New advances in analytic continuation method: novel strategy and studies of mobility and defects in organic semiconductors.

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We unite the advantages of the stochastic optimization (SO) [1] method and recently developed method of consistent constraints (CC) [2] to obtain an effective unbiased SOCC [3] method of solving Fredholm equation of the first kind. Unbiased and effective SOCC formalism is used to obtain mobility of polarons from current-current correlation function and to study distribution of the carrier traps in the field effect transistors based on organic materials

We present the first unbiased results for the mobility μ of a one-dimensional Holstein polaron [4] obtained by numerical analytic continuation combined with diagrammatic Monte Carlo method in the thermodynamic limit. We have identified for the first time several distinct regimes in the λ-T plane including a band conduction region, incoherent metallic region, an activated hopping region, and a high-temperature saturation region.

We develop a novel method for obtaining distribution of trapped carriers over its degree of localization, based on the fine analyses of the electronic spin resonance (ESR) spectra for low enough temperatures where all carriers are localized [5]. For a single molecule the ESR spectrum S(B) can be represented as derivative of the Gaussian with the width σ_0 determined by the hyperfine splitting. According to the Central Limit Theorem the width of Gaussian is narrowed by the factor $N^{-1/2}$ if the carrier is spread over N molecules. Localized states in solids can be described by probabilities p_i for carrier to occupy the site i. It can be shown that the ESR signal in this case is also represented as derivative of Gaussian but with effective $N = (\Sigma_i \, p_i^2)^{-1}$. In a more complicated case with several types of traps of different origins one can introduce a distribution function D(N) over effective N. The shape of the ESR signal S(B) for distribution D(N) is

$$S(B) = \int_1^{+\infty} D(N) \frac{\partial G}{\partial B}(B,N)\, dN \quad , \qquad (1)$$

where $G(B,N) = \sqrt{\frac{N}{2\pi\sigma_0^2}} \exp\left[-\frac{N(B-B_0)^2}{2\sigma_0^2} \right]$. Integral equation (1), where unknown function is the distribution D(N)**,** is solved by SOCC method revealing the distribution of the traps D(N) over its' effective degree of localization N. To get the distribution of trapped carriers over the binding energies $F(E_B)$ we solve the problem of polaron localization on an attractive impurity by means of direct-space Diagrammatic Monte Carlo (DMC) implemented for the system in the thermodynamic limit [6].

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