Work title: spectroscopic assessment of charge transport in organic semiconductors

Scientific Adviser: Bruevich Vladimir

Organic electronics is a new, rapidly growing field of science, involving the development of electronic devices based on films and crystals of organic semiconductors (OS). These materials have unique advantages, not peculiar to traditional inorganic analogues, such as: flexibility, lightness, transparency and low price. The most important property of semiconductors is carrier mobility - μ. This characteristic determines the performance of key devices of semiconductor electronics, such as a field-effect transistor (FET) and light-emitting transistor (LET). Despite decades of intensive study of charge transport in the OSs, an understanding of the processes underlying its effectiveness remains unclear. In addition, there is the problem of a reliable measurement of μ. In recent studies, it was shown that the nonlocal electron-phonon coupling, which is associated with the existence of low-frequency (LF, <200 cm^{-1}) intermolecular vibrations, plays a crucial role in limiting the mobility in the OSs. However, the theoretical study of the low-frequency oscillatory structure and nonlocal electron-phonon interaction is significantly limited by the capabilities of modern computational methods.

This work is devoted to an experimental study of the effect of nonlocal electron-phonon coupling on the charge transfer process in OSs by Raman spectroscopy.

In the framework of this work, an experimentally measurable spectroscopic parameter (ξ) was proposed for the search for an OS with a weak nonlocal electron-phonon coupling and, therefore, potentially having a high carrier mobility. The correlation between ξ and μ has been demonstrated in a series of well-known highly mobile OSs. In addition, a correlation between the temperature dependence of ξ and μ has been demonstrated for some highly mobile OSs. On the basis of experimental data, a model was tested to estimate the mobility of charge carriers in an OS (spectroscopic mobility — μ_s), which allows one to dispense with the calculation of the nonlocal electron-phonon interaction constant when it is used. A correlation of μ_s and experimentally measured μ for a number of OSs with mobility that is several orders of magnitude is demonstrated.

In addition, using the example of TCNQ and F2-TCNQ crystals, the possibility of using low-frequency Raman spectroscopy to study the nonlocal electron-phonon interaction in various directions of an organic crystal is shown.