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

Financial support: UEFISCDI

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Project timespan: 1.07.2018 – 30.06.2022
Partners and Management

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# Project Teams

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- MS student Sabina Vieriu
- MS student Corina Stoian
## Project Budget

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<th>No.</th>
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<th>2021 (lei)</th>
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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.
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 Universitară, Căciulata, Octombrie 31 - Noiembrie 3, 2018 (oral presentation).

2. New hypercoordinated diorganotin(IV) with dithiocarbamato or tetraorganodichalcogenimidodiphosphinatoligands, E. Denes, N. Chiorean, A. Silvestru, A XXXVII-a Conferință Națională de Chimie, Căciulata, Octombrie 2-5, 2018 (poster).
Dissemination of Results - 2018

Conferences


Dissemination of Results - 2019

Articles


Dissemination of Results - 2019

Articles


Dissemination of Results - 2019

Conferences


Dissemination of Results - 2019

Conferences

4. Novel $\text{[Zn}^{\text{II}}\text{Ln}^{\text{III}}] \text{ luminiscent coordination compounds deposited of graphene}$, A.A. Apostol, T. Mocanu, C. Maxim, I. Mihalache, O. Tutunaru, C. Pachiu, M. Andruh, Romanian International Conference on Chemistry and Chemical Engineering, ediția a 21-a, Constanța - Mamaia, 4-7 septembrie 2019. (poster)

5. Combinații complexe $\text{[Zn}^{\text{II}}\text{Ln}^{\text{III}}] \text{ atașate pe suport de grafenă}$, A. Apostol, T. Mocanu, C. Maxim, I. Mihalache, O. Tutunaru, C. Romanițan, C. Pachiu, M. Andruh, Conferința Naționala a Doctoranzilor din Consorțiu Universitaria, ediția a 2-a, Timișoara, 11-14 noiembrie 2019. (prezentare orală)

Conferences


10. Supramolecular architectures supported by catemers of 2,7-dipyridylfluorene with ortho-, meta- or para- diiodotetrafluorobenzene isomers, Lidia Pop, Ioana G. Grosu, Maria Miclăuș, Niculina D. Hădade, Anamaria Terec, Attila Bende, Ion Grosu, 21st European Symposium on Organic Chemistry, July 14th-18th, 2019, Vienna, Austria. (poster)


14. **Towards the synthesis of new NDI-based shape persistent macrocycles**
Cyril Nicolay, Cătălin Anghel, Ion Grosu, Niculina D. Hădade, International Conference „Students for Students” Cluj-Napoca, 3-7 aprilie 2019, poster

15. **Heterocyclic diorganopnicogen compounds. Synthesis, structure and catalysis**, Anca Silvestru, Răzvan Şuteu, Ana Maria Toma, la 9th International Conference of the Chemical Societies of the South-East European Countries, Târgoviște, România, 8-11 Mai, **2019** (prezentare orală).


Conferences

19. **Main Group heavy metal compounds containing tetraphenylimidodiselenodiphosphinato ligands**, Cristian Silvestru, 14th International Conference on the Chemistry of Selenium and Tellurium, Santa Margherita di Pula (CA), Italia, 3-7 Iunie, 2019 (prezentare orală).

20. **New hypercoordinated triorganotellurium compounds with organophosphorus ligands**, Eleonora Denes, Anca Silvestru, la 14th International Conference on the Chemistry of Selenium and Tellurium, Santa Margherita di Pula (CA), Italia, 3-7 Iunie, 2019 (poster).

Dissemination of Results - 2019

22. Graphene film-supported oriented antimonium nanoplatelets as very efficient catalysts for Michael and Henry additions, CHAOS.V.I. Pârvulescu, (C-H Activation in Organic Synthesis) 6th Workshop, 3-5 April, 2019, Ayia Napa, Cyprus


24. The direct catalytic synthesis of dicarboxylic acids from glucose, N. Candu, M. El Fergani, A. Tirsoaga, V.I. Parvulescu, S. M. Coman, 8th Asia Pacific Congress in Catalysis (APCAT8), 4–7th August 2019, Bangkok, Thailand