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

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## MODEL

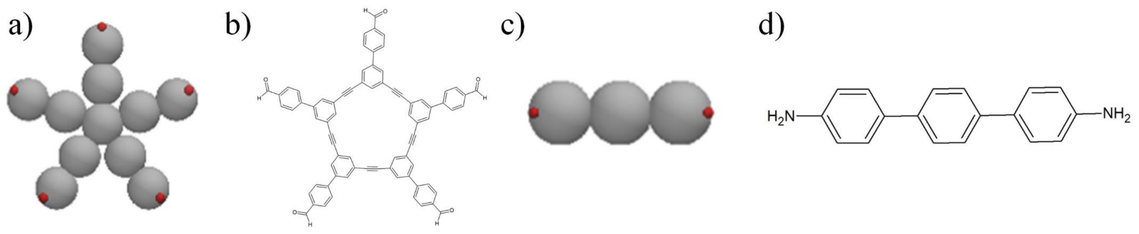



**Figure 1: Schematic representation of molecules used in this paper (a, c). Gray and red segments correspond to the aromatic rings and „active" sites, respectively. Parts b and d show example of chemical compounds, which could reflect the behavior of our model systems.**

The main goal of the model was to reflect the penta-substituted [1] chemical compounds and their mixture with linear molecules, where, for instance, aldehyde or amine groups are attached to terminal phenyl rings [2]. In the latter, the interactions can be described in terms of the so-called „active" sites, presented on red in the Figure above. All of the molecules used in the course of our simulations were treated as flat, rigid bodies. Two main features can be distinguished, namely, the core and the arms. In the former, the segments have been distributed on the vertices of pentagon, with a central atom inside. The latter segments have been tangentially grafted into each of the vertexes of this polygon. For the linear molecules, only the core can be distinguished. The sizes of the segments forming core and arms have been set the same and equal to $\sigma_c$. The bonding distance between particular entities in the main structure has been also assumed to be equal to $\sigma_c$. In the molecular dynamics simulations, the „active" sites, each of size $\sigma_a$, have been defined as the regions entirely embedded into the terminal arms, and the arm-site bonding distance has been abbreviated as $l = 0.4\sigma_c$.

## SIMULATION DETAILS

$$U_{SF} = \begin{cases} U_{LJ}(r) - U_{LJ}(r_{cut}) + U'_{LJ}(r_{cut})(r - r_{cut}) & r < r_{cut} \\ 0 & \text{otherwise} \end{cases}$$

Where $U_{LJ}$ is the standard Lennard-Jones potential and $U'_{LJ}(r_{cut})$ is its first derivative at $r = r_{cut}$.

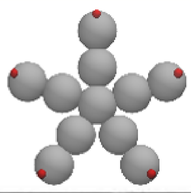
Interactions between entites – core-core (cc), core-active site (ac) and site-site (aa)
$\sigma_{cc} = 1.0\sigma$ and $\sigma_{aa} = 0.2\sigma$
$\sigma_{ac} = 0.5\,(\sigma_{cc}+\sigma_{aa})$ $\varepsilon_{cc} = \varepsilon_{ac} = 1.0\varepsilon$ and $\varepsilon_{aa} = 5.0\varepsilon$
$r_{cut,cc} = \sigma_{cc}$, $r_{cut,ac} = \sigma_{ac}$ - repulsion
$r_{cut,aa} = 2\sigma_{aa}$ - attraction between active sites (only mixed interactions were allowed)

**Simulation method**

All molecular dynamics simulations were perfomed in the *NVT* ensemble using LAMMPS simulation package [3]. To prepare starting configurations of our simulations we have created a single structure of desired architecture and replicated it to obtain 900 pentatopic molecules and from 900 to 5400 linear molecules. One has to note that the total number of atom differed with the architecture of the initial molecule. The size of the simulation cells has been appriopriately adjusted to keep the density and the particles number constant. The simulations were preliminary equilibrated by Berendsen thermostat with the dampening constant for $\tau_B=10\tau$ for $5\cdot10^6$ time steps, and further equilibration for $5\cdot10^7$ time steps, using Nose-Hoover chains approach with $N_{chain}=3$ and with dampening constant equal to $\tau_{chain}=10\tau$. The production runs have been carried out using the Nose-Hoover chains thermostat.

## Results

### One-component system



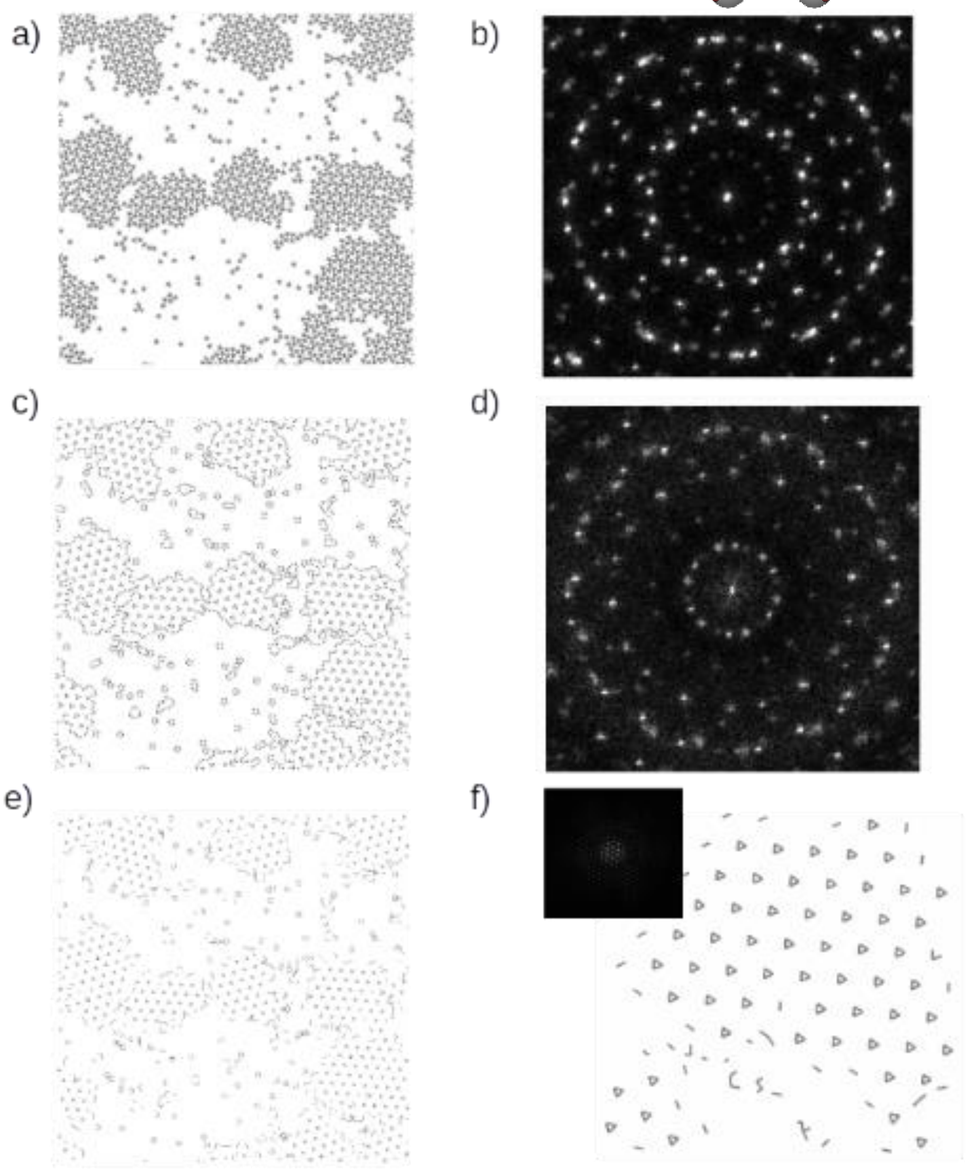
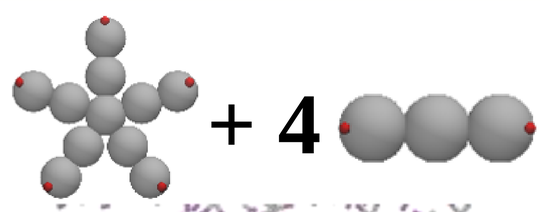



**Figure 2: . Results obtained for pentavalent molecules. Configuration of (a) the system and (b) the corresponding diffraction pattern with respect to the central atom. (c, d) Configuration of the system for (c) non-associated terminal segments and (d) the corresponding diffraction pattern. Part (e) represents different graphical representations of part (c). Part (f) shows the magnified fragment and its diffraction pattern in the inset.**

### Two-component system + 4



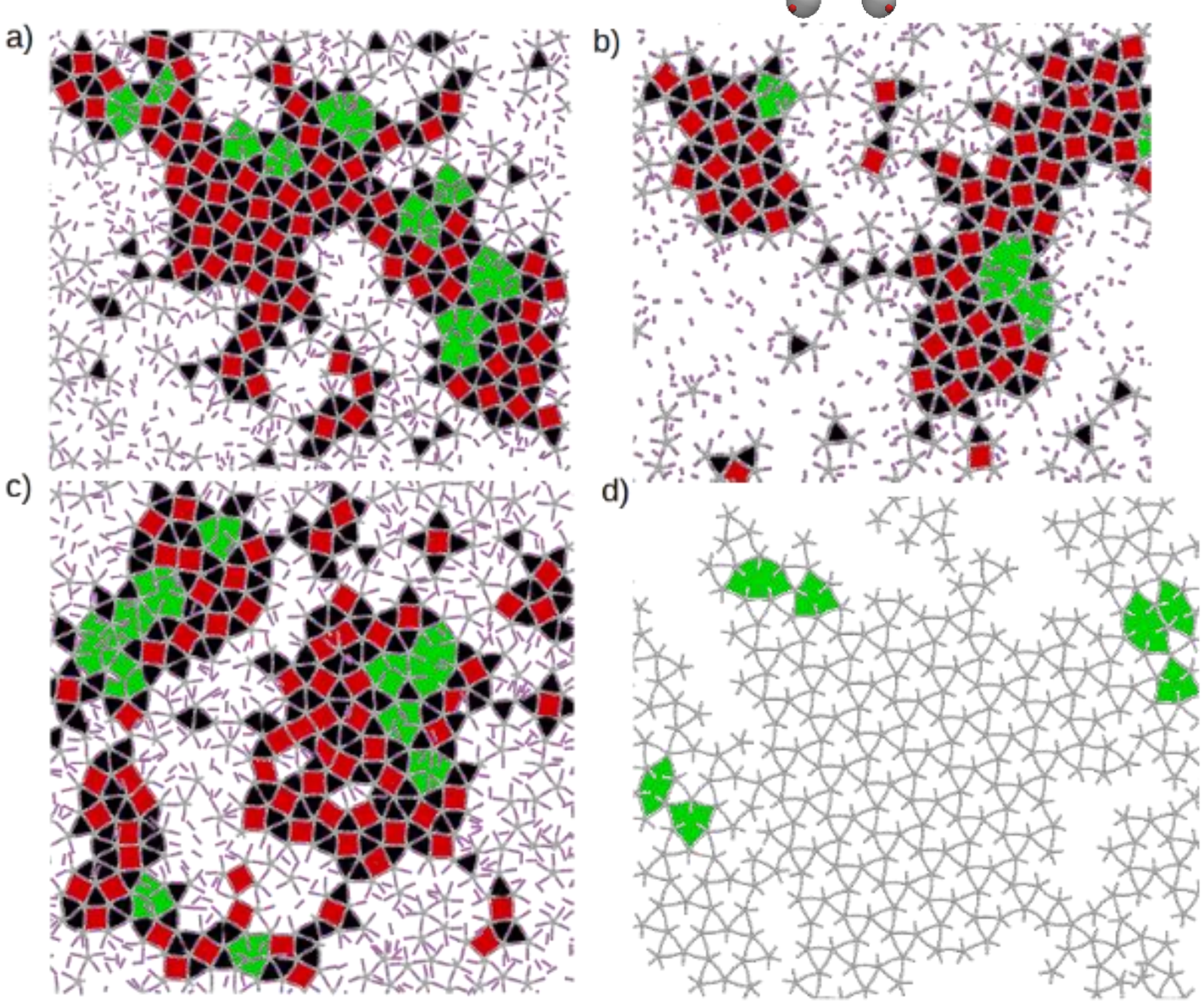



**Figure 3: Fragments of the configurations of mixtures of pentavalent molecules with linear linkers. Part (d) shows the fragment of configuration for a one-component system of pentavalent molecules with elongated arms. Silver and purple segments correspond to the pentavalent molecule and linear molecules, respectively. Particular polygons belonging to this network are colored in red (squares) and black (triangles). The reminiscence of the one-component system is marked in green**

## Conclusions

- **We have found that in the one-component system, voids are ordered into hexagonal network**
- **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**
- **The formation of Archimedean tiling is exclusively related to the the mobility of the linker and not the separation distance between consecutive molecules**

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