
**ROMANIAN ACADEMY**
**INSTITUTE OF PHYSICAL CHEMISTRY "I.G. Murgulescu"**

# *Laboratory of Chemical Thermodynamics*

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# The Characterization of Micro- and Nanostructured Multifunctional Materials Based on a Complex Thermodynamic Approach

***Mode of preparation***

The biographic story

***Properties***

**The Chemical Thermodynamics is a powerful tool in understanding the energy changes involved in the chemical and/or physical phenomena**

•Subtle changes in the energetic parameters
•Nanostructure in relation to defect thermodynamics

The evolution of the properties of materials in use

# Experimental Techniques for Thermodynamic Measurements

## Calorimetry

Total molar quantities

- Heats of reaction
- Heats capacities
- Heats of transformation

## Electrochemical techniques

Standard thermodynamic data of formation

- Energies
- Enthalpies
- Entropies

Partial molar quantities

+

- Chemical Potentials
- Thermodynamic Activities
- Partial Pressures

## Gas Equilibration

Partial molar quantities

- Energies
- Enthalpies
- Entropies

**Redox titration for determination of the average oxidation state in mixed - valence compounds**

- Mn average valence in complex La-Mn perovskites
- Correlation with the oxygen stoichiometry

# OUTCOMES

*The understanding of the property dependence on compositional variables: the key to enable optimization and full exploitation of multifunctional materials*

*A careful evaluation of the trade-off between structure, the grain size (method of preparation), thermodynamic stability*

*The effect of nonstoichiometry in relation to the oxygen vacancies formation in nano and micromaterials*

Correlation between the structural, electrical thermodynamic, and kinetic properties

The defect energies connected with the nanocrystalline state

The oxygen nonstoichiometry in relation to oxygen vacancies formation and the defect thermodynamics

# TASKS

⇒**The grain size effect (micro-, nanostructure) and the influence of the method of preparation on the energetic parameters:**

- **Comparative study of the thermodynamic data in nano- and microstructured compounds**

⇒**The influence of different compositional variables on the thermodynamic properties of micro and nanostructured multifunctional oxide systems:**

- **The influence of the dopants**
- **The effect of the oxygen stoichiometry change in relation to the oxygen vacancies formation**
- **The effect of the global stoichiometry change**

# Laboratory of Chemical Thermodynamics

REFERENCES (selection):


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INTERNATIONAL PROJECTS:

✈Participant in EU project on ***"Improving the understanding of the impact of nanoparticles on human health and the environment"***, ImPart CA, Programme: Priority 3 – NMP, 2005-2007

✈Scientific cooperation with ETH Zürich, Department of Materials - Institute of Nonmetallic Materials, Thermodynamic Group, Switzerland concerning ***"The thermochemical properties of the compounds in the La-Sr-Mn-O system"***. Agreement on the scientific collaboration 2001-2005.

✈Scientific cooperation with the Institute of Metallurgy and Materials Science "Aleksander Krupkowski" of the Polish Academy of Sciences, Laboratory of Physical Chemistry concerning **"*The investigation of the influence of phase nonstoichiometry on phase equilibria in Mn-Eu-O system"***. JRC Project 2003-2005

✈Romania - Bulgaria bilateral academic cooperation, ***"Optimization of Hydrogen and Oxygen Electrodes for Proton Exchange Membrane Fuel Cell's Application"*** *JRC Project, beginning with 01.01.2005*

✈Participant (Nov.2004 - June2005) in EU COST Action 525: Advanced Electroceramics: Grain Boundary Engineering, the Project **"*Structural and dielectric studies of incipient ferroelectrics"***

✈Participant in EU "Joule II Programme", Sub-Programme "Energy Conservation and Utilisation" (Contract JOU 2-CT 92-0063 ***"New SOFC Materials and Technology"*****,** (Contract JOU 2-CT 92-0063 ***"New SOFC Materials and Technology"***, 1993-1995

✈The 695/RB(1969-1972) contract with IAEA-Vienna ***"Thermodynamic properties of the uranium oxides***".

# FP 6 EU Programme: Priority 3 – NMP, project on ***"Improving the understanding of the impact of nanoparticles on human health and the environment"***, ImPart CA, 2005-2007

**PROJECT OBJECTIVES:**

To prevent knowledge of the health and environmental implications of nanoparticles from lagging behind the technological advances. In order to do this, ImPart will foster communication links between numbers of regional, national and international initiatives in order to reduce duplication of effort, pool expertise and facilitate co-operation between networks. This will result in an improvement in the understanding of the potential impact of nanoparticles on human health and the environment.

**LIST OF PARTICIPANTS:**

**Chalex Research Ltd. (UK), NFM (IL), Institute of Physical Chemistry "I.G. Murgulescu" (RO), Jozef Stefan Institute (SI), University of Leicester (UK), Kaunas University (LT), University of Munich (D), Technology Codes Ltd. (IRL), University of Craiova (RO), Forschungszentrum Karlsruhe GmbH (D), Verein Deutscher Ingenieure (D), CMP Científica (E), University of Leuven (B), University of Surrey (UK), Temas (CH), Quadrate Digital Media (IRL), National Institute of Research and Development for Technical Physics (RO), Dublin Institute of Technology (IRL), Biomade Technology Foundation (NL), Latvian Society of Toxicology (LV), University of Crete (HE), Rosseter Holding Ltd. (CY).**

**ICF tasks:**

ICF **Laboratory of chemical thermodynamics** (Dr. *Speranta Tãnãsescu*) is involved in all the actions of the project having the principal goal understanding of the short and long term implications of nanotechnology for health and the environment. The contribution in the project is based on the former research experience existing in the Laboratory of Chemical Thermodynamics as concerns the large potentialities offered by the Applied Chemical Thermodynamics to characterize and investigate from the energetic point of view the advanced materials involved in the complex modern systems and the new technologies. Contribution to answer the following questions are expected:

- To what extent can the energetic properties of nanocomposites be predicted from properties of the nanoscale end-members?
- Which is the influence of different compositional variables on the nanophase energetics?
- What environments, besides the now familiar aqueous low temperature setting, are likely to harbor nanoscale phenomena, and how would thermodynamic modelling be affected?
- Which environmental factors and in what extend they are responsible for the interactions between biological and non-biological systems?
- Are the existent thermochemical databases enough comprehensible to prevent or for diminution of ecological hazards?