2D metal-organic frameworks are a class of coordinative polymers, fabricated mainly with the use of self-assembly of simple organic molecules and metal atoms on solid surfaces. Due to their tunable properties (chirality, porosity, composition, etc.) and periodic distribution of organic ligands and metal atoms, such molecular structures are fascinating nanomaterials with potential applications in many fields of science like medicine, pharmacy and chemistry. However, experimental fabrication of supramolecular structures with pre-defined properties is not an easy task. Nowadays the designing of new metal-organic connections stabilized by coordinate bonds is mainly based on the trial and error method. This is related to the variety of available organic ligands and a large number of metal atoms that can be potentially used for this purpose. Moreover, even small changes in the structure of organic ligands can have a profound effect on the morphology of emerging metal-organic connections. Therefore, it is difficult to imagine the future development of supramolecular chemistry without the support of advanced computer modelling. However when large molecular systems are investigated a detailed description of investigated assemblies can be time-consuming (or not possible at all), and unconventional approach is needed. One of the possible solutions is the use of simplified models, in which investigated molecules are mapped on a regular lattice (triangular, square or hexagonal) as a collection of rigid and interconnected segments with properly assigned directional interactions. The most popular organic ligands used as building blocks of 2D metal-organic frameworks are polyphenyl, functionalised molecules composed of similar units (phenyl rings). As connection points between them n-fold coordinated metal atoms (where n = 2-4) like Ag(II), Fe(III), Cu(IV) are frequently exploited. Therefore in many metal-organic systems adsorbed on flat surfaces a mapping of both, linkers and metal centres on regular lattices is possible. This approach can be an especially effective in combination with Monte Carlo (MC) computer simulations.

Taking into account the above-mentioned considerations we would like to verify the hypothesis, that lattice MC simulations can be a complementary tool for experimental studies of complex, self-assembled molecular architectures. In the investigated systems, star-shaped organic molecules will be modelled in a simplified way, but their most important properties like shape, size and functionality will be preserved. Coarse-grained representation of the real molecules/metal atoms adsorbed on solid substrates will allow us to study complex molecular assemblies comprising up to few thousands of components, in a relatively short period of time. The obtained structures will be classified based on their morphology and composition. The proposed theoretical approach can reduce significantly the number of test laboratory experiments which are necessary to prepare metal-organic frameworks with well-defined properties and morphology. Moreover, the findings of our theoretical investigations can be helpful in designing of new functional molecules and programming their interactions to create 2D metal-organic nanomaterials with interesting structure and properties.