

SOFT COMPUTING HYBRID CONFIGURATIONS APPLIED IN CHEMISTRY

IDEI PROGRAMME PNCDI II, Research Grant ID_592, Contract no. 59/2007

This project targets the use of Artificial Intelligence Techniques (neural networks, genetic algorithms, classifiers, fuzzy systems), combined in hybrid heuristic configurations, for modeling and optimization of chemical processes. The synthesis of new materials, based on ferrocene, with liquid crystal properties is considered as a case study. The problems attempted to solve are the subject of complex interdisciplinary research, requiring advanced knowledge in both chemistry and computer science.

The project objectives are organized on two parallel plans, which correspond to the domains of computer science and chemistry. Applying the methods of Artificial Intelligence (AI) to modeling and optimization of chemical systems represents the bridge between the two fields and defines the inter-disciplinary character of our proposal.

Mainly, the scientific goals of the project are:

1) Advanced research oriented toward the elaboration and improvement of techniques based on AI instruments, with a special emphasis on hybrid soft computing techniques that provide computational efficiency and large-spectrum applicability.

2) Synthesis and characterization of ferrocene based new materials with liquid crystal properties.

3) Modeling and optimization of the parameters associated to ferrocene-based materials, making use of soft computing techniques.

Meanwhile, specific goals of the research program *Idei* are as follows:

1) Obtaining scientific achievements at the international level as the result of complex research based on real novelties ("ideas"). Solving the scientific objectives will lead to acquiring advanced knowledge, contributing to generating new scientific and technical knowledge, development and strengthening of those

research directions of scientific and technological top fields, in particular soft computing. The need for "excellency" as the quality level of the Romanian research, in agreement with the international standards, will create the true conditions for the participation in the European programs.

2) Development of the human resource, as a premise for constituting and consolidating of a working team suitable for interdisciplinary research, with both experienced and young researchers and engineers working effectively in AI and chemical synthesis of materials. Promoting young people, preparing them for research, stimulating them adequately to remain to work in research, and supporting them for the highest standards in the field, including Ph.D. degrees, signify important aspects involved within the project.

Starting from the continuous evolution of the life quality, which implies the need for new and higher characteristics of the materials, devices and real systems, the scientific research has to cope with current and future difficult problems. According to the estimated results of the project, the scientific impact of the project will be mainly evaluated by the number and quality of the published papers, related to the scientific level of the chosen journals (their ISI ranking), the quality of the edited monographs, and the scientific level of the Ph.D. theses accomplished within this project.

The social impact is associated to the fact that the project integrates young post-docs, Ph.D. and master students that can develop their talents in research and software product development. Organizing exploratory workshops and research documentation stages in Romania and abroad will represent useful opportunities for the young researchers and for the orientation of their future activity.

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