1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan)

Responsive crystals based on coordination compounds of 3d transition metals with di/tripodal N-donor ligands

1.1. **Project goals:** The project aims at revealing the mechanisms standing behind dynamics taking place in the crystal unity based on studies performed on coordination compounds of 3d transition metals with di/tripodal N-donor ligands by triggering single-crystal-to-single-crystal transformations, analyses of SCXRD data and performing solid-state supportive studies (PXRD, TGA, DSC, IR, solid-state NMR). The findings can be used later on for the preparation of sensing materials.

1.2. **Outline:** Responsive crystals, derived from coordination compounds of 3d transition metals, represent a burgeoning field at the intersection of coordination chemistry, materials science, and nanotechnology. These materials exhibit intriguing responsiveness to external stimuli, such as light, temperature, solvent, and mechanical force, leading to reversible structural transformations and changes in their properties. The responsiveness of these crystals manifests through a range of phenomena, including photochromism, thermochromism, solvatochromism, and mechanochromism. Synthetic strategies for preparing these materials range from traditional solution-based methods to more advanced techniques such as solvo-thermal synthesis. Structural characterization techniques such as X-ray crystallography, spectroscopy, and thermal analysis play crucial roles in elucidating the structure-property relationships and understanding the mechanisms underlying responsiveness in these materials. Their tunable responsiveness and multifunctionality make them promising candidates for addressing challenges in areas such as environmental monitoring, healthcare or energy storage.

1.3. **Work plan:** The work is planned for a maximum of 4 years. The first half of the year would be devoted to getting to know the subject, literature studies, getting familiar with the use of the Cambridge Structural Database and programs needed for the visualisation and analysis of crystal structures. The first year should finish with the synthesis of a range of metal complexes and their crystallisation under different conditions (synthesis and full characterisation of some of the heterocyclic ligands, if needed). Further studies can not be given a proper timeframe. Everything will depend in which direction the experiments will develop. However, they will embrace single-crystal X-ray diffraction analyses of the obtained crystalline products, solving and refining the obtained crystal structures, systematic investigation of the factors that influence the formation of particular supramolecular architectures (e.g. crystallization conditions: the effects of altering solvent, temperature), analyses of intermolecular interactions, and synthetic work to modulate the revealed sensing properties. The studies will be further supported by extended solid-state investigations by applying a range of methods such as PXRD, TGA, DSC, IR, solid-state NMR.

1.4. **Literature** *(max. 7 listed, as a suggestion for a PhD candidate preliminary study)*

1) *I. Senkovska, V. Bon, A. Mosberger, Y. Wang, S. Kaskel,* Adsorption and Separation by Flexible MOFs, *Adv. Mater.* **2025**, 2414724.

2) D. Saito, T. Galica, E. Nishibori, M. Yoshida, A. Kobayashi, M. Kato, *Reversible and Stepwise Single-Crystal-to-Single-Crystal Transformation of a Platinum(II) Complex with Vapochromic Luminescence*, *Chem. Eur. J.* 2022, *28*, e202200703.

3) J. Alen, L. Van Meervelt, W. Dehaen, L. Dobrzańska, *Solvent diffusion through a non-porous crystal 'caught in the act' and related single-crystal-to-single-crystal transformations in a cationic dinuclear Ag(I) complex*, CrystEngComm, 17, (2015), 8957-8964.

4) L. Dobrzańska, G. O. Lloyd, C. Esterhuysen, L. J. Barbour, *Guest-induced conformational switching in a single crystal*, Angew. Chem. Int. Ed., 45, (2006), 5856-5859.

1.5. **Required initial knowledge and skills of the PhD candidate**

The candidate should have a passion for lab work and be familiar with synthetic lab equipment, as well as with basic methods of compound characterisation ($^{1}H/^{13}C$ NMR in solution, MS, IR, melting point determination). Familiarity with SCXRD and PXRD will be an advantage.

1.6. Expected development of the PhD candidate's knowledge and skills

The candidate, after finalisation of this project, should be well familiar with basic organic synthesis methods, as well as metal complexation, with methods for single-crystal X-ray diffraction analysis of small molecules and techniques for solid-state characterisation: powder X-ray diffraction, thermal analysis (TGA, DSC), solid-state NMR as well as the techniques to trigger single-crystal-to-single-crystal transformations. Moreover, the candidate will have the opportunity to feel part of the research community by participating in conferences and/or workshops as well as writing papers and grant proposals.