# Study of Electronic Processes in Organic Semiconductor Devices: Atomic and Mesoscopic Scale Modeling and Computer Simulations

**Murat Mesta**

**Abstract:**

Recent advancements in organic materials has resulted in a new field in technology called “organic electronics” promising properties such as mechanical flexibility and large area production. A particularly exciting class of devices are organic light-emitting devices (OLEDs) and organic solar cells(OSCs), whose optoelectronic character have not been fully understood due to their disordered structure that localizes charge-carriers not in energy bands but in specific molecular states (sites). Computer simulations are essential in this sense where we can address both the steady-state and time-dependent behavior of devices at the mesoscale, and atomic properties using fully ab initio approaches at the molecular level. We perform Monte Carlo simulations to study charge and exciton dynamics in a multilayer OLED. In the first part of the talk, I will present our simulation results of emission profile, current-density, and efficiency analysis agreeing well with the measurements. The time-dependent response of a conducting polymer is simulated using a master equation approach modeling dark-injection and impedance spectroscopy of hole-only transport. In the second part, I will show the results of our computational screening of materials used in polymer solar cells using the density functional theory simulations and machine learning. We calculate polymer properties from a tight-binding approach over DFT results then build a grammar variational autoencoder machine learning tool trained on thousands of DFT results to estimate the properties of molecules outside the set of our calculations.