Synthesis of transition metal oxo-complexes as precursors of functional materials (Description for the general public)

Recently, along with the dynamic progress in the field of functional material-based technologies, the development of new, effective, hence clean synthesis method of such materials is of high interest. One of the most fascinating effects of this trend is the relentless search of novel molecular precursors, which enable effective transformations in mild-conditions bottom-up processes. A real challenge is to make the direction of chemical transformations and properties of the resulting material dependent on the precursor's molecular structure. Rational precursor design also makes the syntheses closer the ideas of green chemistry, for example, by applying new solventless synthesis techniques. Considerable interest in complexes bearing a central oxo ligand is based on both their structural uniqueness as molecular building blocks of functional materials, as well as their application in catalysis. A prominent group of oxo-complexes are those involving the M₄O core. Complexes of this type are characterized by the presence of a four-coordinate oxo-centre surrounded by four metal ions placed in the vertices of a tetrahedron. In the simplest case, such a core can be stabilized by six organic anions, every of which bridging two metal cations, which results in their pointing of 6 fundamental directions (left, right, up, down, forward, backward). The involvement of scientific community in the research concerning oxo-complexes, especially those based on Zn₄O units, increased significantly after the discovery of Metal-Organic Framework (MOF) materials, which are highly promising in the context of energy storage. Nevertheless, until recently, the studies on their synthesis and properties were non-systematic, and still the lack of universal and effective preparation method is visible. One of the most prominent groups of oxo-complexes are, oxo-amidate clusters of the type $[Zn_4(\mu_4-O)(NHOCR)_6]$, which were demonstrated, developed in our group, to be excellent precursors of functional materials, but also serve as en excellent example of how by altering a reaction system precursor we can direct the transformation to obtain a completely different group of resulting materials.

Our recent studies lead to establishing of a synthesis method of oxo-zinc complexes, which was universal in terms of the used stabilizing carboxylate/amidate ligand. The primary goal of this project is the development of efficient synthesis pathways of oxo-amidate complexes also for transition metals, and their application as pre-organised molecular precursors of functional materials. Within the framework of the presented project, we plan to develop novel methods based on the use of inorganic salts as metal source instead of organometallic transition metal compounds, which are difficult to prepare and handle, we plan to use only easily-accessible inorganic salts. New oxo-metallic complexes will be synthesized by means of mild-condition synthesis (e.g. using water as substrate) in the processes, which will be as universal in terms of the used metal centre as possible. In these pioneering studies we focus on the model examples of oxo-cobalt and oxo-iron amidates, since oxo-complexes of these metals are still rarely reported, despite being very promising in terms of practical applications.

The presented project involves the evaluation of the obtained oxo-complexes as effective mildconditions precursors in the mechanochemical synthesis of MOFs and metal oxide nanoparticles. The complexes obtained within the frameworks of this project will be subjected to mechanochemical reactions in the chosen model systems. The reactions will be interesting not only because of the utilization of novel oxoamidate precursors, but also the possibly unique properties of the resulting materials. Cobalt/iron oxide nanoparticles are known as effective catalysts and nanomagnets. Also, the controlled bottom-up formation of MOFs based on Fe- and Co-based nodes was not possible until recently, and is still very uncommon. Fe-MOFs and Co-MOFs are likely to be applied as porous catalysts and redox-active materials.