# Ultrathin piezoelectric transition metal compounds with defined oxygen and chalcogen content

The scientific objective of the submitted research project is to carry out a systematic study of the piezoelectricity in ultrathin membranes of Transition Metal compounds with definied oxygen and chalcogen content. Piezoelectricity in Transitions Metal Dichalcogenides (TMDC) materials has been increasingly explored due to their unique atomically thin nature and large surface area to thickness ratio. Accordingly, piezoelectric materials are useful for a variety of sensing, actuating, energy generation and conversion applications. Various theoretical and experimental investigations have estimated piezoelectric coefficients of 0.2–1 $pmV^{-1}$ for graphene and hBN, 2–10 $pmV^{-1}$ for most TMDCs. Another interesting category of 2D materials are Janus monolayers, which can show stronger piezoelectricity than their standard TMDC counterparts.

$MoO_2$ crystallizes in a monoclinic structure which is centrosymmetric. This along with delocalizing of electrons across differing Mo-O bond lengths leads to an unusual metallic-like conductivity thereby precluding expectations of conventional piezoelectric behavior. Observed apparent piezoelectric behavior of $MoO_2$ and conclude its origins to the formation of the so-called electret state. The 2D $MO_2$ flakes synthesized via CVD at high temperature, contain defects and voids which act as prime spots for trapping charges before the growth process completes and sample is cooled down to room temperature. In short, the 2D flakes possess frozen dipoles.

We put forward a thesis that there is a transition between the piezoelectricity in $MX_2$ and the apparent piezoelectricity in $MO_2$ and this state depends on the composition of the mixed $M(X_xO_{1-x})_2$ layer. As a part of the project, we want to synthesize using the CVD method $MO_2$ materials with a defined chalcogen content and then examine its piezoelectric response. In addition, we want to develop a methodology for the production of materials such as Janus type MSO and develop doping of TMDC materials with oxygen. We believe that in these types of materials the piezoelectric effect depends on the percentage of exchange of chalcogen atoms (X) with oxygen in a MSO layers.

To verify the hypothesis, we intend to:

i) fabrication of the ultrathin membranes from TMDC and TMO bulk crystals,
ii) synthesis of the TMDC and TMO with defined No. of layers using CVD methods,
iii) synthesis of the Janus layers using plasma assisted CVD methods,
iv) syntesis of TMO/TMDC and TMO/Janus hybrids,
v) structural and strain investigations of the produced membranes using Raman spectroscopy and XRD methods,
vi) structural characterizations of the materials surface of the obtained flakes using AFM and HR-S/TEM microscopic methods,
vii) PFM assisted piezoelectrical studies of the doped materials,
viii) HR-EBSD assisted HR-SEM strain investigations and simulations.

Such a combination of techniques related to the synthesis and characterization using the AFM, TEM, SEM microscopic methods and additional methods such as Raman spectroscopy and X-ray diffraction will allow to characterize the synthetised materials and prove the thesis put forward in the project.

The research program will be carried out by research teams: Łukasiewicz Research Network – PORT, whose leader and principal investigator is dr. hab. eng. Alicja Bachmatiuk and the Wrocław University of Technology - Department of Nanometrology at the Faculty of Microsystem Electronics and Photonics - headed by dr hab. eng. Jarosław Serafińczuk.

We are fully convinced that two-dimensional van der Waals crystals, and in particular membranes made on their basis, are a very promising topic that gives the opportunity to conduct many interesting and innovative research experiments. Most of the research planned by the project will be pioneering for these materials. We are convinced that this type of materials will be very intensively researched in the coming years, and the proposed technologies will be conducted by the experiments and the research techniques developed will be a guarantee of valuable scientific results.