Project Title: Metal Organic Frameworks: from GREEN Synthesis to GREEN Applications

Project code: Cod PN-III-P4-PCE-2021-0089
Contract no: PCE24/2022
Project acronim: MOFGREEN

Program 4: Basic and frontier research
Type project: Exploratory research projects- Competition 2021

Contracting Unit: UEFISCDI (Executive Unity for Financing the Superior Education, Research, Development and Innovation)

Contracted Unit: "Coriolan Dragulescu" Institute of Chemistry

Period: 32 months (May 2022-December 2024)

Total Value: 1.200.000 Lei

Amount in 2022: 226.860 Lei
Amount in 2023: 524.140Lei
Amount in 2024: 449.000 Lei

Project leader: Dr. Aurelia VISA

Project members:
Dr. Bianca MARANESCU
Dr. Lavinia LUPA
Dr. Laura COCHECI
Dr. Nicoleta PLESU
Dr. Gheorghe ILIA
Dr. Adriana POPA
Dr. Simona Muntean (May-August 2022)
Dr. Lavinia MACARIE
Drd. Samuel TOLEA (September 2022-December 2024)
Student masterand Marcela IOSIVONI (September 2022-December 2024)

Project Summary:

The project scope is to develop new technology for organic pollutants (OPs) removal from wastewater by using new adsorbent materials, metal organic frameworks (MOFs) modified with ionic liquids (ILs) through adsorption followed by electrochemical and/or photocatalytic regeneration.
By the specific objectives, in the framework of the project, we are planning to perform researches by two main directions: The first direction of present project is the synthesis and characterization of new adsorbent materials starting from di, tri or tetra phosphonic acids or phosphono carboxylic acid, namely MOFs modified with ionic liquids. The main motivation of this project is the second research direction, namely potential application of metal organic frameworks modified with ionic liquids for organic pollutant removal combined with electrochemical and/or photocatalytic regeneration of the adsorbent material. Using the ILs for

the MOFs modification increases the efficiency and selectivity of the obtained adsorbent materials. The combination of advanced properties of MOFs with the advantages of the ionic liquids, being used a very small amount of ILs, leads to a decreasing of the capital and operating costs and make it easy to scale up.

Publications mentioning the project to the Acknowledgements sections:

1. Maranescu B, Visa A. Applications of Metal-Organic Frameworks as Drug Delivery Systems. *International Journal of Molecular Sciences*, 2022; 23(8):4458 (I.F.=5.6)
2. Marganovici, M.; Maranescu, B.; Visa, A.; Lupa, L.; Hulka, I.; Chiriac, V.; Ilia, G. Hybrid Coordination Networks for Removal of Pollutants from Wastewater. Int. J. Mol. Sci. 2022, 23, 12611. (I.F.=5.6)
3. Plesu N., Maranescu B., Mihali M., Visa A., The electrochemical oxidation of spent metal organic framework impregnated with ionic liquid, phenol degradation, *J. Compos. Sci.*, 2023, *accepted in 05.12.2023* (I.F= 3.3)
4. Ardelean R., Popa A., Visa A., Dragan E.S., Davidescu C.M., Synthesis, characterization and applications of copolymers functionalized with aminophosphinic acid pendant groups as high performance adsorbents for acetylsalicylic acid, *Polym. Bull.,* 2023, *under review,* manuscript nr. POBU-D-23-01104 (I.F.=3.2)
5. Lupa L., Tolea N., Iosivoni M., Maranescu B., Plesu N., Visa A., Performance of ionic liquid functionalized metal organic frameworks in the adsorption process of phenol derivatives, *RSC Advences*, 2023, under review, manuscript nr.: RA-ART-11-2023-008024 (I.F.= 3.9)

Book charter:

Visa A., Plesu N., Ilia G., Maranescu B., (Q)SAR methods used in MOFs studies, in Springer Handbook of Chem- and Bioinformatics edited by Jerzy Leszczynski, 2023 *under review*

Conference participation

Oral presentations:
2022

1. **Visa A.,** Maranescu B., Popa A., Lupa L., Metal organic frameworks: from green synthesis to green applications, **Conferinta Nationala de Chimie, Editia XXXXVI**, 4-7 Octombrie 2022, Calimanesti-Caciulta, Romania
2. **Plesu N.,** Maranescu B., Macarie L., Visa A.,Anticorrosive effect of phosphonate metal organic frameworks on mild steel, **Conferinta Nationala de Chimie, Editia XXXXVI,** 4-7 Octombrie 2022, Calimanesti-Caciulta, Romania
3. **Visa A**., Maranescu B., Lupa L., Ionic Liquids-modified Metal Organic Frameworks: Preparation and Application in Adsorption, **9th IUPAC International Conference on Green Chemistry (9th ICGC**), 5-9 September 2022, in Athens, Greece O-144, pag. 335
4. **Visa A**., Metal Organic Frameworks: Diversity in Structure and Green Applications, **14th Green Chemistry Postgraduate Summer School**, 3-9 July 2022, Venetia, Italia, pag 43 – **invited speaker**

2023

5. Visa A., Maranescu B., Plesu N., Lupa L., Greener alternatives for phosphonate Metal Organic Frameworks synthesis, ***Smart Diaspora 2023***, 10-13 Aprilie 2023, Timisoara, Romania, O-26
6. Visa A., Maranescu B., Lupa L., Metal(II) coordination polymers based on bisphosphonates or mixed imidazole ligands and bisphosphonates: green syntheses and applications,***8th International Workshop of Materials Physics***, ***Book of Abstracts,*** 17-19 Mai 2023, Magurele, Romania, O-10, pag. 32
7. Visa A., Greener Alternatives for Phosphonate Metal-Organic Frameworks Synthesis and Applications, ***15th Green Chemistry Postgraduate Summer School,*** 2-7 Iulie **2023**, Venetia, Italia **invited speaker**
8. Plesu N., Maranescu B., Visa A., The electrochemical oxidation of spent metal framework impregnated with ionic liquid, phenol degradation, ***4th International Conference on Phosphonate Chemistry, Science and Technology, ICOPHOS-4,*** 2-4 of October **2023**, Heraklion, Crete, Greece, Lecture 19
9. Visa A., Iosivoni M., Maranescu B., Lupa L., Green Alternative Approaches to the Synthesis of Metal Organic Frameworks, ***4th International Conference on Phosphonate Chemistry, Science and Technology***, ***ICOPHOS-4,*** 2-4 of October **2023**, Heraklion, Crete, Greece, Lecture Lecture 4

Poster presentation:

2022

1. Visa A., Plesu N., Macarie L., Popa A., One-step solvent-free mechanochemical synthesis of metal chitosan powder, **Conferinta Nationala de Chimie, Editia XXXXVI,** 4-7 Octombrie 2022, Calimanesti-Caciulta, Romania

2023

2. Iosivoni M. Maranescu B., Visa A., Phosphonate metal organic frameworks as environmentally friendly adsorbent materials, ***New trends in Chemistry Research, Book of Abstracts*** Editia a 15-a, 21-22 Octombrie 2023**,** pag. 83
3. Visa A., Maranescu B., Lupa L., Green Alternatives for Synthesis of Metal Organic Frameworks, ***49th IUPAC World Chemistry Congress*****,** ***Book of Abstracts,*** 20-25 August 2023, Haga, Olanda, pag. 737
4. Maranescu B., Visa A., Lupa L., Heterogeneous catalyst based on vinyl phosphonate in sustainable syntheses, ***8th International Workshop of Materials Physics***, ***Book of Abstracts,*** 17-19 Mai 2023, Magurele, Romania, P5, pag 81

Event disemination:

European Researcher Night, 30 September **2022,** Nokia Campus, Timisoara
European Researcher Night, 29 September **2023,** Nokia Campus, Timisoara

Training of human resources in the project

To integrate young researchers in the team and to support/train them in research careers:
PhD students: Drd. Samuel Tolea;
Master students: Iosivoni Marcela; Buftea-Bercea Giulia Roberta; Cojocaru Monica-Adriana

Drd. Samuel TOLEA - completion of doctoral thesis entitled *Chemically modified materials with ionic liquids applied in wastewater treatment*, date of defense 21 September 2023

Preparation of dissertation in cotutelle:

1. Dissertation title: M Phosphonic organic metal networks as environmentally friendly adsorbent materials; Student: Iosivoni Marcela-Georgiana; Coordinators: dr. Bianca Maranescu (UVT)/dr. Aurelia Visa (ICT)
2. Dissertation title: Mechanochemistry, an alternative method for the synthesis of metal-organic networks; Student: Buftea-Bercea Giulia Roberta; Coordinators: dr. Bianca Maranescu (UVT)/dr. Aurelia Visa (ICT)
3. Dissertation Title: Metal organic networks: heterogeneous catalysts for methylation reaction; Student: Cojocaru Monica-Adriana; Coordinators: dr. Bianca Maranescu (UVT)/dr. Aurelia Visa (ICT)

Progress Reports:
Stage I: May - December 2022
Stage II: January-December 2023

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