

Problems with the Gaussian density of states in organics: definite solution, ambiguous, and hardly any solution

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Disordered organic materials are the basis of organic electronics with organic light emitting diodes for displays and lighting, organic field-effect transistors (OFET) and circuits made with them, and organic solar cells. Almost twenty years since the pioneering work of Bäessler [1] on hopping transport in disordered organics it is widely accepted that the density of states (DOS) is a Gaussian. From the application of various numerical models for the mobility, a variance of the order of 100 meV seems to be typical. Although a large number of device modelling using the Gaussian DOS has been published, support of design and technology of devices by full two-dimensional simulation is required. Until recently this possibility was not completely implemented in the simulation programs as sDEVICE [2] or ATLAS [3] due to peculiarities of the Gaussian DOS. We discuss here three problems important for implementation and application.

Fast and efficient numerical simulation requires analytical expressions for the carrier density (as the Fermi integral for the square-root DOS). Alternatively, the numerical integration of the product of the DOS and the Fermi distribution is in principle possible and for some cases of non-parabolic bands available. For the Gaussian DOS we developed an analytical approximation for the carrier density (Gauss-Fermi integral) [4] which is meanwhile implemented in sDEVICE [2]. Detailed testing and comparison with experimental OFET current characteristics is in progress but is also connected with further problems.

For the Gaussian DOS an enormous amount of theoretical work on the mobility has been done and published. The extended Gaussian disorder model (EGDM) [5, 6] (describing the dependence of the mobility on temperature, carrier concentration, and field) was to our opinion a first highlight after Bäessler, followed later by the extended correlated disorder model (ECDM). However there exist many other models, also from recent times, with different dependencies. There remain serious ambiguities: Which model is applicable to a given organic material, which parameters should be used or how one can determine them, are the models sufficient for application at high concentrations and high fields?

Most problematic is the question what the band edge is and how to determine it. As a routine method the valence band edge is determined by ultraviolet photoemission (UPS). However, this method probes regions of the DOS which are unoccupied in devices and transport takes place

at much lower energies not accessible up to date by UPS. Moreover, the upper part of the UPS spectrum below the gap is rather broad compared with the narrow hopping transport DOS. Thus we do not really know where this DOS is situated. We supposed [7] that the transport DOS is the narrower tail of the broader UPS distribution. With some uncertainty one can then fix the position of the Gaussian transport DOS on the binding energy scale. But there remains a further problem, namely where is the band edge situated relative to the maximum of the Gaussian DOS. The method presented in [7] is not unique and we will discuss several other possibilities, but until now without a definite choice. It might be that the injection into a Gaussian DOS requires a new theoretical treatment and its implementation beyond the traditional one.

References

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