Annotation for master's thesis

«Calculation of intermolecular interaction to predict the crystal packing motif of organic semiconductors»

Master student of group 225 Gultikov N.V.

Scientific adviser: Ph.D. Sosorev A. Yu.

In this work was developed a theoretical method for predicting the crystal packing motif. In our method, the interaction energy is the sum of the interaction energies of various dimers. We don’t take into account the influence of external factors, such as pressure and temperature. To find the interaction energy of dimer molecules, the geometry of the molecule itself was initially optimized using DFT. Then dimers were created, whose geometry was also optimized using DFT. In our technique, we assume that all the proposed types of crystal packings consist of such types of dimers, whose geometry is optimized. Based on the data of numerical calculations, the binding energy between the dimer molecules and, accordingly, the total energy of interaction of the molecule with its environment for the selected types of crystal packings have already been calculated. The higher the total interaction energy, the more energy-efficient the system is to be in this state, to have a certain crystal packing.

Using DFT, the geometries of monomers and different types of dimers were optimized and their ground state energies were obtained for all molecules under study. The total interaction energies of the assumed types of packagings for all the studied molecules, which in our approximation is made up of the interaction energies of dimers, are calculated. Based on these calculations, crystal packings are successfully predicted. However, for octafluoronaphthalene, the technique gave the wrong packaging.