ACADEMIA ROMÂNĂ
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HABILITATION THESIS ABSTRACT

Functional materials based on d-block metal coordination complexes: luminescence and/or mesomorphism

Domain: ***CHEMISTRY***

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The present habilitation thesis presents the most relevant scientific, academic and professional results of the author after defending her PhD thesis at University of Calabria, Department of Chemistry and Physics, Laboratory of Inorganic and Coordination Chemistry, Cosenza, Italy (June 2005).

The thesis is structured in three main chapters, as follows: i) in *Chapter I* the main scientific, professional and academic results linked to the published results in the main research area of the candidate are presented, respectively *d-block metal coordination complexes with optimized optical (mesomorphic, photophysical) properties by "smart" molecular engineering*, highlighting the results obtained since she is the Head of Program 4 of "Coriolan Drăgulescu" Institute of Chemistry (ICT), Romanian Academy (January 2017); ii) *Chapter II* describes her scientific and professional development plans, whereas iii) *Chapter III* includes a list of references.

New *d*-block metal coordination complexes with luminescent and/or liquid crystalline properties were designed, synthesized and characterized following the optimization of their properties by "smart" molecular engineering and investigating the relationship molecular structure-supramolecular structure-photophysical properties in condensed phases (crystalline and/or liquid crystalline). The complexes are presented according to the central metal, *i.e.* Ag(I) (Section I.1.1), Ir(III) (Section I.1.2), Cu(I) (Section I.1.3), Zn(II) (Section I.1.4) and Pt(II) (Section I.1.5). Single crystal X-ray diffraction studies on model compounds were used to explain the molecular and supramolecular organization in condensed states. The optimisation of specific desired properties was carried out according to the applicative field proposed; more specifically two targets were followed: thermotropic luminescent low temperature metallomesogens are highly researched in electrooptics for obtaining polarized emission and water soluble luminescent *d*-block metal coordination complexes with sensitive photophysical properties for biomedical applications (theranostic agents, bioimaging, biosensing).

For the first target, liquid crystalline luminescent *d*-MCC coordination complexes were designed and obtained, their mesomorphic and photophysical properties being accurately described. For the second target, luminescent *d*-block metal coordination complexes were appropriately functionalised to give water solubility. In this ambit, the first examples of lyotropic-chromonic-like mesomorphism with bulky metal centres like Ir(III) and Ag(I) coordination complexes were reported. The luminescent properties of the Ir(III) complexes were studied in solution, liquid crystalline and condensed (powder solid or crystalline) states. Following also biomedical applications, the inclusion of luminescent Ir(III) chromophores in mesostructured silica framework, “soft” amphiphilic surfactant aqueous systems or in the silica shell of gold nanoparticles was carried out for multiple purposes: to reduce the unwanted aggregation quenching of luminescence, to increase the stability by shielding of the chromophore against chemical, thermal or photochemical degradation or to obtain hybrid nanocomposites as theranostic agents. The sensitivity of the photophysical properties of the chromophore to the molecular environment is showed to be an excellent tool to determine the position of the chromophor in the system.

In the present thesis, the current state-of-the-art in the field of luminescent *d*-block metal coordination complexes is summarized in comparison to the results of the candidate, reporting several outstanding achievements: low temperature luminescent liquid crystalline phases with sensitive properties and the first reports on lyotropic-chromonic-like mesomorphism in Ir(III) and Ag(I) coordination complexes. The latter can bring important advances in the re-definition of chromonic liquid crystals or the description of a new and original class of functional ordered dynamic *d*-block metal based materials. Moreover, the obtainment of hybrid nanoplatforms containing a highly luminescent Ir(III) complex for simultaneous cellular imaging, photodynamic and photothermal therapies of cancer, that exploits synergistically photodynamic and photothermal effects as a result of the coupling between the photophysical properties of the *d*-block metal complexes with the thermoplasmonic effect of the gold nanospheres is described.

Finally, the perspectives and future research directions that will further contribute to the scientific development of the candidate and her research group from ICT are presented in *Chapter II*. This comprises both the following of the research applicative directions described in the thesis in electrooptics and biomedical fields, using new designed strategies that will bring important and innovative developments, and extension of the research domain in inorganic chemistry related fields.