UDK 547.854.5 PIEZO-RESPONSIVE DROP-CAST VANILLIN–BARBITURATE NANOFILMS Nebalueva A.S. (ITMO University), Muravev A.A. (ITMO University), Scientific supervisor – prof. Skorb Ekaterina Vladimirovna (ITMO University)

In this paper, a concept of piezo-responsive hydrogen-bonded organic frameworks based on vanillin– functionalized barbiturates was developed The compounds under study, vanillin-barbiturate and ethylvanillin-barbiturate, were analyzed using optical microscopy, PFM methods, it was shown that the piezoelectric response of the vanillin moiety changes markedly with an increase in the length of the ether substituent.

The development of "smart" surfaces is one of the most urgent tasks in materials science. Currently, the search is underway for organic and bioorganic molecules with a piezoelectric response in order to increase the biocompatibility. Therefore, piezosensitive materials built on hydrogen-bonded frame structures are of great interest. These assemblies can find application in many fields.

In this paper, we took barbituric acid and vanillin/ethylvanillin as the initial components of the reaction. Replacement of the substituent at ether oxygen atom of vanillin moiety from methyl to ethyl group enhanced stacking interactions resulting in needle (methyl group) or star-shaped aggregates (ethyl group). This type of assembly was observed by SEM (Scanning Electron Microscopy). Our system was modeled by computational chemistry (Quantum Mechanic) using quantum chemical calculations, we investigated the formation of which supramolecular assembly is advantageous and how the different structure of assembles affects the appearance of crystals and the properties of these supramolecules. This gave a several-fold increase in piezoelectric effect. In PFM, an alternating voltage is applied between the needle pressed to the sample surface and the sample. In the presence of a piezoelectric effect, the sample changes size under the influence of voltage, which leads to the appearance of vibrations of the probe pressed against it. We examined this response not only in the crystals themselves, but also in films created on the basis of the initial components used in the work, using a gelation agent. The piezoeffect was observed in films as well.

Thus, supramolecular assemblies with different properties were obtained by changing the structure, and since piezosensitive materials are in demand in sensorics, the systems designed and described by us can also be used in this industry.