Ferroelectric perovskite oxides: The interplay between surface and bulk polarization

(Ferroelektryczne tlenki perowskitowe: pomiędzy powierzchniową a makroskopową polaryzacją)

There is no need to convince anyone that the world desperately needs new methods of energy harvesting, which are cheap and renewable. One of the most interesting ideas is the use of thermal energy, but not the energy stored in the Earth's crust, but the one much more readily available as it comes from the air. If we imagine a material whose paraelectric-ferroelectric phase transition occurs near room temperature, such a material will change its phase twice a day depending on the ambient temperature (see Figure 1), generating electric charges due to the piezoelectricity and pyroelectricity effects. Therefore polarization fields in the bulk affecting its surface can help in catalytic or, if supported by light, photocatalytic reactions such as water decomposition and hydrogen production.

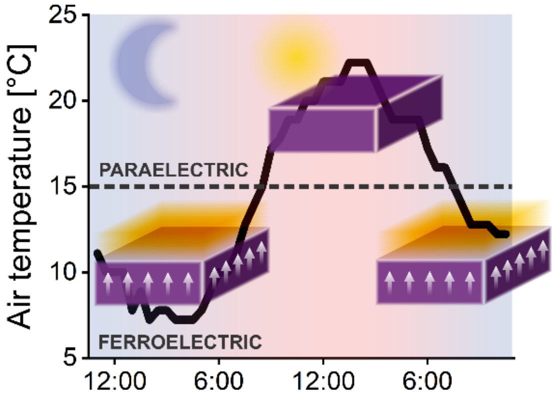

Figure 1. Plot of the air temperature registered on Thursday, May 5th, 2022, in Kraków, Poland, with a potential paraelectric-ferroelectric transition in a perovskite crystal (with T_c approx. 15°C) used to generate charges and electric fields on the surface.

This project involves research on a special class of ferroelectric materials, i.e. inorganic oxide perovskites with an ABO_3 structure. Importantly, these are non-toxic and relatively easily accessible materials. The aim of the project is to investigate the basic surface properties of perovskites, since many of them have not been thoroughly studied so far, and to correlate the phase transitions occurring in bulk crystals with changes in the surface structure manifested in electric fields generated. Due to the access to materials whose crystalline structure remains unchangeable after doping but the temperature of the ferroelectric-paraelectric transition changes (e.g. $KTaO_3$ doped with niobium), the specific goal is to select such an admixture that the transition temperature will be around 0-20°C, which would in turn allow to take advantage of the fluctuations in the daily temperature. The project involves also the use of the oxidation-reduction reaction in perovskite oxides, which would potentially allow for much simpler control of the phase diagram. The final step in the research will be to observe specific catalytic reactions occurring on perovskite ferroelectric surfaces during phase transitions.

Due to the complexity of the research problem posed, the project involves the use of many experimental techniques to obtain comprehensive information on the behavior of both bulk materials and their surfaces. The most sensitive Atomic Force Microscopy techniques in contact and non-contact modes as well as spectroscopic and diffraction methods will be used. Most of the research will be carried out in ultra-high vacuum conditions (comparable to space vacuum) and in ultra-low temperature conditions, starting from 4 K up. International cooperation with groups from Prague and Vienna will allow access to the state-of-the-art equipment and ensure better interpretation of the results. The project also includes funding to create a small research group, focused on the above-presented research.

Expected results of the project are publications describing new surfaces of ferroelectric perovskites prepared by breaking in vacuum, their electrical properties and crystal structure. Since only a few of the available surfaces are described in literature ($SrTiO_3$(001), $KTaO_3$(001)) however in journals such as Science and Nature, this guarantees the success of this project. Further tasks are also predicted to be potentially significant due to the presentation of various possibilities for controlling the phase transitions in crystals and their subsequent use in real (photo-) catalytic reactions on surfaces.