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HABILITATION THESIS ABSTRACT

Switchable structures: from molecular to supramolecular level

Domain: ***CHEMISTRY***

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This habilitation thesis presents some of the most important scientific, professional and academic achievements obtained after defending the PhD thesis, entitled "Contributions to the synthesis of organic ligands for obtaining complexes with potential liquid-crystalline properties" at the Politehnica University Timișoara, Faculty of Chemical and Environmental Engineering, on November 17, 2005, confirmed by the Order of the Ministry of Education and Research No. 5657 /12.12. 2005.

The habilitation thesis entitled "Reversible structures: from molecular to supramolecular level" has the following structure:

Part A: Summary of the thesis written in Romanian and English;

Part B: Scientific, professional and academic achievements, and future plans of scientific and academic career development;

Part C: 10 relevant scientific articles that partially illustrate the scientific achievements from the thesis.

Section B is divided into three chapters; in the first and second chapter are presented the achievements, respectively the development plans from a scientific, academic and professional point of view, and in the third chapter are presented the bibliographical references, which served me as a source of inspiration for personal research, but also my own works underlying this thesis.

The first part of Chapter B1.1 contains a brief chronological description of the reference points that were the basis of the scientific results of the thesis, some points on the thematic field of the thesis at international level with highlighting the need to design and study the reversible structures from the point of view of fundamental and applied research.

The results of scientific research are divided into two subchapters according to the two research directions, namely:

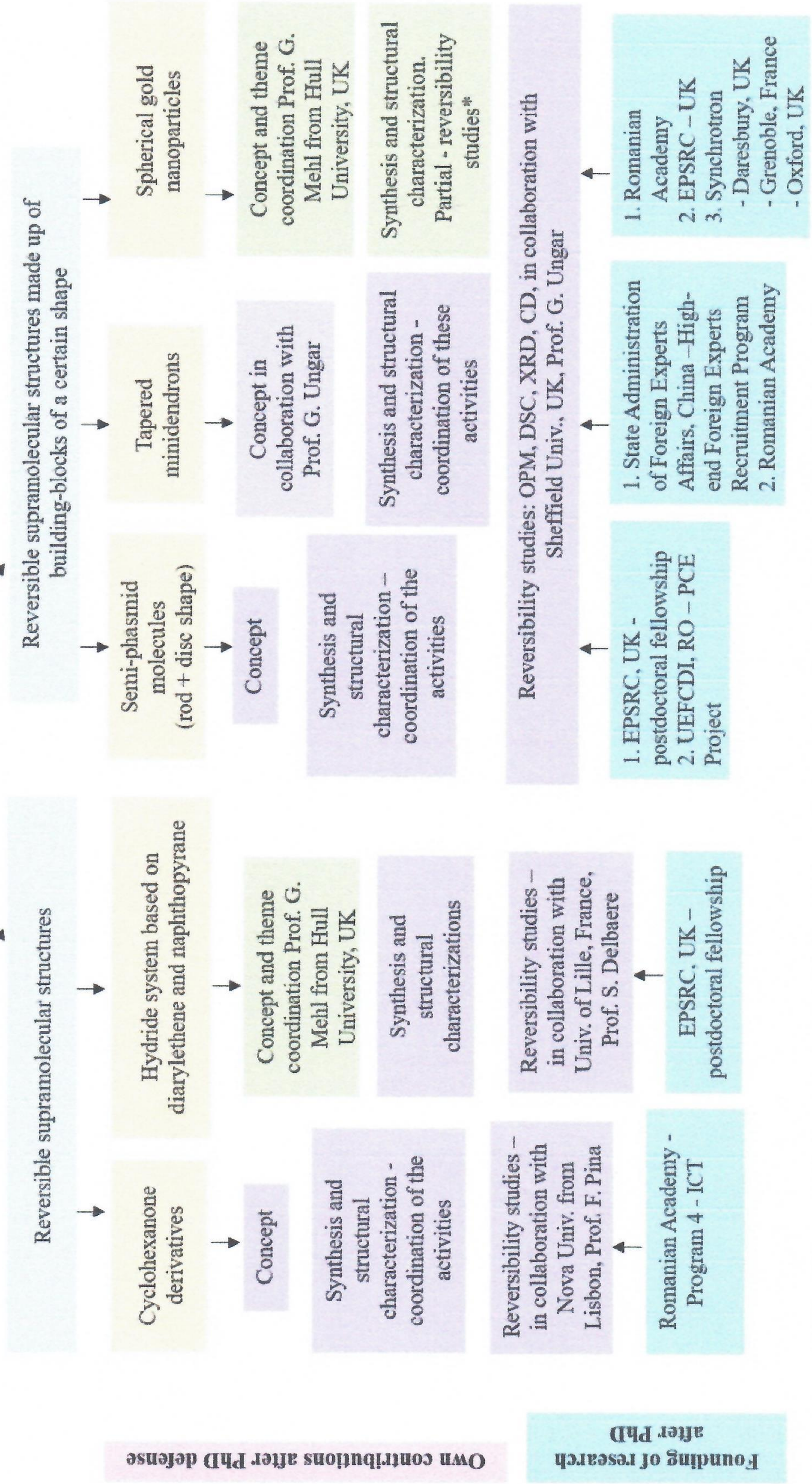
- Synthesis, characterization and investigation of molecular structures with multiple states at the molecular level, in which reversibility is achieved under the action of external stimuli (pH, light, temperature). Two types of molecular structures were studied: curcumin analogues based on cyclohexanone and a hybrid molecular system containing diarylethene and naphthopyran moieties. For all these compounds the network of chemical reactions and the reversibility parameters have been established.

- Synthesis, characterization and investigation of molecular or supermolecular structures capable of self-assembling and/or self-organization in liquid-crystalline supramolecular structures. These processes are reversible at the supramolecular level and take place with phase transitions under the action of temperature; in other words, phase transitions are accompanied by changes in the way of self-organization or self-assembly of molecules, therefore the properties of new created supramolecular structures are different from those of the initial structures. The results of this research direction are divided into three subchapters: the first subchapter is represented by spherical gold nanoparticles functionalized with rod mesogens or cholesterol; the second chapter refers to mono-taper and di-taper shapes minidendrons of 3,4,5-trialcoxi benzoic, and in the last subchapter are presented the results on semi-phasmidic molecules (mixed form).

The beginning of the description of the studies and the results obtained for each category of compounds mentioned above, contains a brief presentation of the context in which the results were obtained, their originality and their personal contribution to obtaining them, and at the end of each category of compounds are the conclusions related to the study carried out. The summary of scientific research, own contribution and collaborative relationships that have contributed to the achievement of the scientific results, as well as the sources of funding are presented schematically in following graph:

THE SUMMARY OF SCIENTIFIC RESEARCH

Reversible structures



Own contributions after PhD defense

Founding of research after PhD

* The synthesis, structural characterization and partial reversibility studies were performed during PhD thesis. The reversibility studies obtained by XRD were performed after defending the doctoral thesis. The result regarding reversibility studies obtained during the PhD and later are fully presented a better understanding, but also for the fact that these methods are complementary.

The chapter B1.2. of this thesis summarizes the most important achievements of the candidate's academic and professional activities since defending the PhD thesis, covering the period January 2006 – present. Thus, in the academic activities with respect to the following aspects are highlighted: academic teaching, coordination of diploma projects and dissertations, coordination of the Program 4 of ICT in the period 2014-2016 and coordination of one research theme within the Program 4 of ICT, covering the period January 2012-present, contributions to research infrastructure for academic activities and managerial activities carried out mainly as deputy director at ICT and Coordinator of ICT Research Program. Professional achievements during the same period are briefly presented in terms of scientific publications, coordination of research projects, research and specialization internships, presentations at national and international conferences, involvement in the organization of symposiums, conferences and workshops, membership of working bodies as an expert, awards, expert evaluator of European projects, reviewer of ISI-listed magazines in the field of expertise and membership of professional associations.

Chapter B2 succinctly presents the main directions of future scientific and academic activities. Regarding scientific activities, the two research directions will be developed, namely: (i) obtaining new reversible molecular structures by designing, synthesizing and studying molecular structures with multiple/multifunctional states; these new molecules will contain two type of reversible units (one or two photochrome units and one "halocrom" unit as chalcone); (ii) obtaining reversible structures at the supramolecular level with liquid-crystal properties, containing functional groups (fluorophore moiety). For these structures, the properties can be modulated and switched by external stimuli.

The development plan regarding the academic activity in general, the following paths are considered: integration of undergraduate and graduate students in the candidate's research team along with the new PhD students, coordination of doctoral students in order to carry out the research plan and doctoral thesis and guidance of PhD students on how to conduct an ethical research and to develop their competences in the management of a research topic. Also, on the professional development plan, I will continue to consider in the short and medium term my managerial contribution in the implementation of the RO-OPENSREEN infrastructure project won this year; and in the long-term raising funds to support the research directions that I intend to develop.