polarons and ferroelectricity

at atomic scale on oxide perovskite surfaces

Dominik Wrana1,\*, Igor Sokolović2, Jesus Redondo1, Pavel Kocán1, Aji Alexander1,

Martin Setvin1,2

# 1Department of Surface and Plasma Science, Charles University, Prague, Czech Republic

2Institute of Applied Physics, TU Wien, Austria

\*autor korespondencyjny: dominik.wrana@mff.cuni.cz

    Although perovskite oxides share many common properties, *e.g.*, ABO3 chemical formula or a high dielectric constant, the interest in these materials is driven by unique properties such as colossal magentoresistance, transport properties, superconductivity, ferroelectricity or charge ordering. In this talk I will focus on understanding the atomic origin of the two last properties and their relation to (photo-)catalytic applications.

            In order to showcase those mechanisms, two perovskite oxide single crystals were chosen: Ferroelectric BaTiO3 and incipient-ferroelectric KTaO3. As both are insulating, low temperature non-contact atomic force microscopy (nc-AFM) microscopy, equipped with a qPlus sensor, was employed. As it will be presented, electric fields emerging from the same metallic tip can cause permanent crystal distortions or charge ordering, depending on the atomic structure of the perovskite surface.

            In order to compensate the surface polarity, bulk-terminated KTaO3(100) develops two alternating domains of KO and TaO2 [1]. Excess electrons injected from the AFM tip form quasiparticles called polarons (charges coupled with lattice distortions) which can be further shaped into 1D or 2D structures by emerging electric fields.

            Different mechanism applies in the case of BaTiO3(100), a model ferroelectric perovskite. When cooled down to 4K it adopts a rhombohedral crystal structure, where titanium atoms can easily break the symmetry causing a spontaneous polarization. I will present that a biased tip placed a few nanometers above the surface allows for reversible manipulation of individual atoms on the surface, writing and erasing polarized ferroelectric domains.

[1] Setvin, Martin, et al. "Polarity compensation mechanisms on the perovskite surface KTaO3 (001)." Science 359.6375 (2018): 572-575.