Research Projects For Young Research Teams

PNII-RU-TE-2012-3-0390 (contract no. 13/26.04.2013)

Rationally designed coordination polymers as precursors for oxide nanomaterials

Project timespan: 1.05.2013 - 30.09.2016

Project Leader:
Dr. Carmen Stefanescu (Paraschiv)
Project Summary

The main goal of the present proposal is to open a new interdisciplinary research direction and to build a team of experts in both fundamental and applicative research.

We aim to develop rational synthetic strategies leading to novel metallosupramolecular architectures with pre-established structures by linking homonuclear alkoxo-bridged Zn(II) nodes into lattices with polycarboxylate and/or divergent N-donor ligands. These will be further used for the preparation of nanosized ZnO materials.

The physico-chemical properties of both precursors and ZnO particles will be investigated.

The interdisciplinary interaction of scientists with expertise in diverse areas (metallosupramolecular chemistry, synthesis of materials, materials characterization, and physics) will provide a better insight into the properties of the obtained systems.
Main objectives

- to design and synthesize new metallosupramolecular architectures
- to investigate the possibility of reassembling the obtained systems by solvothermal treatment in order to obtain new network topologies
- to develop protocols for the preparation of nanosized ZnO materials from the newly synthesized compounds and to check their physico-chemical properties
- to establish coordination polymers structural characteristics – synthetic methods – oxide features correlations
- to investigate the parameters governing the thermal, pressure and light induced properties of compounds and search for potential applications
**Methodology**

- **Zn source**
- **Aminoalcohol**
- **Zn(II) alkoxo-bridged node**
- **Zn(II) coordination polymer**
- **Solvothermal treatment / Calcination**
- **ZnO**

**Ligands**

- **Anionic polycarboxylic ligands**
  - ![Polycarboxylic Ligands](image)
- **Anionic pyridinecarboxylate ligands**
  - ![Pyridinecarboxylate Ligands](image)
- **Neutral N-donor ligands**
  - ![N-donor Ligands](image)
Main research facilities

National Institute for R&D in Electrical Engineering
ICPE-CA

Bruker TENSOR 27
FTIR Spectrometer

Memmert Humidity chamber HCP108

Bruker D8 ADVANCE Diffractometer

FESEM-FIB Workstation Auriga
Carl Zeiss SMT

Simultaneous thermal analysis
Netzsch STA 409 PC Luxx®
Main research facilities

University of Bucharest, Faculty of Chemistry

STOE IPDS II X-ray diffractometer on single-crystals

EuroVector EA3000 CHNS-O Elemental Analyzer

Institute of Physical Chemistry “Ilie Murgulescu”, Romanian Academy

JASCO FP-8300 Spectrofluorimeter
Research team

Project leader:
Dr. Carmen-Alina STEFANESCU (PARASCHIV), Senior researcher III, National Institute for R&D in Electrical Engineering ICPE-CA

Team members:

1. Dr. Andrei CUCOS                   Senior researcher III, National Institute for R&D in Electrical Engineering ICPE-CA
2. Dr. Gabriela HRISTEA              Senior researcher I, National Institute for R&D in Electrical Engineering ICPE-CA
3. Dr. Beatrice-Gabriela SBARCEA     Researcher, National Institute for R&D in Electrical Engineering ICPE-CA
4. Dr. Diana-Beatrice VISINESCU      Senior researcher II, Institute of Physical Chemistry “Ilie Murgulescu”, Romanian Academy
5. Dr. Catalin MAXIM                 Senior researcher III, University of Bucharest, Faculty of Chemistry
6. Teodora MOCANU                    Ph.D. student, University of Bucharest, Faculty of Chemistry*
7. Eng. Laura-Ileana CHIOSE          Technician, National Institute for R&D in Electrical Engineering ICPE-CA

*The Ph.D. student follows Ph.D. programs of the University of Bucharest. Her experience in the synthesis, crystallization and characterization of alkoxo-bridged systems is very useful for the project.
1. ZnO nanoparticles obtained by wet chemical methods, Carmen Paraschiv, Gabriela Hristea, Gabriela Sbarcea, E-MRS Fall 2013, 16-20 september 2013, Warsaw, Poland

2. Structural and optical properties of doped Zinc Oxide thin films, Beatrice – Gabriela Sbarcea, Carmen Paraschiv, Jenica Neamtu, Sorina Mitrea, E-MRS Fall 2013, 16-20 september 2013, Warsaw, Poland


3. Polycarboxylate-assisted synthesis of ZnO nanoparticles, Carmen Paraschiv, Andrei Cucos, Gabriela Sbarcea, Delia Patroi, Virgil Marinescu, 5th EUCHEMS Chemistry Congress, 31st August – 4th September 2014, Istanbul, Turkey (poster)


5. Alternative approaches for ZnO-graphene nanocomposites designed for supercapacitors, Gabriela Hristea, Carmen Paraschiv, Mihai Iordoc, 5th EUCHEMS Chemistry Congress, 31st August – 4th September 2014, Istanbul, Turkey (poster)


5. Synthesis, structure, TG+FTIR analysis and solid-state conversion to ZnO of new coordination compounds constructed from Zn(II), Bis-Tris and divergent N-donor ligands, Andrei Cucos, Carmen Paraschiv, Gabriela Sbarcea, Catalin Maxim, Virgil Marinescu, Sergiu Shova, 3rd Central and Eastern European Conference on Thermal Analysis and Calorimetry (CEEC-TAC3), 25 – 29 August 2015, Ljubljana, Slovenia (poster)

6. Synthesis and characterization of new Zn(II) extended structures based on amino-alcohols and polycarboxylic acids, Carmen Paraschiv, Andrei Cucos, Sergiu Shova, Diana Visinescu, 19th Romanian International Conference on Chemistry and Chemical Engineering” (RICCCE 19), 2 – 5 September 2015, Sibiu, Romania (poster)

7. Synthesis and characterization of new Zn(II) coordination compounds constructed from Bis-Tris and divergent N-donor ligands, Andrei Cucos, Carmen Paraschiv, Catalin Maxim, Sergiu Shova, 19th Romanian International Conference on Chemistry and Chemical Engineering” (RICCCE 19), 2 – 5 September 2015, Sibiu, Romania (poster)

Conferences - 2016

1. Coupled TG+FTIR analysis and conversion to ZnO of new coordination compounds constructed from Zn(II), amino-alcohols and divergent N-donor ligands, Cucos A., Paraschiv C., Sbarcea G., Marinescu V., Shova S., Maxim C., XV Russian and International Conference on Thermal Analysis and Calorimetry (RTAC-2016), 19 – 23 September 2016, Sankt-Petersburg, Rusia (poster)


