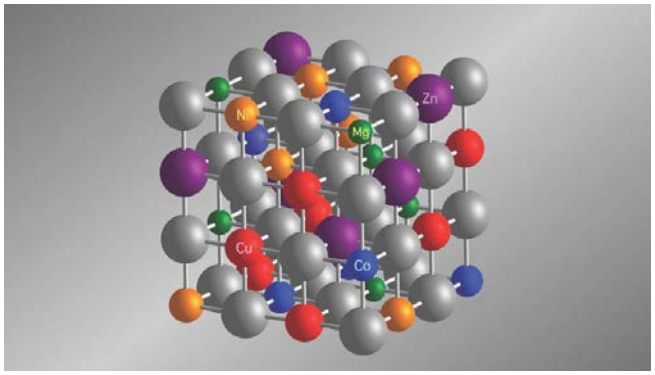
Description for the general public

Concept of materials, which structures are stabilized by high configurational entropy, has been one of the most influential in materials science during last decade. The first group of materials designed using such approach were high-entropy alloys (HEAs). However, this idea has been carried even further to create high-entropy alloy nitrides (HEANs) and in 2015 a new group of materials was developed - high-entropy oxides (HEOx).

The general idea in all these groups is to stabilize solid solutions structures by high configurational entropy, what can be accomplished by mixing number of components (at least five) in equimolar or near-equimolar proportions. Due to the high number of components the cations are distributed randomly at the atomic scale, throughout the whole crystal structure. The visualization of such behaviour is presented in the image below, which shows the entropy-stabilized oxide made from five different oxides. Such approach to materials design drastically differs from the conventional one, in which ordered structures such as spinels and perovskites are synthesized. At the same time, it often leads to extraordinary properties, resulting from the synergistic effects, lattice distortion and other factors typical for high-entropy materials.



Despite their very short history, the HEOx materials are already in the centre of attention of multiple scientific groups. The initial studies of their electrical properties show that high-entropy oxides may have a huge potential as solid-electrolytes, which can be used in e.g. new generation of lithium batteries, characterized by much higher performance in terms of charging speed and capacity. Other potential applications are just awaiting discovery.

The main objective of this project is to investigate microstructures, stabilities and basic properties of the new high-entropy oxides systems. Until now only a few potential compositions of HEOx have been investigated, with most of them being developed from the first synthesized HEOx material, namely (Co,Cu,Mg,Ni,Zn)O. In the current project a much wider range of possible compositions will be studied in search of optimal materials, which would be even better base for further modifications than the mentioned one. To obtain this goal, a group of compatible base oxides will be selected, basing on their crystal structures, ionic sizes, molar volumes, as well as binary phase diagrams, with potential candidates being CoO, CuO, FeO, MgO, MnO, NiO and ZnO. The various quinary subsystems of the selected group will be studied, to determine the most stable ones. They will be further studied to find out which of them are characterized by the most promising electrical properties and therefore have the highest potential for further development. The choice of materials will also allow to study influence of each of the components, significantly expanding our understanding of high-entropy oxides and processes which govern the formation of solid solution structures.