Exploring surface-chemistry driven effects in ferroelectrics

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Project background and description

Ferroelectrics are polar materials with applications in devices that range from sensors and actuators to memories and neuromorphic computing. More recently these materials known for their spontaneous polarization (and switching) have shown great promise for applications aimed at electrochemistry and controllable surface chemical reactions,[1] including water splitting,[2, 3] and piezo-catalysis.[4]

The ability to control their polarisation is what makes ferroelectric surfaces promising, as tuneable and dynamic platforms for electrochemical reactions. Importantly, the surface dynamics are a direct result of the interplay between internal and external fields, a phenomenon known as screening. In typical ferroelectric devices, charge compensation is achieved through the screening provided by the metallic electrodes. However, any deviation from this ideal scenario, including the presence of surface charges, will directly affect the screening dynamics and hence the ferroelectric properties. Importantly, ferroelectric surfaces allow carrier separation and reversibility, overcoming species recombination. An additional dimension for tuning the surface reactivity can be achieved through their pyroelectric effect through temperature modulation of polarisation. Thus, ferroelectric polar surfaces are extremely interesting entities, where the possible controlled exchanges between the chemical species in a chemical environment and the polarisation states can be exploited to tailor surface reactivity for electrochemical, catalytical,[5, 6] and other energy harvesting applications.[1, 2, 7-10]

Up to date, most of studies have focused on epitaxial thin films or bulk systems demonstrating their feasibility. However, systematic exploration of size effects, along with temperature-polarisation coupling for different surface interaction strengths, is needed, particularly in a dynamic manner. Additionally, free-standing ferroelectrics have recently attracted great interest as they exhibit interesting effects that differ from the bulk[3, 11-13] and could be good candidates to further tailor surface reactions. For example, previous work has directly imaged the dynamic response of a free-standing $BaTiO_3$ to different environments,[14] providing proof that free-standing thin films as a promising candidate to further tailor surface reactions.

In summary, this is a complex phenomenon and the current understanding of this remains an open theoretical and experimental challenge. The aim of this project is to experimentally investigate ferroelectric surfaces under different chemical environments, and as a function of temperature, using in-situ transmission electron microscopy techniques by mapping the evolution of the domain structure. The understanding of this behaviour is a crucial aspect for the development towards novel applications aimed at electrochemistry and controllable surface chemical reactions.

The project will use in-situ heating and atmosphere (gas) in the transmission electron microscope (TEM). A substantial part of this project involves the development of sample preparation techniques and use of new image analysis methods. Furthermore, specific parts of the project will be carried out in collaboration with world-leading advanced electron microscopy centres such as the Ernst Ruska-Centre, leading experts in the field of ferroelectrics and machine learning.

Entry requirements: Applicants are expected to possess a first or upper-second class degree in physics, chemistry, mathematics, or a relevant discipline (or an equivalent overseas qualification), or a lower second-class degree along with a Master's degree.

How to apply: Applications should be submitted via the Direct Applications Portal.

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