Highlights

ACTIVITY E Advanced materials and techniques for organic electronics, biomedical and sensing applications 2020

Electronic properties of one-dimensional pentacene crystals

C. Nappi[1], F. Romeo[2], E. Sarnelli[1,]

[1]CNR-SPIN Institute of Superconductors, Innovative Materials and Devices, UOS-Naples, Naples 80126, Italy
[2]Physics Department "E. R. Caianiello" , University of Salerno, Fisciano 84084, Salerno, Italy
[3]INFN, Naples Division, Naples 80126, Italy

NANO EXPRESS 1, 030002 (2020)

We have studied the charge transport properties of a 1D pentacene crystal with a general view to provide clues in understanding the peculiar physics of the organic semiconductors. In the tight binding approximation, and neglecting hydrogens, we have calculated the energy band structure of the pentacene solid system allowing for a variable coupling Γ between molecules. In this way we can range from the coupling of a tight packing structure, close to that of a graphene nanoribbon (Γ~3eV), to the loose packing one of a weak interacting pentacene aggregate (Γ → 0eV). Our model illustrates how an energy bandgap opens up and evolve in amplitude, reaching a maximum of ~1.4 eV in correspondence of Γ=1.74 eV. This maximum value is characterized by a crossover in the energy bands between HOMO LUMO and secondary HOMO LUMO levels. The subsequent evolution with Γ consists in a lowering of the bandgap amplitude, up to zero (existence of a second metallic point) and a regrowth, up to the energy difference between HOMO and LUMO of an isolated pentacene molecule (1.3eV). Next, we used the model to calculate the conductance of an assigned micrometric length portion of crystal and simulate a gate operation in a voltage range of a few ten of volts (Figure 1) . No specific disordered has been introduced in the regular crystal structure, while we have considered a generic scattering mechanism represented by a phenomenological relaxation time τ. We obtain typical conductance values of 0.01–0.2μS with a relaxation time of 1fs. After having derived the relationship between conductance and mobility of the 1 D model, we have obtained mobility values as a function of the gate voltage (Figure 2) for two significant cases of semiconductive crystals with moderately low overlap integrals: Γ=0.15 eV and Γ=0.12 eV (corresponding to a bandgap of Eg=1.05 eV and Eg=0.6 eV, respectively) obtaining mobility values in very good agreement with the observed values of literature.

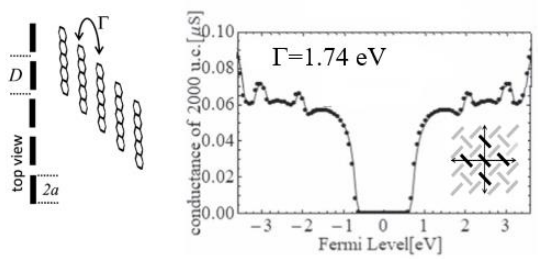

Fig. 1: (Left) Schematic representation of a one-dimensional pentacene crystal studied in this work. Γ is the (distance dependent) inter-molecular hopping energy. (Right) Calculated conductance of a 2000 unit cell long (L~1μm) pentacene crystal vs chemical potential, for Γ=1.74eV. The bandgap energy of the crystal is maximum for this value (E_g=1.4eV). A relaxation time τ of 10^{-15} s was used.

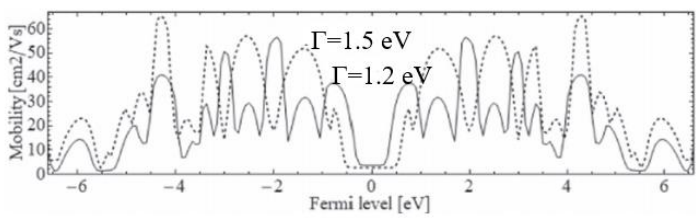

Fig. 2: 1D pentacene crystal mobility as a function of the Fermi level calculated in the present model with Γ=1.5eV and Γ=1.2eV. The obtained mobility values span the range between 10 cm^2/Vs and 50 cm^2/Vs which is compatible with the accepted experimental values from the literature. In close vicinity of the Fermi level of the pristine system (E_F=0) the channel conductance can be effectively controlled by using a back gate, the latter observation being relevant to set the device working point for applications.