



**Centrul de Chimie Organica  
al Academiei Romane "C.D. Nenitescu"**



**UNIVERSITATEA DIN  
BUCUREȘTI**  
VIRTUTE ET SAPIENTIA



**Institutul National de Cercetare si Dezvoltare  
pentru Tehnologii Criogenice si Izotopice**

**BRINGING TOGETHER QUANTUM SIEVING PROCESS AND NEW METAL-ORGANIC  
FRAMEWORKS SYNTHESIS TO DEVELOP  
A NEW HYDROGEN ISOTOPE SEPARATION TECHNOLOGY  
(HYSO-MOF)**

**Financial support: UEFISCDI**

**PN-III-P2-2.1-PED-2019-2079 (469PED/23.10.2020)**

**Project timespan: 2020 – 2022**

# Partners and Management

**Coordinator (CO) – Universitatea din București, Facultatea de Chimie**

**Project leader: Acad. Marius ANDRUH**

**Partner P1 – Centrul de Chimie Organică al Academiei Române “C.D. Nenițescu”, București**

**Team P1 leader: Dr. Simona NICA**

**Partner P2 – Institutul Național de Cercetare și Dezvoltare pentru Tehnologii Criogenice și Izotopice, Râmnicu Vâlcea**

**Team P2 leader: Dr. Mihai VARLAM**

# Project Teams

## **CO Members:**

Conf. Dr. Augustin M. Mădălan

Lect. Dr. Ruxandra Gheorghe

Drd. Cristian Spînu

## **Partner 1 Members:**

Dr. Andreea Dogaru (căș. Horga)

Dr. Anamaria Hanganu

## **Partner 2 Members:**

Dr. Adriana Marinoiu

Dr. Anisia Mihaela Bornea

Ing. Marian Curuia

# Project Budget

No.	BUDGET CHAPTER (EXPENSES)	2020 (lei)	2021 (lei)	2022 (lei)	TOTAL (lei)
1	SALARIES	66.261	158.000	73.739	298.000
2	LOGISTICS	7.600	94.500	40.900	143.000
3	TRAVEL	600	27.000	17.400	45.000
4	INDIRECT COSTS	17.615	65.375	31.010	114.000
	TOTAL	92.076	344.875	163.049	600.000

# Summary

The project proposes a systematic study of a non-polluting technology for hydrogen isotope separation using metal-organic frameworks (MOFs), based on a chemical quantum sieving (CAQS) mechanism.

Our strategy involves classical reactions conditions and cheap materials. The starting point of this study is  $^3_{\infty}[\text{Cu}_2(\text{mand})_2(\text{hmt})]\cdot\text{H}_2\text{O}$ , a 3D MOF structure, previously synthesized in our laboratory, made of binuclear  $\text{Cu}_2\text{O}_2$  nodes, hexamethylenetetramine and mandelic ion linkers. This material exhibits permanent porosity, thermal stability and, due to its texture, capacity of  $\text{H}_2$  capture and storage.

As the pore size plays an important role in determining the diffusion kinetics and the overall separation, we shall investigate the ability of isostructural MOFs to separate hydrogen isotopes. Firstly, the Cu(II) ion will be replaced by Zn(II). Secondly, a screening of various organic species (hydroxyacids and new adamantane-pyridines) as linkers will be undertaken.

Ultimately, we propose to develop an innovative hydrogen isotope separation technology for the most efficient permanent porous MOF material, using an in-house assembled cryogenic (down to 20 K) thermal desorption mass spectrometer, unique in Romania, existing only at ICSI Rm. Vâlcea.

# Objectives

- (O1)** Concept development: study of the ability of the starter system,  $^3_{\infty}[\text{Cu}_2(\text{mand})_2(\text{hmt})]\cdot\text{H}_2\text{O}$ , to act as a chemical quantum sieve for hydrogen isotope separation.
- (O2)** Optimization of MOFs architectures based on the effect of the metal ion; when the Cu(II) ions are replaced by Zn(II) ones.
- (O3)** Optimization of MOFs architectures based on the substitution of the mandelic bridge within the  $\text{Cu}_2\text{O}_2$  nodes with various hydroxy-carboxylates.
- (O4)** Design and synthesis of new organic neutral tetrahedral spacers (adamantane-pyridines) replacing the hexamethylenetetramine within the starter system.
- (O5)** Modulation of the pore size: building MOFs based on the newly designed and synthesized adamantane pyridine spacers.
- (O7)** Optimizing MOFs properties by post-synthetic processes.
- (O8)** Evaluation of the solid structure, thermal stability and selective sorption capacity of MOFs.
- (O9)** Demonstration of the concept functionality by elaboration of a sustainable isotope separation technology involving selection of the best isotopologue MOF adsorbent tested with the home-built cryogenic thermal desorption mass spectrometer.