

When the dimensionality of the system decreases, defects play an increasingly important role. It is intuitively clear that while a point defect will not affect much the electronic transport in a bulk system, single defect in a 1D system (e.g. atomic chain) may completely block the conducting channel. The characteristics of 2D materials (2DMs), which are in between these two limiting cases, are strongly influenced by imperfections. Defects can appear during the growth, or as 2D systems consist of essentially surface only, during processing or characterization in, e.g. transmission electron microscope (TEM). Grain boundaries or interfaces between different 2DMs in lateral heterostructures can be referred to as defects as well. Most of defects deteriorate the properties of materials. At the same time, defects and impurities can be useful and may open new possibilities for tuning materials properties. The examples include doping and defect-related chemically active sites for functionalization and catalysis. In this project, by using multi-scale atomistic simulations, we plan to study point and line defects in a broad range of 2DMs including transition metal dichalcogenides (TMDCs), as well as monochalcogenides, and understand how the defects influence the electronic, magnetic and catalytic properties of these systems. The project will be carried out in a close collaboration with several experimental groups focused on fabrication and characterization of 2DMs (specifically using TEM). Introduction of impurities and alloying, which corresponds to a high concentration of impurities, will also be investigated. The mechanisms of defect production under electron beam in TEM will be studied as well, with the main focus on electron-beam mediated etching.