Formation of Archimedean Tessellation Found in the Mixtures of Pentatopic and Linear Molecules

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Abstract

Supramolecular chemistry is of particular interest for past few decades. Many either theoretical or experimental papers have been published about various classes of molecules, which are able to self-assembly on solid surfaces [1, 2]. Particularly interesting are rigid organic compounds of diverse architectures that tend to form different molecular networks by means of directional bonding between “active” groups. Such interactions may be, for instance hydrogen bonding and in the case, when the metal atoms are present - donor-acceptor interactions, which lead to coordinate bonding between metal and active groups. Hence, ability to self-assembly could be used in material chemistry and especially for producing new class of the so called "smart materials". Their application is mainly focused in fields like photonics, electronics, drug delivery systems and so on.

In this work, we present the results of molecular dynamics simulations for two cases, (i) single-component systems involving the tetra-, penta- and hexatopic [3, 4] molecules and (ii) for their mixtures with linear and V-shape particles. For the latter case, we have changed the chemical composition of the mixture and checked its influence on the formed ordered structures. We have found that, in the mixture of a pentavalent molecule and linear linker, the Archimedean tiling has been formed, which has not been the case in the single-component system. We have concluded that, for this case, the mobility of the linker is the driving force.

All of the formed structures have been further characterized by several quantities such as bond order parameter and other distribution functions.

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FIGURES

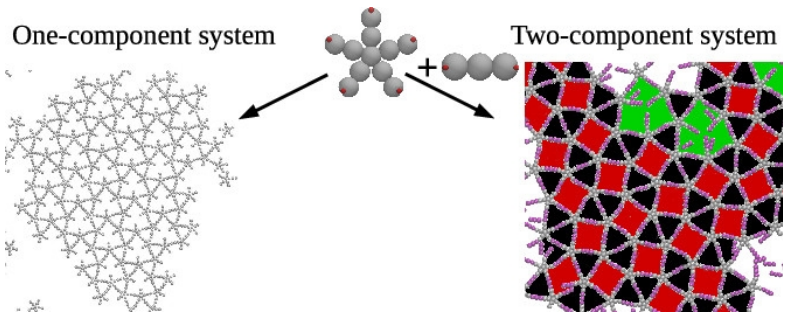

Figure 1: Presentation of different networks fromed by pentatopic molecule either in one-component system or two-component system with linear linker.