Two-dimensional (2D) materials can be defined as crystalline structures, 2D allotropes, with a single layer (or a few layers) of atoms or chemical compounds. The extraordinary properties of these 2D materials have opened new opportunities for scientists and engineers and have dominated nanomaterials science nowadays. Actually, graphene (and its derivatives) is the most researched 2D material up to now, followed by transition metal dichalcogenides (TMDC), such as MoS_2. Generally, 2D materials can be classified as elemental, compounds, or van der Waals heterostructures. Recently, very interesting group of 2D materials has appeared, namely, layered transition metal carbides, nitrides, and carbonitrides, so-called **MXenes**. Basic structures of MXenes consist of a sequential layers of a transition metal (TM) and carbon or nitrogen C(N), for example, TM-X-TM, or TM-X-TM-X-TM, with chemical formulas TM_2X, and TM_3X_2, respectively, and X = C or N. The family of MXenes has expanded rapidly since the discovery of Ti_3C_2 in 2011. Preliminary results obtained for MXenes clearly demonstrate that these materials could provide breakthrough on many areas of materials science, chemistry, and physics. However, the understanding of their properties and physical processes is far of being complete or even satisfactory.

The main objective of the project is to provide deep understanding of physicochemistry of recently discovered and only weakly explored new family of MXenes, and further, through the *experiment aided computationally driven materials design,* to determine functional nanostructures that could be utilized in next generation of functional devices in the field of **plasmonics**, **spintronics**, and **thermoelectricity**. With the developed *experiment aided modeling tool,* we intend to proof the **main hypotheses of this project**: (i) MXenes can be very good materials for plasmonics and outperform other 2D materials considered for this purposes up to now, (ii) MXenes constitute family of good thermoelectric materials, particularly for applications at higher temperatures, and (iii) through the suitable functionalization, one can synthesizes semiconducting phases, and also ferromagnetic MXenes with Curie temperature above room temperature. This gives us unique opportunity to build spin field effect transistor (spin FET) entirely on the basis of one material.

The methodology employed to reach the main objective of the project is based on development of multi-scale modeling tool that should provide reliable quantitative predictions for real systems that are technologically available, usually not perfect and with some degree of disorder, and not only for 'idealized' perfectly ordered structures studied up to now. The realization of this computational tool will be facilitated by close cooperation with experimental group. The synergy between theoretical and experimental research, should generate cost-effective research scheme that can lead to novel and important results. The developed computational scheme in the framework of atomistic theory should provide quantitative reliable predictions for stability of the structures, their equilibrium morphology and geometry, electronic, optical, magnetic properties, and simultaneously allowing us to calculate charge, spin, and heat transport in functionalized MXenes systems that can contain few hundreds thousand of atoms. The tool has to account for the following physical and chemical factors that determine the properties of the structures based on MXenes: (i) shape of flat or bent flakes: (ii) existence of edges, (iii) internal structural defects, (iv) remnants from the technological process (F, O, OH) usually randomly distributed over the surface, (v) possibility of alloying, (vi) existence of the intentionally introduced functionalizing atoms and molecules, and (vii) external electric and magnetic fields. Close cooperation with the experimental group will allow us to verify our modeling tool, assess reliability of predictions, and fine-tune the model.

The development of the computational scheme will constitute big achievement in the computational nanoscience and theory of condensed matter, and the tool can be broadly used for other materials systems in the future. We are aware that the spin FET hypothesis has character of the ***high risk - high reward research***. In spite of huge effort invested in the spin FET issue, no research group succeeded to build well functioning device on the basis of single material, and hybrid structures are rather ineffective.

The realization of the project will bring solutions to novel and important problems, therefore, contributing substantially to the basic physics, chemistry, and material science. In addition, proposing new functional structures for plasmonics and thermoelectricity, and pointing out the new option for realization of spin transistor, the project will contribute to the issue of energy storage, energy conversion, and future nanoelectonics, all challenges that are extremely important for the development of our civilization.