We first review the current state-of-the-art in the field of organic electronics and then focus on organic solar cells, which we define as solid-state cells in which the semiconducting materials between the electrodes are organic, be them polymers, oligomers, or small molecules. We describe the optical and electronic processes that take place in such cells and turn our attention briefly to: (i) optical absorption and exciton formation; (ii) exciton migration to the electron donor – electron acceptor interface; (iii) exciton dissociation into charge carriers, resulting in the appearance of holes in the donor component and electrons in the acceptor component; (iv) charge carrier mobility; and (v) charge collection at the electrodes [1-3].

In the second part of the presentation, we underline the complexity of the processes taking place at the nanoscale at the donor/acceptor interfaces and highlight the molecular understanding that comes from a computational approach combining electronic-structure theory calculations, molecular mechanics / molecular dynamics simulations, and Monte Carlo simulations [4-6].

References: