Thursday 5 March 2020
16:00 Room: OFLG/402
TFI-LMX SEMINAR

Surface structure, defects and reactivity of perovskite oxynitrides

Guest Speaker: Ulrich Aschauer
Department of Chemistry and Biochemistry, University of Bern

The smaller band gap compared to pure oxides yields a superior light-absorption efficiency of perovskite oxynitride photocatalysts. While the bulk structure and properties of these materials have been extensively studied by computational methods, significantly less is known about their surfaces and consequently their photocatalytic reaction mechanisms. In this talk, I will present results of our density functional theory (DFT) calculations, highlighting anion-ordering phenomena at perovskite oxynitride surfaces, the effect of defects on their oxygen-evolution reaction (OER) activity as well as the potential of strain engineering these materials to become ferroelectric photocatalysts.