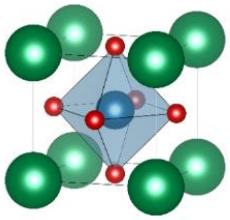
High entropy oxides for energy conversion

Entropy may be described as a thermodynamic quantity indicating the inaccessibility of a system's thermal energy for conversion into mechanical work, often interpreted as the degree of disorder or randomness in the system. It can be used not only to describe theoretical thermodynamic systems or processes but also to describe the disorder in crystalline materials. The first materials to be described as high entropy ones were metal alloys. However, today the idea of multicomponent materials is not only limited to alloys but since recently also to other materials including oxides.



High entropy oxides (HEO) are a new class of multicomponent oxides stabilized by configurational entropy. The key point of the high-entropy stabilization concept is the combination of a large number of cations (usually five or more) in solid solution in equiatomic proportions, which results in the formation of a single-phase structure. Within this project mainly two crystallographic structures will be studied, namely: perovskites and fergusonites. The representation of unit cells, the smallest crystal building blocks, of these structures is presented in Figure 1. These types of structures are very interesting because of their possible applications as materials for energy conversion devices like fuel cells and electrolyzers. The project aims to synthesize various compositions of HEO materials and to determine their properties. Both previously known compositions and new modifications of existing compounds will be produced and measured.

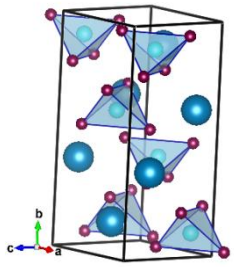


Figure 1 Graphic representation of the main two structures to be studied in the project: perovskite (up), and fergusonite (bottom).

The main methods used in the project are: X-ray diffraction – to determine the materials crystalline structure; Scanning electron microscopy – to determine samples morphology and possible phase separations; Differential scanning calorimetry – to determine samples heat capacity; Thermogravimetry – to determine material's mass change upon hydration and/or oxidation; Electrical measurements – to determine the conductivity of synthesized specimens. All these measurements will allow the project team to describe the materials synthesized very thoroughly.

The project output will influence not only the field of materials science but also, as it tackles issues with materials for energy conversion, will help in developing a new more sustainable European society.