

## Project Details

<b>Final Registration Code</b>	PN-III-P1-1.1-TE-2019-1534
<b>Project Title (Romanian)</b>	Noi materiale multifuncționale bazate pe lantanide
<b>Project Title (English)</b>	New Lanthanide-based Multifunctional Materials
<b>Project Acronym</b>	LantMat
<b>Contracting Authority</b>	UEFISCDI
<b>Project Host Institution</b>	University of Bucharest
<b>Project Duration / Run Period</b>	24 Months / 21.10.2020 - 20.10.2022
<b>Total Funding</b>	431.900,00 lei

## Project Summary

The progress of a technology-driven society requires the development of materials with enhanced capabilities and new properties. Among alternatives, heterometallic coordination polymers are one interesting candidate not only because they exhibit various and interesting structures, but also for their potential applications as state-of-the-art materials in magnetism, catalysis, sensors, ion exchange, fluorescent lamps, or electroluminescent devices.

The advantage of heterometallic frameworks over their single-metal counterparts arises from synergetic properties evolving from having lanthanides and transition metal ions close together; this may generate novel multifunctional materials with properties which could not be obtained in homometallic systems.

Heterometallic coordination polymers with targeted properties should contain two components:

- (a) a new 3d-4f heteronuclear node, as the carrier of the desired magnetic, chiral, or luminescent properties;
- (b) a spacer with tunnable size and properties.

## Project Summary

As most previously described 3d-4f systems focus on the magnetic exchange interaction in the  $\text{Cu}^{\text{II}}\text{-Ln}^{\text{III}}$  pair, with rare examples for  $\text{Ni}^{\text{II}}\text{-Ln}^{\text{III}}$  pair, we will try to design, obtain and characterize new heterometallic nodes containing scarcely studied  $\text{V}^{\text{IV}}\text{O-Ln}^{\text{III}}$ ,  $\text{Cr}^{\text{III}}\text{-Ln}^{\text{III}}$ ,  $\text{Mn}^{\text{II/III}}\text{-Ln}^{\text{III}}$ , and  $\text{Fe}^{\text{II/III}}\text{-Ln}^{\text{III}}$  pairs, in order to elucidate the nature of 3d-4f magnetic exchange interactions within them.

Another element of novelty arises from the study of rarely studied 3d-4f systems containing a trivalent 3d metal ion ( $\text{Cr}^{\text{III}}$ ,  $\text{Mn}^{\text{III}}$ , or  $\text{Fe}^{\text{III}}$ ). Once the 3d-4f molecular magnets, chiral, or luminescent compounds are obtained, we will connect them, using various organic spacers and metalloligands, into heterometallic coordination polymers in order to increase their stability and enhance their properties. For  $\text{Gd}^{\text{III}}$  derivatives, magnetic refrigerants may be obtained using this strategy.

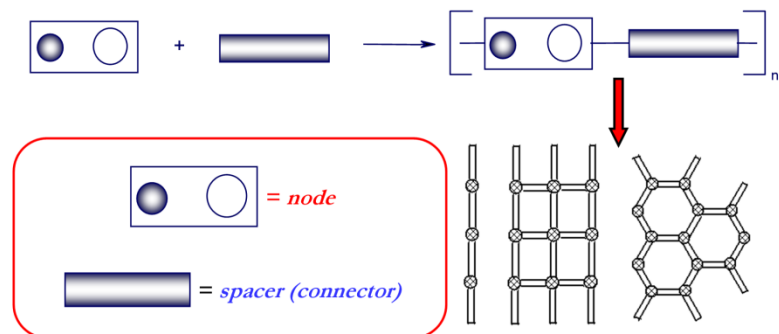


Illustration of the “*node and spacer*” approach

# Project Summary

The objectives of the project are:

(I) the synthesis of novel 3d-4f heteronuclear complexes containing: (a)  $V^{IV}$ - $Ln^{III}$ ,  $Cr^{III}$ - $Ln^{III}$ ,  $Mn^{II/III}$ - $Ln^{III}$ , or  $Fe^{II/III}$ - $Ln^{III}$  pairs, if magnetic properties are targeted; (b)  $Zn^{II}$ - $Ln^{III}$  or  $Cd^{II}$ - $Ln^{III}$  pairs when luminescent properties are desired. Once the new complexes are obtained and structurally characterized, their magnetic and luminescent properties will be investigated and analyzed in order to improve the design with the aim of enhancing their properties.

(II) the synthesis of coordination polymers using as nodes the previously synthesized 3d-4f heteronuclear complexes and as linkers various organic spacers or metalloligands. The design of coordination polymers with various network topologies is based on Robson's highly efficient "node and spacer" approach, which usually yields the desired solid-state architecture.

Magnetic and luminescent properties of the novel compounds will be tested and results will be disseminated through papers in leading journals, as well as oral or poster communications in international conferences in the field.

# The Implementation Degree of the Project

**Phase I / 2020 (20.10.2020 - 31.12.2020):** Synthesis and characterization of new heteronuclear 3d-4f complexes.

**Activity 1.1.** Synthesis of different classes of new *building-blocks*

New complexes will be synthesized using transition metal ions ( $V^{IV}O$ ,  $Cr^{III}$ ,  $Mn^{II/III}$ ,  $Fe^{II}/Fe^{III}$ ,  $Co^{II}/Co^{III}$ ,  $Ni^{II}$ ,  $Cu^{II}$ ,  $Zn^{II}$ ,  $Cd^{II}$ ) and lanthanide ions and Schiff or Mannich bases as ligands.

**Deliverables**

Phase report

# The Implementation Degree of the Project

**Phase II / 2021 (01.01.2021 - 31.12.2021):** Synthesis and characterization of the new 3d-4f complexes to be used as nodes and of metalloligands to be used as spacers (part two). Synthesis and characterization of new coordination polymers based on the previously synthesized molecules.

**Activity 2.1.** Synthesis of different classes of new *building-blocks* (part two)

**Activity 2.2.** Structural characterization of the new 3d-4f/4d-4f *building-blocks* and evaluation of their magnetic and luminescent properties

**Activity 2.3.** Synthesis of new coordination polymers using 3d-4f *nodes*.

## Deliverables

Phase report

Project site

Scientific papers and communications

# The Implementation Degree of the Project

**Phase III / 2022 (01.01.2022 - 20.10.2022):** Synthesis of new coordination polymers using 3d-4f *nodes* (part two).

**Activity 3.1.** Synthesis of new coordination polymers using 3d-4f *nodes*. (part two)

**Activity 3.2.** Investigation of magnetic and luminescent properties of the new complexes

**Activity 3.3.** Analysis of the properties and structure of the new complexes and dissemination of the scientific results.

## **Deliverables**

Phase report

Update of the project site

Scientific papers and communications