# Book of Abstracts

# 15th International Conference "Advanced Carbon Nanostructures" ACNS'2021

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# Simulation of supramolecular microporous structures on the basis of carbon nanotubes and toluene coordinator molecules

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A numerical experiment on the formation of supramolecular structures based on arrays of single-walled carbon nanotubes (SWCNTs) and coordinator molecules was carried out in this work, using the method of molecular dynamics (MD), as it allows to observe the development of a model structure in time. A mechanism formation of supramolecular structures based on nanotubes and coordinator molecules has been employed as a working hypothesis for simulation model [1].

An array of three nonchiral SWCNTs with a diameter of ~ 1 nm and a length of ~ 5 nm, coordinated by toluene was chosen as the object of study. The numerical experiment was carried out in a cubic simulation cell with 10 nm edges, with maintained temperature of 298 K. Calculations were performed using the TINKER software package [2] using the OPLS-AA universal potential [3].

At the first stage three parallel SWCNTs were fixed in the central part of the simulation cell. Then, 200 toluene molecules were injected into the cell in random order. After that, the energy minimization algorithm was launched with fixed position of the nanotubes. The calculation was carried out until the value of the total energy of the simulation system stabilized. At the second stage, the condition for fixing the nanotubes was removed, allowing them to move freely along the simulation cell together with the toluene molecules. At this stage SWCNTs formed a supramolecular structure with coordinating molecules, which moved along the simulation cell. At the third stage, toluene molecules were removed from the simulation cell in small portions. Selection of molecules for removing was carried out one by one in a random manner based on the Monte Carlo method.

As a result of simulation procedure, it was found that the toluene molecules "move apart" SWCNTs and orient them parallel to each other, creating triangular-type array. The gradual removal of coordinator molecules makes it possible to preserve the coordination of the nanotubes and create porosity in the space between them. The supramolecular structure occurs to be stable even, when a small number of toluene molecules (up to 6) remain in the simulation cell. At the same time coordinator molecules are distributed between SWCNTs closer to the center of the newly formed supramolecular structure.

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