



UNIVERSITATEA DIN
BUCUREȘTI
VIRTUTE ET SAPIENTIA



Universitatea Babeș-Bolyai
Cluj-Napoca

FUNCTIONALIZED HIERARCHICAL STRUCTURES ON GRAPHENE EXHIBITING MAGNETIC, ADSORPTION AND CATALYTIC PROPERTIES

Financial support: UEFISCDI



UNITATEA EXECUTIVA
PENTRU FINANTAREA
INVATAMANTULUI
SUPERIOR, A CERCETARII
DEZVOLTARII SI INOVARII

Project Code: *PN-III-P4-ID-PCCF-2016-0088* (1 din 01/07/2018)

Project timespan: 1.07.2018 – 30.06.2022

Partners and Management

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Leader: Acad. Cristian Silvestru

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Project Teams

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Project Budget

No.	BUDGET CHAPTER (EXPENSES)	2018 (lei)	2019 (lei)	2020 (lei)	2021 (lei)	2022 (lei)	TOTAL (lei)
1	SALARIES	307.500	670.000	985.000	1.235.000	387.500	3.585.000
2	INVENTORY	343.240	2.340.000	277.500	268.000	136.760	3.365.500
3	MOBILITY	45.000	99.000	99.000	40.000	30.000	313.000
4	OVERHEAD	148.935	251.000	324.750	373.250	138.565	1.236.500
	TOTAL BUDGET	844.675	3.360.000	1.686.250	1.916.250	692.825	8.500.000

Abstract

The present research proposal aims to develop a series of directions which are less or non-explored to date in the chemistry of graphene. Its objectives rely on the experience of the four participants in organic synthesis, organometallic chemistry, molecular magnetism and catalysis. The project will stimulate not only the enhancement of the value of previously synthesized compounds by the partners, but also the development of an original chemistry. The hierarchical organization of organometallic – classical transition metal complexes on graphene surface is a step forward in materials science. The design of 3-D frameworks incorporating graphene is original and opens interesting perspectives for applications. The grafting of magnetic and luminescent complexes on graphene could bring an important added value in molecular magnetism. The catalytic processes to be investigated are carefully selected, in order to address important problems in organic synthesis, environmental protection and energy. The project will focus on the following major objectives: (i) design of networks by covalent connections between the decorated graphene sheets; (ii) design of graphene-based hybrid materials with appropriate organometallic/metalloid units as ligands for transition metals; (iii) single molecule magnets and luminescent molecules grafted on graphene; (iv) functionalization of graphene with macrocycles, cryptands and rotaxanes for organocatalytic reactions; (v) development of multifunctional catalysts for controlled cascade reactions; (v) applications in catalysis (the valorization of the CO₂ emissions; the hydrogenation of nitro-alkenes and mixtures of acetylene-ethylene; C-C and C-N coupling reactions) and gas sorption. A special attention in these studies will be addressed to the investigation of the catalytic mechanisms.

Objectives

The main objectives of the present project are:

O1. Assembling hierarchically organized architectures incorporating graphenes.

O2. Exploring graphene-grafted SMMs and luminescent molecules.

O3. Gas storage and gases separation with rational designed hierarchical architectures.

O4. Investigation of the newly designed hierarchical (supra)molecular architectures grafted onto graphenes in catalysis.

Dissemination of Results - 2018

Conferences

1. *Sinteza și caracterizarea de noi compuși organometalici ai stibiului(III) și bismutului(III) de tipul $[2-(GF^*)C_6H_4]_nMX_{3-n}$ ($M = Sb, Bi; n = 1-3; GF^* = -CH=O, -CH=NCH_2C_6H_4N-2', -CH=NCH_2C_6H_4N-4'$), F.-A. Adăscăliței, C. Silvestru, la Conferința Școlilor Doctorale din Consorțiul Universitaria, Căciulata, Octombrie 31 - Noiembrie 3, **2018** (oral presentation).*

2. *New hypercoordinated diorganotin(IV) with dithiocarbamate or tetraorganodichalcogenimidodiphosphinato ligands, E. Denes, N. Chiorean, A. Silvestru, A XXXVII-a Conferință Națională de Chimie, Căciulata, Octombrie 2-5, **2018** (poster).*

Dissemination of Results - 2018

Conferences

3. *Synthetic "host molecules", mechanically interlocked and self assembled architectures: from design to applications*, Ion Grosu, A XXXVII-a Conferință Națională de Chimie, Căciulata, Octombrie 2-5, **2018** (plenary lecture).

4. *New pyridine/hydroquinone based [2]rotaxanes: synthesis of the building blocks* Teodor-Aurelian Cucuiet, Cătălin Anghel, Niculina D. Hădade, Ion Grosu, A XXXVII-a Conferință Națională de Chimie, Căciulata, Octombrie 2-5, **2018** (poster).

5. *Conformational versatility of a new macrocycle based on 1,3-dioxane units*, Alexandra Bogdan, Andreea Pentronela Crișan, Ionuț-Tudor Moraru, Ion Grosu, A XXXVII-a Conferință Națională de Chimie, Căciulata, Octombrie 2-5, **2018** (poster).