The materials with a 2D atomic structure (flat, one layer) have drawn attention of researchers for years. The practical applications of graphene sheets, nanotubes can be observed in many areas from electronic industry up to civil engineering (e.g. concrete with nanotubes fillers). The carbon based materials are well known and have applied in many fields, but also other chemical elements which can be used to create 2D structures like molybdenum or compounds like molybdenum disulphide (MoS_2), tungsten diselenide (WSe_2) and others. The stable configurations of atoms in such materials are known but only for typical configurations.

The goal of the project is create a method for intelligent design new 2D atomic stable nano-structures with prescribed properties based on molybdenum. The research will be conducted on the base of authors experience with carbon based flat structures. The change of atom type or use of compound leads to complications during computer simulations (change of type of inter atomic potentials, modification of optimization tools). The goals of the project are both to create a method, software tools for its verification and generation of new molybdenum flat structures with prescribed properties. The nanostructures obtained during the intelligent design based on a memetic optimization process should have stable configuration (minimum energy) and prescribed properties (e.g. orthotropic mechanical, thermal properties of material).

The optimization of flat structures, distribution of atoms in periodic cell of structure, based on molybdenum may be performed with use of optimization techniques and molecular simulations. The optimization algorithms should be resistant to locking in local optimum but also able to obtain exact value of global optimum. Such features can be found in memetic (also called hybrid) algorithms. The objective functions depend on minimum energy criteria or predefined properties of microstructure. The objective function can be evaluated on the basis of numerical simulation of atomic structure. The simulations should be close to the real structure, so the models used, especially interatomic potentials used in the simulations are critical.
The ab initio, molecular statics and dynamics will be used during realization of the project. The objective function will depend on results of numerical simulations.
Nanostructures based on carbon (C) and molybdenum (Mo) can be considered as alternative though graphene till now are definitely more popular than molybdenum. Some researchers think that expectations concerning graphene are overdone.
To illustrate an attempt to the different alternatives in the field of 2D materials one can propose the following vivid comparison. Considering graphene as the tip of the iceberg the discovery of alternative 2D materials is a pioneering attempt to show the rest of this iceberg.