Motivation
The material TaS$_2$ is a Van der Waals material like graphene, consisting of layers bonded only by Van der Waals bonds. There exist different orderings of the atoms within the layer, so-called polytypes (Figure 1). Each of these polytypes has different interesting properties, such as Charge Density Waves (CDW’s)[2] or superconductivity.

Project
In the Low Energy Electron Microscope (LEEM) we observe different spectroscopic reflectivity curves for TaS$_2$ samples, which correspond to these different polytypes. To identify which curve corresponds to which polytype however, a comparison with simulations is needed.

There is existing software (e.g. https://physics.mff.cuni.cz/kfpp/povrchy/software) to simulate these reflectivity curves. This bachelor project will consist of understanding the issues involved with these simulations, simulating the different polytypes using this software in order to identify these polytypes in the experimental data.

Student profile
You have affinity with programming and working with different programming languages and you like to apply programming to physical problems.

Figure 1 Different polytypes of TaS$_2$: the CDW exhibiting 1T phase, the superconducting 2H phase and the 3R phase. Figure adapted from [1]

Figure 2: Measured spectroscopic reflection curve of different areas of a TaS$_2$ sample.

[2] https://www.nature.com/articles/srep07302