florina Pogăcean, Stela-Maria Pruneanu

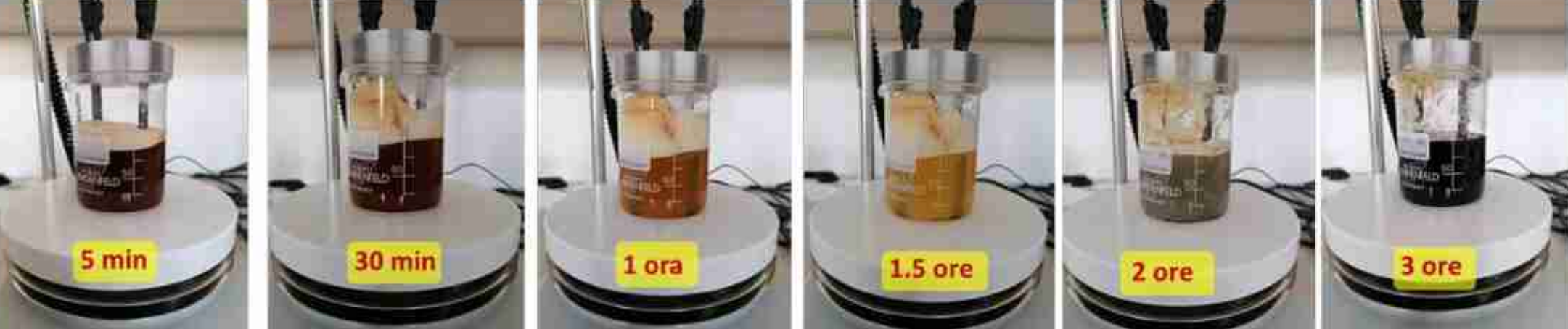
### 1 MOTIVATION

Due to improper usage or the insufficient withdrawal periods, the abusive use of sulfamethazine as a growth promoter in the veterinary sector has led to numerous public health problems associated with the accumulation of antibiotic residues in the environment, and the existence of worrisome amounts in the animal-derived food products destined for human consumption. The invention refers to a green strategy for the production of nitrogen-fluoride co-doped graphene material together with the applicability of this new nanocomposite material in the sulfamethazine electrochemical detection.



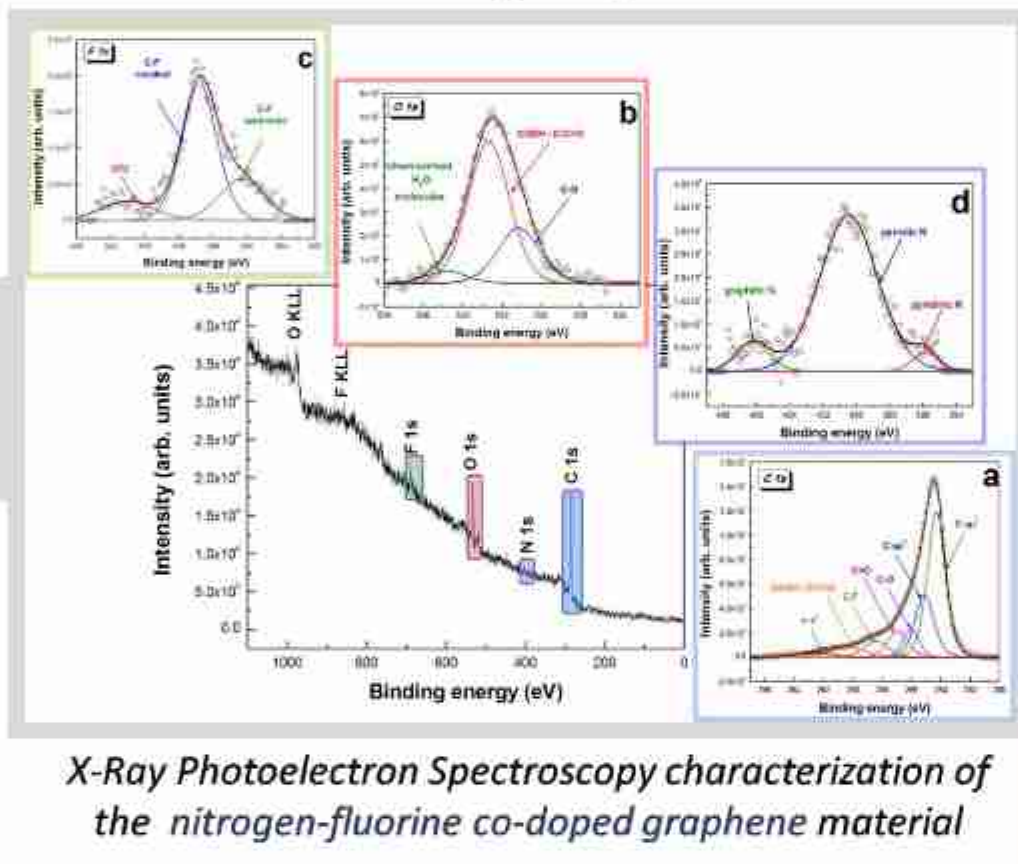
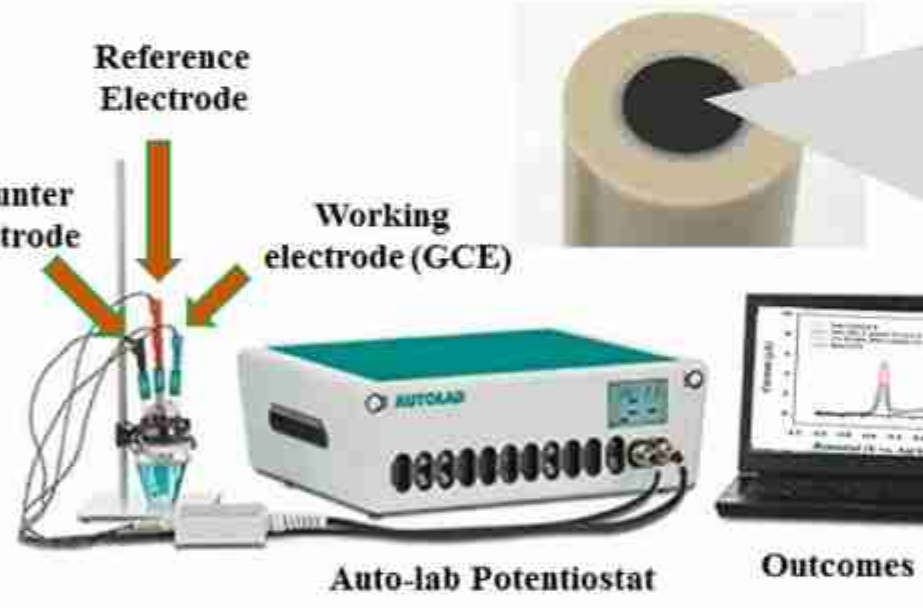
### 2 RESULTS

A simple, quick, economically advantageous and environmentally friendly protocol was established based on graphite rod electrochemical exfoliation in instant coffee.



A homemade electrochemical cell was constructed from a 150mL glass beaker with a Teflon cover provided with two holes centred at a distance of 2cm. The cell was filled with an electrolyte solution prepared by dissolving under magnetic stirring, at room temperature, 250mg commercially available instant coffee powder Nescafe in 100mL ultrapure water followed by the addition of 372mg potassium chloride in order to obtain a homogenous salt aqueous solution of concentration 0.05M. Two pure graphite rods were immersed in the electrolyte being fixed in the Teflon cover. Next, a Mesit (Slovakia) power source was set to apply DC voltage (6V) on the two graphite rods which served as anode and cathode in the so-build electrochemical cell, under continuous magnetic stirring, at room temperature. The experiment was stopped after a total of 4 hours. The obtained black solution underwent successive filtration and dialysis steps before being dried by lyophilization. The black resulting powder was further characterized from morphological and structural point of view. For the sensor fabrication aliquots of 0.5  $\mu$ L from a colloidal suspension of exfoliated graphene in DMF (2mg/1.5mL) were subsequently drop casted and dried under ambient conditions up to a maximum volume of 8.5 $\mu$ L. The efficiency of nitrogen-fluoride co-doped graphene material in sulfamethazine assay was tested using cyclic voltametric and amperometric approaches.

Electrochemical testing set-up and glassy carbon electrode having its active area modified with the new nitrogen-fluoride co-doped graphene nanocomposite



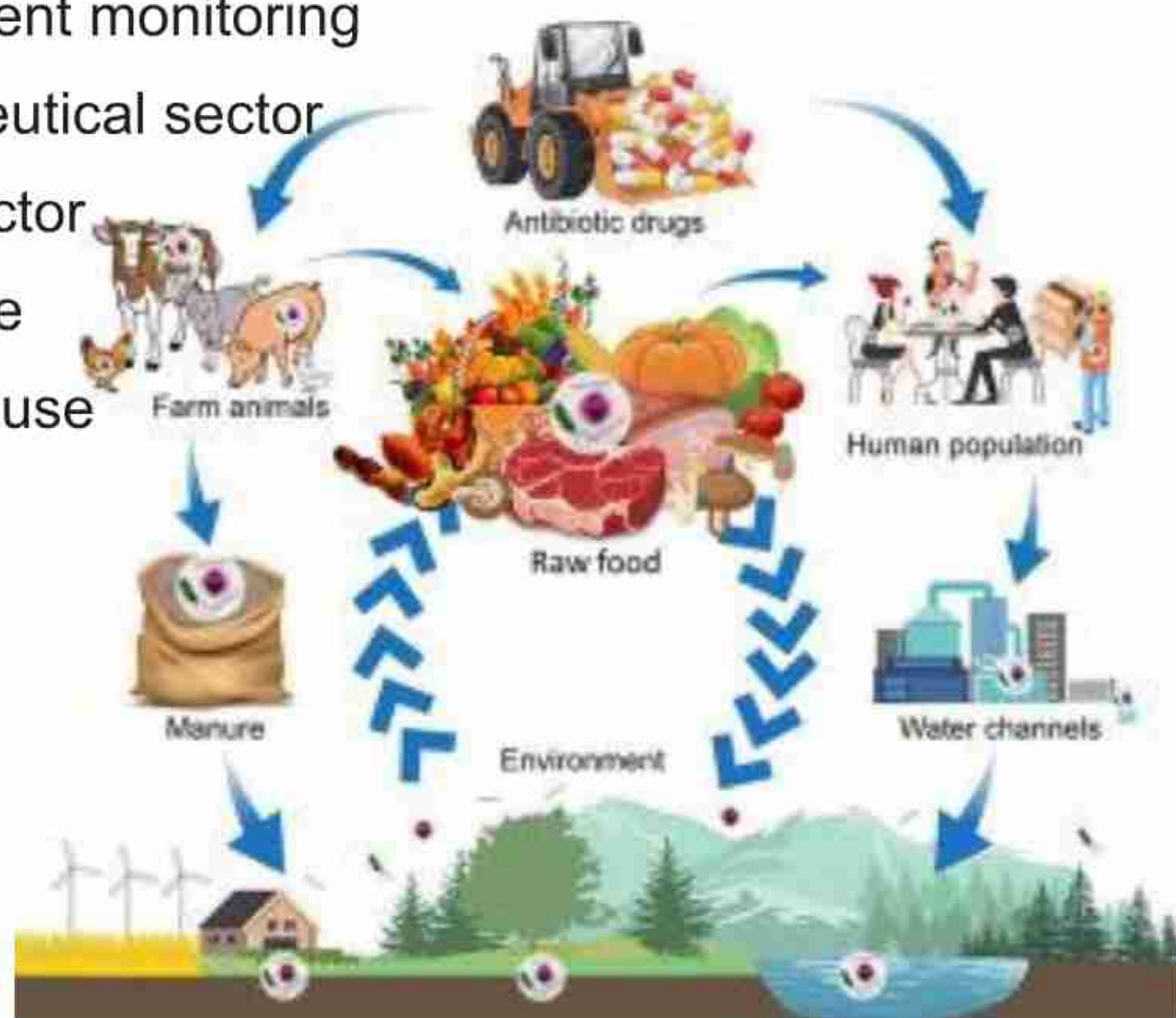
### HIGHLIGHTS

- The direct in-situ co-doping of graphene material without the usage of nitrogen or fluorine containing chemical precursors via electrochemical exfoliation of graphite in instant coffee electrolyte solution, at low applied bias
- Remarkable enhancement of the voltammetric response of the modified electrode attributed to the excellent electro-catalytic activity of co-doped graphene
- Increased efficiency and selectivity of the developed experimental model, with low detection and quantification limits (0.924nM), over a wide concentrations range (0.0028 – 100  $\mu$ M).

### 3 APPLICATION

The developed electrochemical protocol has an extended range of applicability in different fields

- food industry
- environment monitoring
- pharmaceutical sector
- health sector
- agriculture
- domestic use



Furthermore such modified active surfaces can be integrated and employed as sensing elements in the construction of miniaturized sensing platforms.

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## Non-metallic bioelectrodes based on electroconductive polymers

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### 1 MOTIVATION

- Bioelectronic medicines (BiEM) – a next generation class of closed-loop implantable neurostimulators for treatment of diseases: epilepsy, Parkinson's, pain, hypertension etc. [1].
- BiEM – record biological signals to monitor impaired body functions → deliver therapeutic stimulation pulses when sensing a dysfunction.
- Recording and stimulation – through bioelectrodes implanted in targeted organs.
- The present bioelectrodes are metallic (Pt, Pt/Ir) → several orders stiffer than biological tissues → move relative to the tissue during tissue motions → unstable recording and stimulation operations, tissue/bioelectrode damage, scar tissue formation → reduce/cancel the therapeutic effects.
- Conclusion: the need of softer bioelectrodes.**
- Our solution: non-metallic bioelectrodes made from the polymer polypyrrole (PPy) = much softer than metals [2].**

### 2 RESULTS

We made two types of PPy-based electrodes:

- recording electrodes:** from 300  $\mu$ m nylon filaments coated with a 20  $\mu$ m thick layer of PPy doped with naphthalen-2-sulfonic acid (PPy/N – Fig. 1) and used such electrodes to record biological signals (Fig. 2).
- stimulation electrodes:** from a 35  $\mu$ m (valleys) to 70  $\mu$ m (hills) thick PPy/N film (Fig. 3) and used such electrodes to stimulate living organs (Fig. 4).

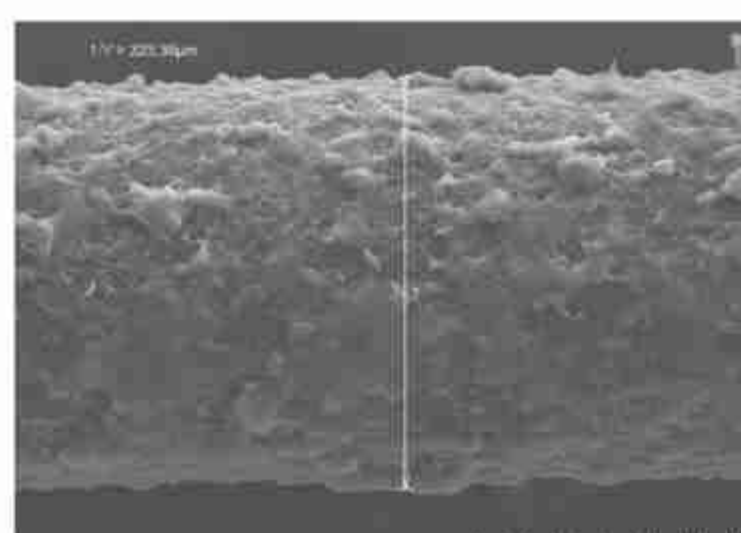


FIG. 1. PPy/N deposited on a nylon filament.

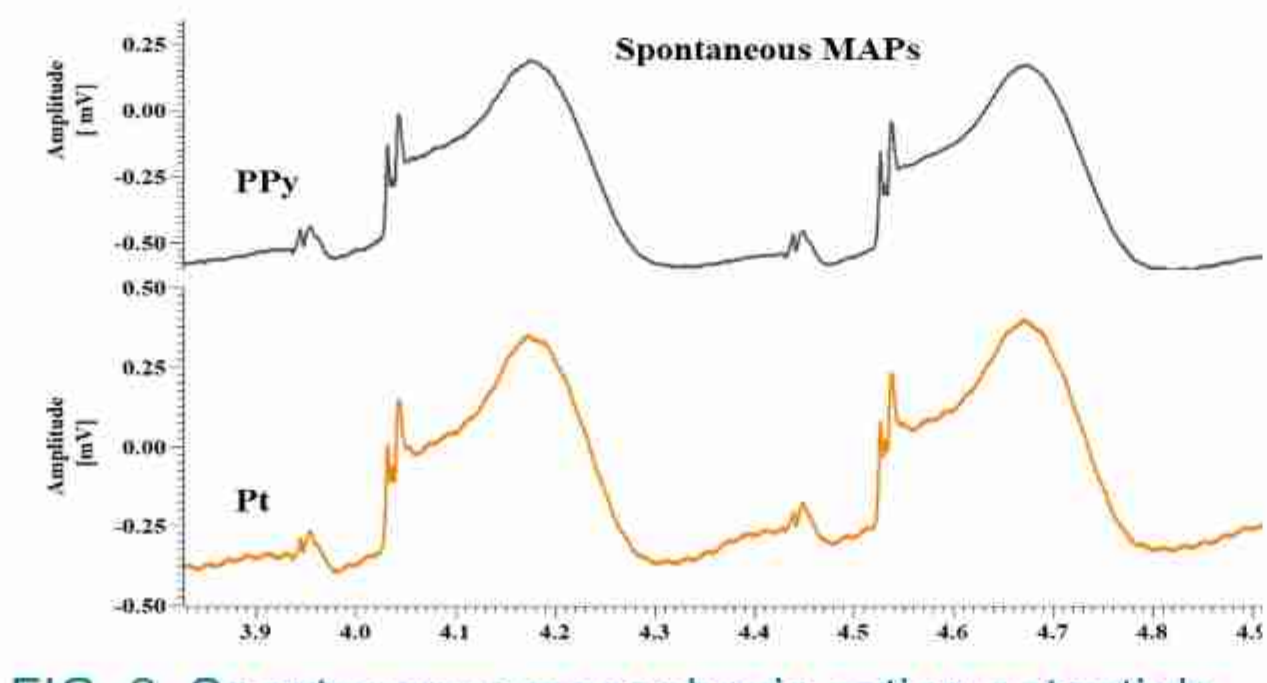


FIG. 2. Spontaneous monophasic action potentials (MAPs) recorded from a chick embryo heart with electrodes made from nylon filaments coated with PPy/N (PPy) vs. MAPs recorded with platinum electrodes (Pt).

### HIGHLIGHTS

- Bioelectronic medicines (BiEM) is an emerging class of therapeutic stimulators.
- The interface between BiEM and body organs – through bioelectrodes implanted in those organs.
- The present metallic bioelectrodes are too stiff and therefore unsuitable for advanced closed-loop BiEM.
- We successfully tested non-metallic bioelectrodes made from the conductive polymer polypyrrole.
- Patent Application No. A/00635/2024 concerning polymer-based bioelectrodes was filled .

### 3 APPLICATION

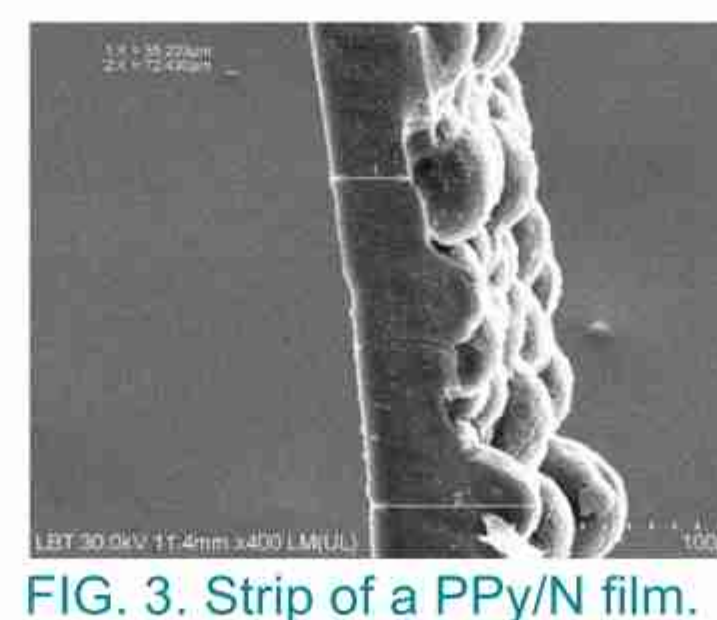


FIG. 3. Strip of a PPy/N film.

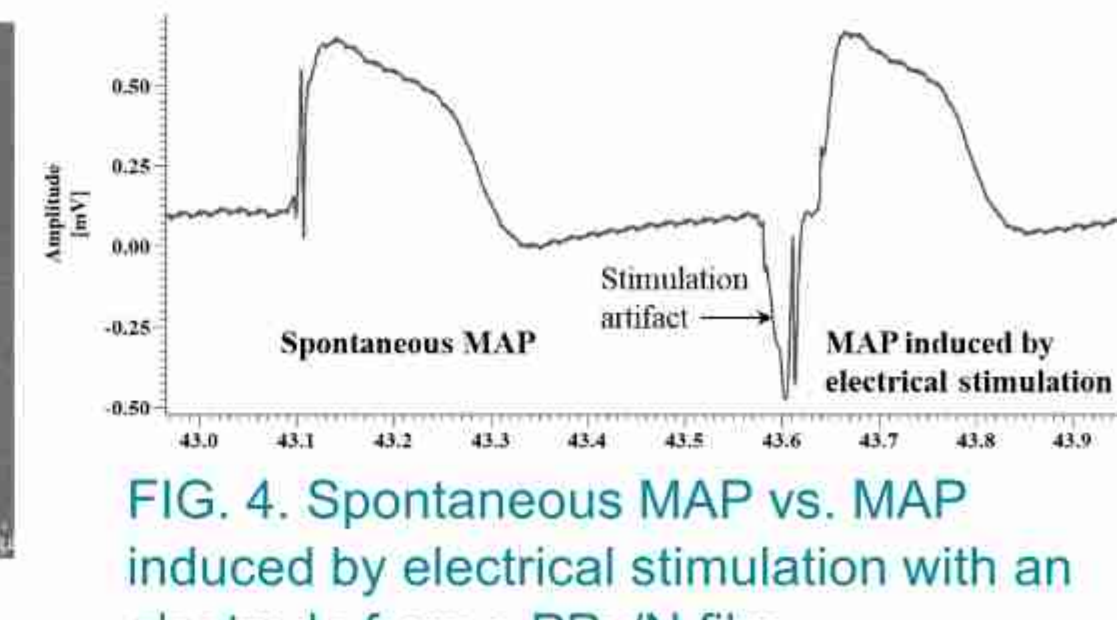


FIG. 4. Spontaneous MAP vs. MAP induced by electrical stimulation with an electrode from a PPy/N film.

- Thin layers of PPy/N are able to conduct :
  - ✓ biological signals from a living organ to a recording device;
  - ✓ stimulation impulses from a stimulator to a living organ.
- Such PPy/N layers deposited on strong, soft and flexible substrates could be used to make non-metallic bioelectrodes for BiEM.
- The PPy/N solution and several polymer-based bioelectrodes configurations were claimed in Patent Application No. A/00635/25.10.2024.

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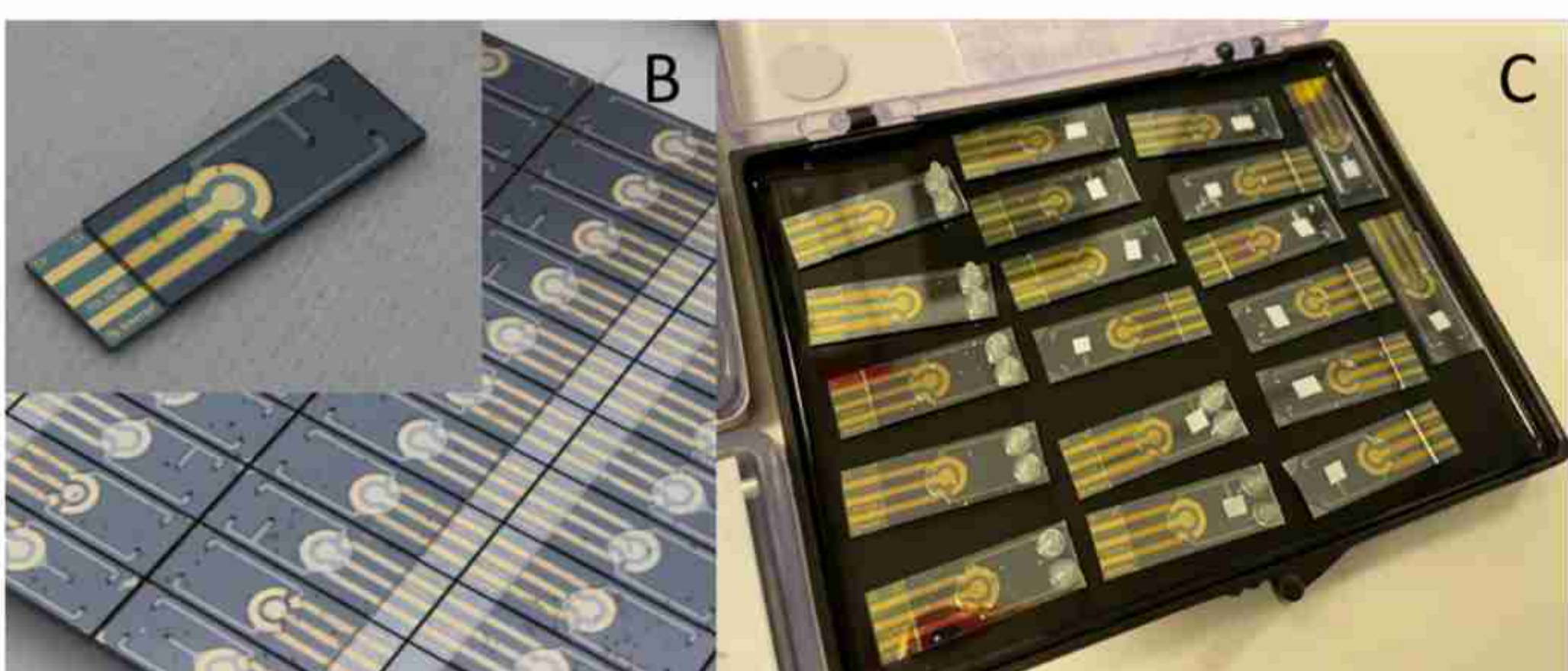


## Template-directed electrodeposition of plasmonic micro/nanostructured interconnected hemisphere-void lattice on gold electrodes for (EC-)SERS applications

Nicoleta Toșa, Alexandra Fălămaș, Septimiu Tripon, Denisa CuiBUS, Cosmin Farcău, Rebeca Moldovan, Bogdan-Cezar Iacob, Ede Bodoki, Karolina Milenko, Elizaveta Vereshchagina

### 1 MOTIVATION

The invention addresses the challenge of creating quasi-three-dimensional structured gold films through electrochemical processes for use as substrates for analytical investigations based on enhanced Raman scattering and electrochemical potential modulation (EC)-SERS. The process can be used in the laboratory, as well as at a large scale for the development of macroelectrodes.



Images of fabricated electrochemical SERS gold sensors

### 2 RESULTS

The process involves first constructing a gold electrode on a non-conductive substrate by magnetron sputtering. The gold layer is then covered with a compact hexagonal lattice of 460 nm polystyrene spheres through convective self-assembly. Using an electrochemical deposition process, gold micro/nanostructures in the form of interconnected negative hemispheres are created on the gold electrode. The setup for metal electrodeposition operates without a reference electrode, allowing controlled formation of plasmonic gold micro/nanostructures solely in the presence of electric current.

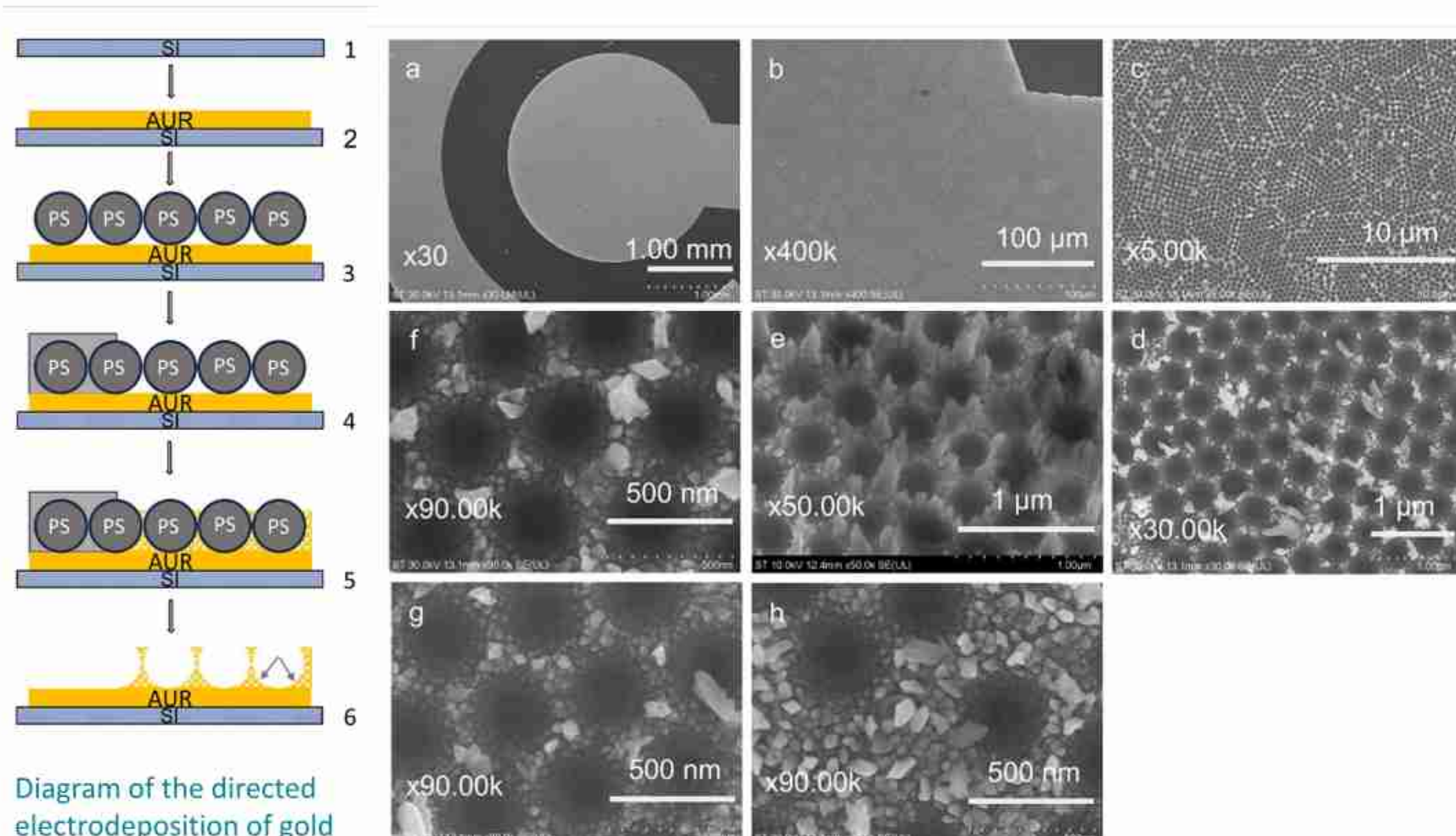


Diagram of the directed electrodeposition of gold nanostructures shaped as interconnected negative hemispheres on gold electrodes.

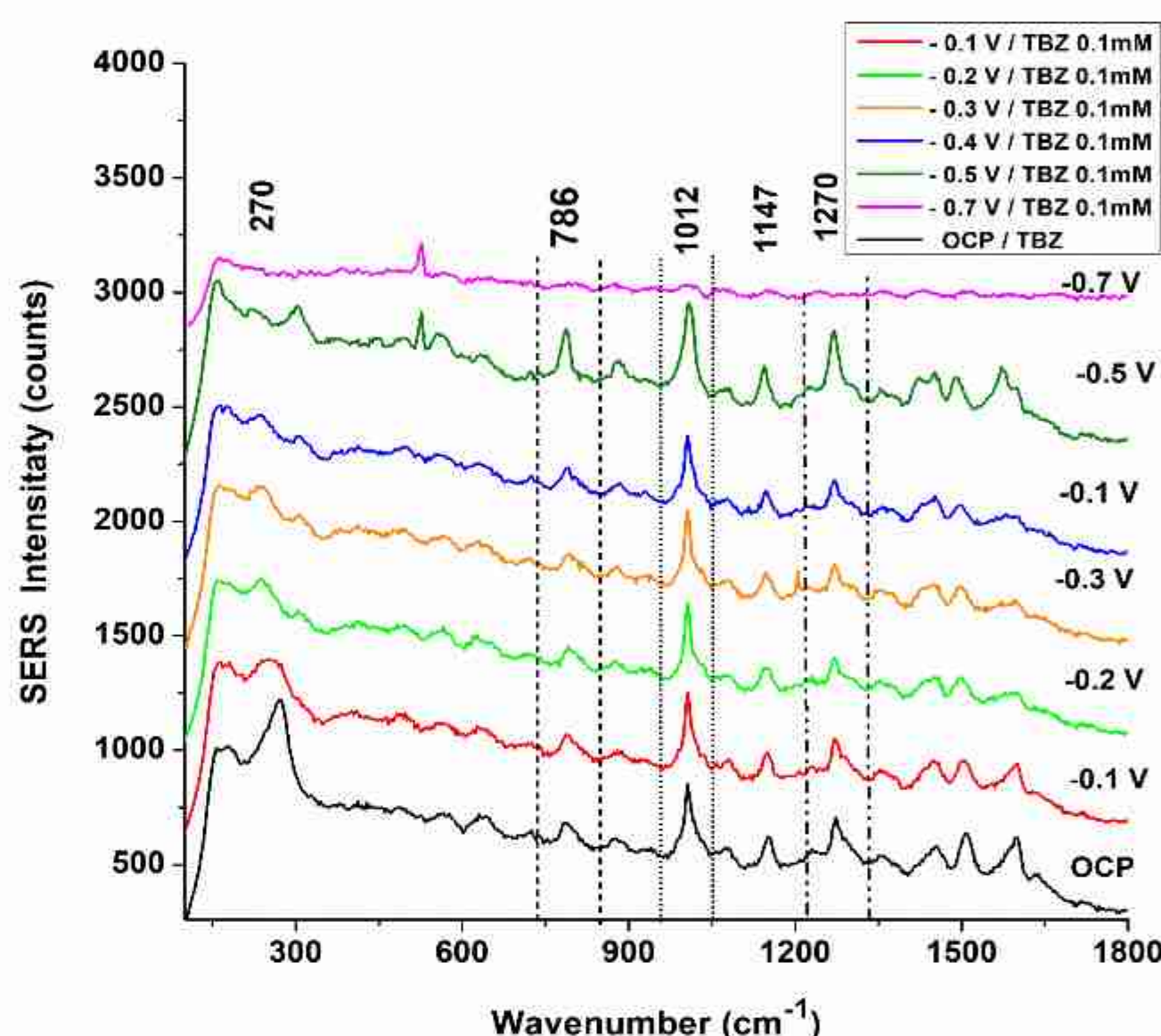
Scanning electron microscopy (SEM) micrographs of plasmonic micro/nanostructures in the form of INH on gold electrodes after the removal of polystyrene spheres at magnifications ranging from x220 (a) to x90,000 (h)

### HIGHLIGHTS

- Quasi three-dimensional structured materials shaped as interconnected negative hemispheres created from noble metals through electrodeposition processes;
- The SERS substrates are applied for the EC-SERS detection of thiabendazole pesticide detection.
- Patent Application: a 2024 00225 / 29/04/2024
- Abstract publication: BOPI No.2/28.02.2025

### 3 APPLICATION

EC-SERS is a potent surface analysis technique for *in situ* analysis of adsorption behaviors and chemical changes at electrode surface, with important applications in environmental monitoring and protection. The gold electrodes developed here were applied for the detection of pesticides, such as thiabendazole (TBZ). The potential-dependent SERS spectra shown in figure present Raman bands assigned to TBZ molecules (786, 1012, 1270  $\text{cm}^{-1}$ ). The spectra also show the dependence of Raman bands enhancement on the applied potential. These results suggest the means to enhance the sensitivity of TBZ SERS detection by electrochemical effects, which will serve for improving the limit of detection in future practical applications.



SERS spectral response, with electrochemical potential modulation and in open circuit, of a gold electrode decorated with interconnected negative half-shell plasmonic micro/nanostructures network in the presence of aqueous solution of thiabendazole  $10^{-4}\text{M}$ , mixed with phosphate saline buffer solution (PSB) 0.1M and potassium chloride (KCl) 0.05M.

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## Portable cold plasma microreactor for fast processing of the liquid samples

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### 1 INTRODUCTION

Cold plasma is effective for facilitating chemical reactions because of its electron temperature, which usually ranges from 10,000 to 100,000 K, corresponding to an energy range of 1 to 10 eV. Cold plasma in solution is an innovative and environmentally friendly approach that simplifies synthesis processes, reduces reagent usage, shortens reaction times, and enables processing under ambient conditions.

### 2 RESULTS

The portable microreactor described in this invention has been designed and built for chemical reactions assisted by cold plasma. Its purpose is to provide users with a versatile, simple, and robust device. The reaction cell of the microreactor consists of a coaxial arrangement of two tubes, positioned vertically. The liquid sample, in the form of a film, passes through an electrical discharge (plasma)

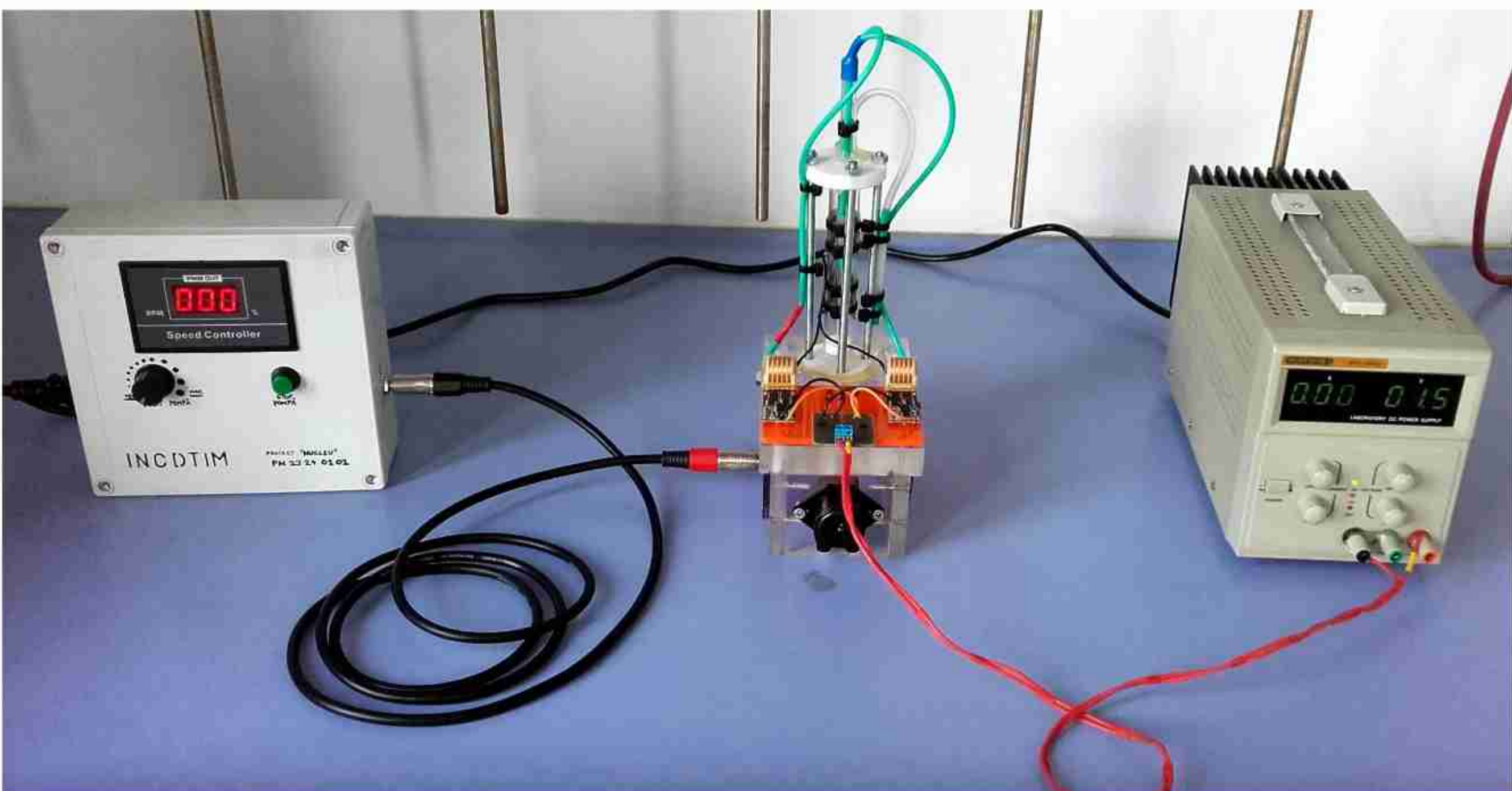
### HIGHLIGHTS

- Cold plasma
- Plasma chemistry
- Portable cold plasma microreactor
- Plasma-assisted reactions in solution

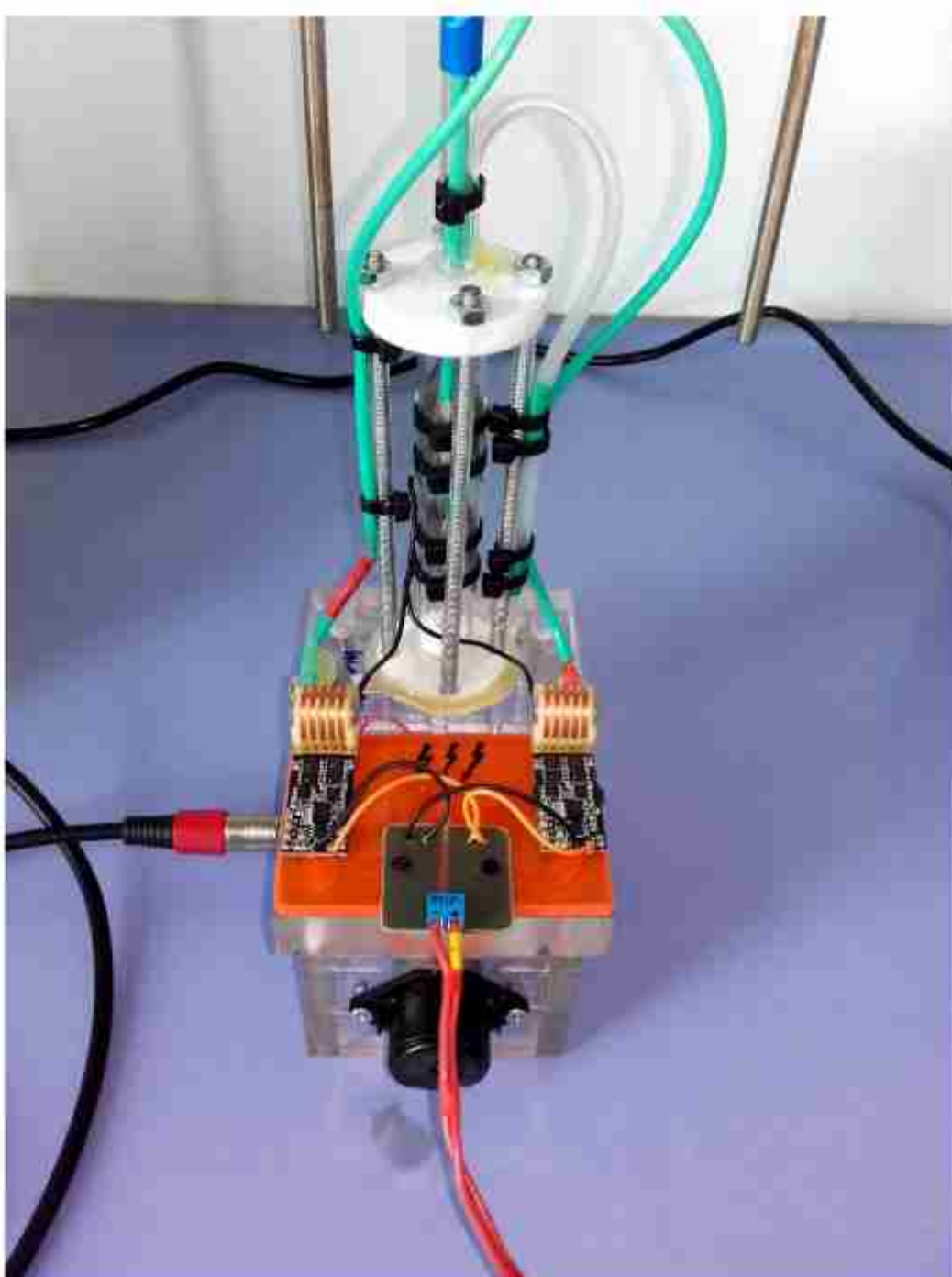
that is initiated between the active cylindrical electrode (inner) connected to a high-voltage source and the ground electrode (outer). A peristaltic pump reirculates the liquid sample through the reaction cell during the processing within the electrical discharge.

### 3 APPLICATION

- Organic reactions in plasma-liquid system



Cold plasma microreactor



Cold plasma reaction cell

### REFERENCES

- Maria Coroș, Cristian Tudoran, Gabriela Blăniță, Diana Lazăr, Inventors, INCDTIM assignee, *Portable cold plasma microreactor for fast processing of the liquid samples*, Romanian patent application 00712/18.11.2024.

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