# 1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan)

## **Project title:**

Design of new deep eutectic solvents and their practical application.

#### 1.1. Project goals

Chemometric design and synthesis of new deep eutectic solvents (DESs)

Application of new DESs for recovery of metal ions and the release of drugs and therapeutic substances.

Optimization of the method for preparing polymer inclusion membranes (PIMs) for metal ions separation and the release of drugs and therapeutic substances.

Determination of operational parameters influencing the membrane transport effectiveness. Identification of the membrane morphology change during the membrane transport process. Elaboration of mathematical model for the description of the transport kinetics.

### 1.2. Outline

Nowadays, metals such as cobalt, nickel, cadmium, zinc, and indium are critical and strategic because they are difficult to substitute in a particular industrial application. Therefore recovery of these metals from so-called secondary resources (various wastes) becomes increasingly important. Understandably, developing more efficient, economical, and environmental-friendly processes capable of recovering metals from poor and complex feed materials is still a priority. Among numerous separation techniques applied to recover valuable and/or toxic metals from wastewater, the membrane techniques seem most appropriate.

One of the intensively developing research directions is the application of polymer inclusion membranes (PIMs) for the recovery and/or separation of metal ions from aqueous solutions. PIMs are obtained by slow evaporation of a volatile organic solvent from a polymer, carrier, and plasticizer solution. The carrier binds to the substance present in the feed solution and enables (or facilitates) the transport through the membrane. One of the new research directions is the application of deep eutectic solvents (DESs) as carriers in PIMs. DESs are a new class of safe, efficient, simple, and low-cost solvents characterized by significant depressions in melting points compared to those of the neat constituent components. Compared to typical carriers, DESs possesses many advantages, such as very low vapor pressure, non-flammability, thermal and electrochemical stability, and the ability to dissolve organic and inorganic substances depending on the structure. Due to their properties, they can also be called "green solvents". The main advantage of DESs is the possibility to design a compound having specific and desired properties through the appropriate selection of a hydrogen bond donor (HBD) and a hydrogen bond acceptor (HBA) forming the DES. The ease of synthesizing new DESs with unique properties makes it possible to use them in PIMs to recover metal ions from electroplating wastewater, electronic waste, sewage sludge, etc. as well as for the controlled release of drugs and therapeutic substances.

#### 1.3. Work plan

Chemometric design and synthesis of new deep eutectic solvents.

Preparation and optimization of the composition of polymer inclusion membranes.

Examination of the membrane structure by contact angle measurements, vibrational spectroscopy (FT-IR, Raman), atomic force microscopy, scanning electron microscopy, etc., and determining the membrane structure effect on the transport effectiveness.

Application of response surface methodology for optimization of transport selectivity and efficiency.

Elaboration of physicochemical model for membrane transport kinetics description.

Application of optimized membranes for recovery and separation of metal ions from real wastewater solutions (electroplating, e-waste) and controlled release of drugs and therapeutic substances.

#### 1.4. Literature

[1] European Commission, Report on ad hoc working group on defining critical raw materials. Report on Critical Raw Materials for the EU, 2014, available at

http://ec.europa.eu/growth/sectors/raw-materials/specific-interest/critical/index\_en.htm.

- [2] A. K. Dwamena, Separations 2019, 6, 9.
- [3] Deep Eutectic Solvents, Y. Marcus, Springer Nature Switzerland AG, 2019.
- [4] Deep Eutectic Solvents Synthesis, Properties, and Applications, D. J. Ramón, G. Guillena (Eds), Wiley-VCH Verlag GmbH & Co. KGaA, 2020.

## 1.5. Required initial knowledge and skills of the PhD candidate

Knowledge about general, physical, and polymer chemistry.

Self-discipline.

Motivation to achieve the goal (i.e. PhD degree).

## 1.6. Expected development of the PhD candidate's knowledge and skills

Ability to design deep eutectic solvents with desired properties.

Better understanding of physicochemistry of membrane transport.

Practical knowledge and skills in membrane morphology analysis.

The ability to work independently.

Gaining experience in analyzing according to principles of good laboratory practice (GLP).

The advanced ability of data processing and statistical/chemometric analysis.