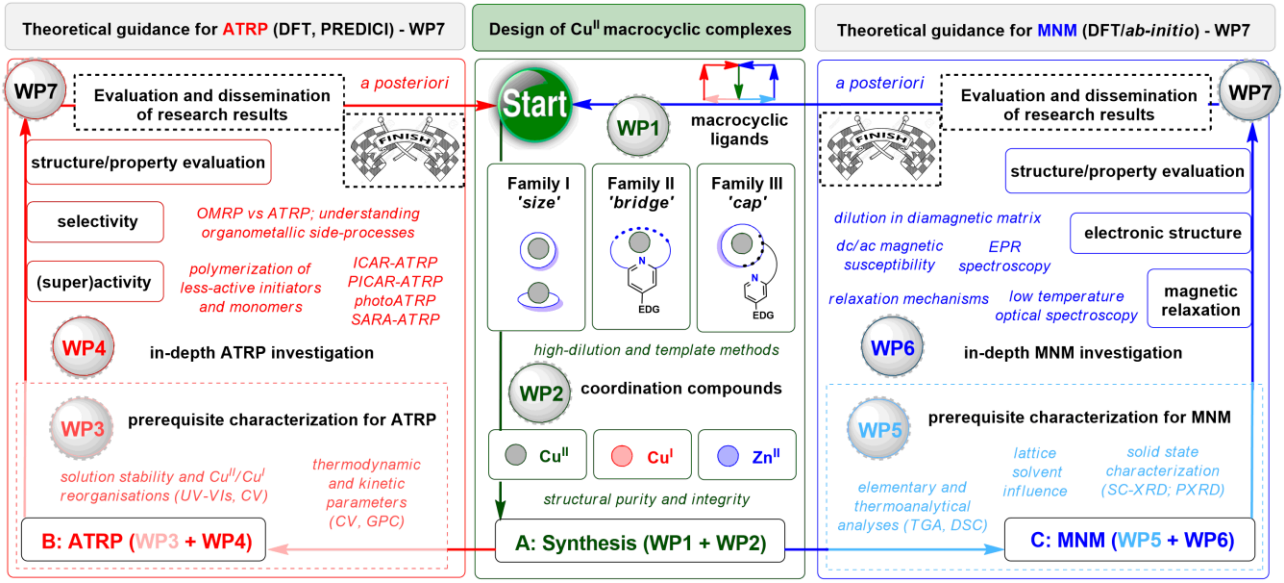
Aim of the project

The rational design and modification of molecular architectures is of prime importance for predictive generation of advanced functional materials. These in turn should find applications towards solving some of the global-nature problems, such as (but not limited to) environmental sustainability or the Big Data problem. In the present project we aim to synthesize and study a series of rationally designed copper(II) macrocyclic complexes, which are envisaged to improve our understanding of molecular nanomagnetism (MNM) as well as function as superactive Atom Transfer Radical Polymerization (ATRP) catalysts.

Concept and work plan

The work plan can be divided into seven Work Packages **(WPs)** – **each representing specific objective** – which are gathered in three structured sections **A-C**. Section **A** (green) covers ligand/complexes synthetic parts, Section **B** (red) focuses on studies related to ATRP, whereas Section **C** (blue) covers the MNM related investigation.



Please note that we introduce the concept of the "**ongoing design of new compounds**", that proceeds through the three-level functionalization method. We start from the *a priori* design of the target molecule **TM1** on the grounds of literature survey, theoretical calculations and/or existing data. Upon successful synthesis (**A:** WP1+WP2), we proceed to the prerequisite WPs from sections **B** (WP3) and **C** (WP5) to determine if **TM1** exhibits the appropriate properties/features necessary for the in-depth investigation (ATRP - WP4; MNM - WP6). This approach saves time and resources, but simultaneously increases our understanding of the structural design to ensure envisioned properties. Specifically, we can determine what hinders the positive outcome, and therefore *a posteriori* design of new target molecule **TM2** that is devoid of the drawbacks of **TM1** can be achieved. These will be ensured by theoretical guidance (DFT, *ab initio*, semiempirical methods) that is the subject of WP7, with the ultimate goal of demonstrating the ***Multifunctional character of copper(II) macrocyclic complexes in atom transfer radical polymerization) and molecular nanomagnetism.***

Anticipated results

Proposed macrocyclic ligand families will increase the robustness of the ATRP process and its versatility for the construction of various polymeric materials, but also contribute to fundamental understanding of free radical chemistry, coordination chemistry, controlled radical polymerization and catalysis. In addition, insight into the rarely studied nature of the Cu^{II}-based nanomagnets will be pursued, particularly regarding their design principles and how the spin-nuclei coupling translates into the relaxation mechanisms in these classes of compounds. As such, a multifunctional character of the planned architectures will be demonstrated and eventually they will contribute to solving some of the global challenges. The proposed activities should have significant scientific and educational impact and may additionally affect commercial production of new polymers by ATRP and accelerate The Second Quantum Revolution.