Description for general public

Piezo- and ferroelectric materials play an important role in everyday life. They are used e.g. ultrasonography, echolocation devices, ferroelectric memories (FeRAM), and many others. The most popular this type of material is lead zirconate-titanate ($PbZr_{1-x}Ti_xO_3$). Due to the toxicity of lead, there is a necessity of finding materials with similar properties but more enviroment-friendly. The most promising candidate are bismuth-based perovskites $BiMO_3$. In both, Pb- and Bi-based perovskites the same mechanism is responsible for piezo- and ferroelectric properties. The lone pairs $6s^2$ on the Pb^{2+} or Bi^{3+} ions are responsible for large structural distortions and, as a result, a large ferroelectric polarization. However, the ferroelectric properties of Bi-based perovskites are limited by different types of defects.
These defects are responsible for harmful from applicational point of view leakage currents. The first purpose of this research project is analysis of native defects (e.g. Bi- or O-vacancies) in selected $BiMO_3$ perovskites by using density functional theory. Next, we will analyze different substitution of dopants, to determine the best candidates to eliminate harmful effects from vacancies.
The second stage of the research will be to determine the conditions of occurance of the phases of Bi-based perovskites with the desired properties. The effect of both, hydrostatic and chemical pressure on pervoskites $BiMO_3$ (M=Al, Ga, In) will be investigated. In case of chemical pressure, the solid solutions e.g. $Bi_{1-x}RE_xMO_3$ (RE=Y, La, Ce; M=Al, Ga, In) will be investigated.