Modeling of charge transport in conjugated oligomer crystals

In recent decades, active fundamental and applied research in the field of organic electronics based on organic semiconductor materials has been conducted. One of the most promising types of organic semiconductors are crystals of conjugated oligomers. Recently, it has been shown that a new type of organic semiconductors, oligothiophene-phenylens, combine high charge carrier mobility and effective luminescence, which makes them very promising for optoelectronics. However, reliable experimental measurement of mobility requires technically complex manufacturing of samples, and the palette of organic materials is infinitely diverse. In this regard, the theoretical evaluation of mobility is in demand.

The aim of the paper is a theoretical estimate of the mobility of charge carriers in oligothiophene-phenylene crystals, as well as suggestions for ways to improve it. The simulation is performed using methods based on the Markus model for charge transfer, the parameters of which are the reorganization energy and the transfer integrals. Using the quantum-chemical model, the charge mobility in crystals of various conjugated oligomers promising for organic electronics and optoelectronics is estimated. In this case, charge transport in oligothiophene-phenylene crystals is modeled for the first time. It is shown that the reorganization energy of the molecules decreases with increasing size, and the transfer integral strongly depends on the mutual arrangement and on the structure of the molecules. The applicability of various methods of calculation is also discussed. Based on these data, the most promising oligothiophene-phenylene materials were identified and ways of increasing the efficiency of charge transport in crystals of this class were proposed.