The ultimate objective of the project is to construct a general theoretical model which would enable fast prediction of self-assembled structures created by organic star-shaped functional molecules adsorbed on solid substrates. The proposed research focuses on theoretical modeling of the self-assembly of organic molecular superstructures adsorbed on crystalline surfaces and it aims at designing new two-dimensional molecular architectures sustained by short-range directional interactions. The main research subject are the adsorbed overlayers comprising simple multi-armed functional organic molecules which can form intermolecular hydrogen or halogen bonds to produce ordered 2D organic nanostructures. An important objective of the project is to study the influence of such factors as shape, size and functionality of the organic building blocks (number and distribution of interaction centers), adsorbate density, corrugation of the adsorbing surface, temperature and intermolecular interactions on the morphology of the resulting assemblies. Another goal of the project is to determine the ways in which the interactions can be effectively encoded into the building blocks to obtain periodic and random supramolecular structures with presumed architecture. Our main intention is to formulate simple and general rules which would facilitate designing 2D organic supramolecular systems, also porous networks, based on individual properties of the molecular bricks at play. Using computer simulations and simple lattice and off-lattice models we are going to test the hypothesis assuming that accurate de novo structure prediction of such self-assembled overlayers can be made without detailed knowledge about atomic/electronic structure of the interacting components.

The large practical interest in 2D supramolecular nanostructures originates mainly from their broad application potential. These functional systems can serve as, for example, selective adsorbents and catalysts, molecular sensors, photovoltaic elements, magneto-optical responsive materials and molecular switches for future nanotechnological applications. Moreover, recently it has been demonstrated that surface-confined assembly of star-shaped functional molecular units with their subsequent covalent polymerization is a versatile method of fabrication of 2D nanomaterials with largely diversified architectures (networks, graphene, porous graphene, strings etc.). Gaining precise information on how the molecular bricks self-organize in those systems and identifying factors which promote or suppress certain intermolecular connections is crucial for predicting and tuning physicochemical properties of new 2D nanomaterials.

The pioneering character of the project relies on its novel, simple and effective methodology that has not been yet applied to the considered systems. The results of the project will broaden our understanding of the mechanisms governing structure formation in 2D supramolecular assemblies and they will provide hints on how to design new organic overlayers with predefined functions. The obtained results will be valuable contribution to such fields as physicochemisrty of surfaces, nanotechnology and supramolecular chemistry. These findings can be helpful in fabrication of new nanomaterials and nanodevices (e.g. nanoswitches, nanoreactors etc.).