Density of States in Locally Ordered Amorphous Organic Semiconductors: Emergence of the Exponential Tails

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Density of states (DOS) is one of the most important characteristics affecting charge carrier transport in organic semiconductors. The total shape of the DOS in the particular material is typically rather complicated. Fortunately, for the consideration of the charge transport properties at typical operating temperatures the deep tail of the DOS is most important, and the problem becomes much more tractable. Two popular models of the tail are the Gaussian model and exponential model. Here we consider a new mechanism of the formation of the exponential tails in locally ordered amorphous organic semiconductors.[1] The starting point is the model of the qudrupolar glass having the DOS dominated by electrostatic contributions, which is suitable for the description of many nonpolar organic materials. We assume that the quadrupoles are arranged in blocks and the orientations of all quadrupoles in the block is the same while the orientations in different blocks are random. It turns out that for blocks having linear size of about 5 molecules or more the tails become exponential, while for the totally random orientation of all quadrupoles they have the Gaussian shape (Figure 1).

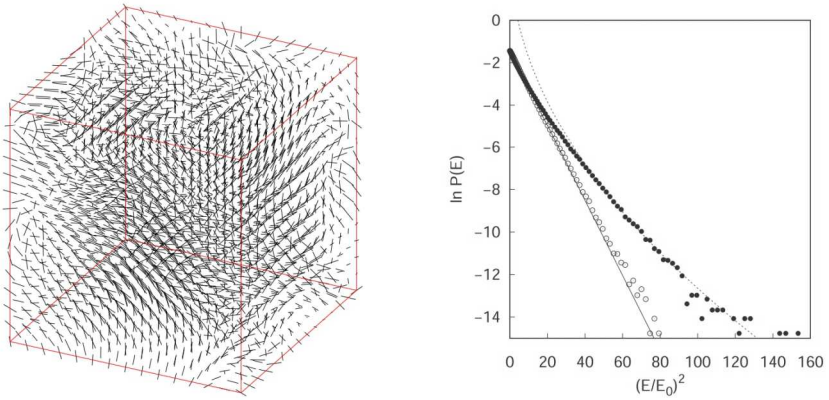

Figure 1. Typical spatial distribution of axial quadrupoles (left) and the DOS for the average linear size of the block equals to 5 molecules (right, empty circles show the low energy tail and the filled circles show the high energy tail, broken line shows the best exponential fit, solid line corresponds to the Gaussian central peak). Parameter $E_0 = eQ/\varepsilon a^3$ is the scale of energy (here Q is the quadrupole moment, a is the lattice scale, and ε is the dielectric constant). We assume that $eQ > 0$, for the opposite sign of eQ the tails are interchanged.

For the quadrupoles having axial symmetry the DOS is asymmetric, while for planar quadrupoles it is symmetric. Particular structure of the blocks is not very important and the only significant parameter is the average size of the blocks (their shape could be random or regular, e.g. cubic, interfaces between blocks could be sharp or smoothed). For this reason we believe that the suggested mechanism of the formation of the exponential tails is rather common and may occur in various organic materials.

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[1] S.V. Novikov, *J. Chem. Phys.* 2021, **154**(12), 124711.