Perovskites as supports for single-atom catalysis

A. Alexander[1], D. Wrana[1,2], P. K. Samal[1], J. Škvára[1], L. Albons[1], J. Redondo[1], L. Fusek[1], I. Píš[2], V. Johánek[1], J. Mysliveček[1], M. Setvin [1]

[1]*Department of Surface and Plasma Science, Charles University, Prague, Czech Republic*

[2]*Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow, Poland*

[3]*IOM-CNR, Istituto Officina dei Materiali, AREA Science Park Basovizza, Trieste, 34149, Italy*

aji.alexander@mff.cuni.cz

Perovskite surfaces attract increasing attention in the catalysis community due to these materials' promising chemical properties, good ability to separate electron-hole pairs in light harvesting, and the presence of ferroelectricity in many perovskites [1]. While perovskites possess a unique set of interesting bulk properties, their surfaces are much less understood; the main open questions are their structural stability and associated chemical reactivity and catalytic selectivity.

This presentation will focus on the atomic structure of doped $KTaO_3-(001)$ and $SrTiO_3-(001)$ perovskite surfaces and the potential to modify their catalytic activity by extrinsic metals, with the main focus on cobalt. I will demonstrate the implementation of combined STM/AFM measurements along with XPS chemical analysis to show the thermal stability and the tendency of the guest atoms to disperse in the form of single adatoms on the polarity uncompensated $KTaO_3$-(001) [2] and $SrTiO_3$-(001) surfaces. The interaction of cobalt with surfaces under various reducing and oxidizing conditions, as well as temperature evolution of absorbed species, will be highlighted. This sheds light on how cobalt's metallic, oxide, and hydroxide phases vary depending on the environment, which is of utmost importance for the realisation of single atom catalysis in perovskite oxides.

[1] Cohen, Ronald E. ***Nature*** 358.6382 (1992)

[2] M. Setvin, M. Reticcioli, F. Poelzleitner et al., ***Science 359***, 572 (2018)