A challenge for modern electronics involves production of densely packed electronic circuits on flexible and planar substrates (flexible nanoelectronics). This is because majority of existing electronic circuits are not flexible, heat excessively and their further miniaturization is stalled due to a minimum size of lithographic masks used for their production. A potential solution might involve 2D materials such as transition metal dichalcogenides (TMDCs), and MoS_2 in particular. However, all electronic circuits heat excessively. Thus, basic research is needed in heat induced reactivity of thin MoS_2 crystals at the length scales for future MoS_2 based circuits, i.e., at the scales of tens and hundreds of nanometers.

The **key research objective of this proposal is to understand the influence of local heating on thin MoS_2 crystals in oxidative conditions. This means to investigate and understand the mechanisms of local heat induced oxidation of thin MoS_2 crystals and related mechanisms of heat induced defects formation within those crystals.** We will concentrate on finding out the types of oxides created on the surface, conditions of their formation, surface distribution and morphology of the arising products, and prowess of the oxidized MoS_2 surface for further oxidation. **We will also study heat induced oxidation of B- or N- doped MoS_2 crystals**, since such doping is expected to yield novel semiconducting materials with different propensity for heat induced oxidation than undoped MoS_2 crystals.

For localized heating we will use the thermochemical nanolithography (TCNL) developed by the PI as well as other local heating methods developed in the course of this proposal. Dry and wet oxidation, defect creation and doping will be realized on MoS_2 substrates via reactive gases and chemical solutions, respectively. Chemistry and microstructure of the oxidized crystals will be characterized via Atomic Force Microscopy (AFM) methods involving imaging and local friction coefficient measurements, Kelvin Probe AFM and Electric Force AFM Microscopy, as well as Scanning Electron Microscopy, photoluminescence, Electron Dispersion X-ray Spectroscopy, X-ray photoelectron spectroscopy and Auger Electron Spectroscopy studies. Electronic properties of the modified MoS_2 crystals will be characterized by I-V curves and electric field effects between various electrodes placed on thermally modified MoS_2 to find the effect of modification on carrier mobility and doping. Experimental measurements will be related to computer simulations such as Molecular Dynamics, Monte-Carlo and Ab initio methods.

Our research team will be well suited to complete this project. Principal Investigator (PI), dr hab. Robert Szoszkiewicz, prof. UW is the main inventor of the TCNL method. He has substantial experience in materials research, AFM methods, nanoscale characterization of 2D materials, as well as MoS_2 modifications via TCNL. The rest of the hired personnel includes two PhD students and two MSc students who together with PI will ensure timely realization of the project. Our research in the Faculty of Chemistry of the University of Warsaw will be complemented by the research of our team members in two leading laboratories specializing in electrical characterization of TMDCs and related computer simulations.