Charles University, Prague, Czech Republic

Open PhD position (net salary 1100-1300 EUR)

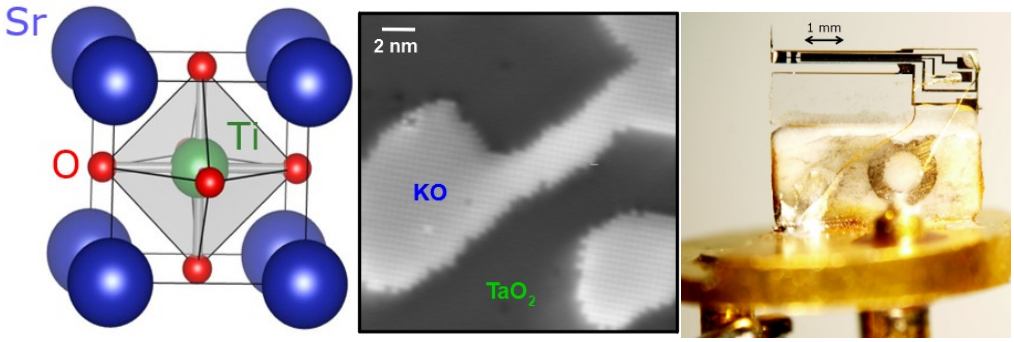
Physical and Chemical properties of perovskite surfaces

Supervisor: Doc. Martin Setvin, Ph.D.

Perovskites (chemical formula ABO_3 [1]) are currently at the forefront of interest in materials research because of their wide applicability in catalysis [2], photocatalysis [3], electronics [4] or spintronics. The class of perovskites contains hundreds of stable materials thanks to the wide choice of A and B cations and further possibilities of doping at all three sites. The surface science of perovskites represents a major challenge mainly due to the ternary composition of the bulk material and consequent complex behaviour of their surfaces.

The focus of this PhD thesis are bulk-terminated surfaces of perovskites from the class of titanates and tantalates (for example $KTaO_3$, $KNbO_3$, $SrTiO_3$ and $BaTiO_3$). A successful preparation of this surface termination has been reported just recently [5,6] and the combined atomic force microcopy/scanning tunnelling microscopy has proven as an invaluable tool for characterization of these surfaces at the atomic scale. The AFM/STM [7] will be supplemented by integral analysis techniques of surface science, such as LEED, XPS, and LEIS. A major aspect of the research will be ferroelectricity (spontaneous electric polarization) [8] often present in these materials, and the opportunities that ferroelectricity offers for production of renewable fuels (photocatalytic and pyrocatalytic effect).

The candidate will be encouraged to spend at least 6 months abroad with one of our collaborators in Austria, Germany or Japan.



Left: Primitive unit cell of a perovskite. Middle: AFM image of a cleaved $KTaO_3$ (001) surface. Right: q-Plus sensor for simultaneous AFM/STM measurements.

[1] R. E. Schaak and T. E. Mallouk, Chem. Mater. **14**, 1455 (2002)
[2] S. Royer, D. Duprez, F. Can, X. Courtois, C. Batiot-Dupeyrat, S. Laassiri, and H. Alamdari, Chem. Rev. **114**, 10292−10368 (2014)
[3] E. Grabowska, Appl. Cat. B: Environmental **186**, 97 (2016)
[4] A. F. Santander-Syro et al., Nature **469**, 189 (2011)
[5] M. Setvin, M. Reticcioli, F. Poelzleitner, J. Hulva, M. Schmid, L. A. Boatner, C. Franchini, and U. Diebold, Science **359**, 572 (2018)
[6] I. Sokolović, M. Schmid, U. Diebold, and M. Setvin, Phys. Rev. Mater. **3**, 034407 (2019)
[7] F. J. Giessibl, Rev. Sci. Instr. **90**, 011101 (2019)
[8] R. E. Cohen, Nature **358**, 136 (1992)

In case of interest, please contact Martin Setvin (martin.setvin.mff.cuni.cz). Deadline for applications is April 15, 2020