DESCRIPTION FOR THE GENERAL PUBLIC

Spin-crossover (SCO) materials compose the family of switchable systems based on metal ions and organic or inorganic molecules, which are responsive to external stimuli, such as temperature or light, and reveal at least two different states differing in magnetic and other physical properties. The first state of such a material is named ″high-spin state″. It exhibits a stronger magnetic response related to the higher number of unpaired electrons in incorporated metal ions. In contrast, the second state, named ″low-spin state″, shows a weaker magnetic response due to the lower number of unpaired electrons in the inbuilt metal ions (see Scheme below). **SCO materials are based on transition metal ions, such as Fe^{2+}, Fe^{3+}, or Mn^{3+}, surrounded at the molecular level by properly designed organic or inorganic molecules, so-called ligands**. SCO materials can demonstrate the switching between a ″high-spin state″ and a ″low-spin state″ by multiple external stimuli, including temperature, light, pressure, mechanical action, electric field, and various chemicals. Moreover, the SCO effect can affect not only the magnetic signal from the material but also many other physical properties, including optical, such as the material's color or its ability to emit light (i.e., luminescence), electrical, such as electrical conductivity, or mechanical ones (e.g., change of the crystal's size). As a result, SCO materials are great candidates for multiple applications. Among them, the broadest attention is devoted to the construction of **sensors for physical or chemical stimuli** as well as to the usage of SCO materials as components of **data storage devices** as some of these materials reveal the co-existence of a ″high-spin state″ and a ″low-spin state″ at the identical conditions (so-called bistability of these two spin states) with the ability to switch between them using, e.g., light irradiation.

In this project, we will focus on the design, synthesis, and investigation of **novel spin-crossover materials** emphasizing the temperature- and pressure-induced switching of their optical properties. We aim to prepare the new generations of **thermochromic materials**, i.e., showing the changes in optical properties by temperature, and **piezochromic materials**, i.e., exhibiting the modulation of optical properties by pressure. Our primary goal is to achieve material candidates for applications in optical sensors of temperature, pressure, or both of these physical stimuli. For the specific cases of SCO materials showing the mentioned spin bistability, we will explore their potential applications in data storage. We will construct new **SCO materials by linking two ionic molecular components**: cationic SCO-active metal complexes (M1) and functionalized molecular anions, often also based on metal ions (M2). The SCO materials will first be prepared in a crystalline form, which is of significant importance for their structural characterization. Next, the temperature- and/or pressure-induced SCO effects, the related change in the magnetic signal, and the concomitant switching of optical properties will be studied. We will investigate the **thermo- and piezochromism in diverse optical properties**: (i) **linear optical properties** (whose output light intensity depends linearly on the irradiation intensity), including **light absorption** (related to color change) and **photo-luminescence** (light emission after absorption of photons), (ii) **non-linear optical properties** (whose output optical light is non-linearly dependent on the irradiation intensity), such as **second-harmonic generation** (i.e., generation of light of double frequency in comparison to the irradiation light), and (iii) **chiro-optical properties** related to the combination of chirality and optics, including **circularly polarized luminescence** (differential emission intensity of right and left circularly polarized light for enantiomeric materials). We will also attempt to prepare **multifunctional SCO materials** linking a few different properties. Best-performance materials will be processed into **thin films** that are more convenient for application in devices. Therefore, this project is focused on novel functional switchable materials with clear application horizons. However, the discovery of **new physical phenomena** arising from linking the SCO phenomenon with optical effects, along with an understanding of the related mechanism of light-matter interaction, will be of critical importance.