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How Microstructure Defines Function in Organic Conjugated Materials: Insights from Modelling

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Organic conjugated materials have attracted an increasing interest over the years for their use in organic opto- electronic devices such as light-emitting diodes, solar cells, or field- effect transistors as a result of their low cost, light weight and ease of processing from solution. The improvement of the device performances requires a deep understanding of the electronic processes taking place in these devices down to the molecular scale. Especially, the way organic conjugated molecules or polymer chains organize in the solid state appears as a critical parameter to control in order to fine tune the materials electronic and photophysical properties. In our laboratory, we have developed a multi-faceted modeling scheme that encompasses classical molecular dynamics, quantum-chemistry, non-adiabatic quantum dynamics and kinetic Monte Carlo simulations to assess multiple fundamental opto- electronic processes occurring in conjugated materials used in devices. Here, we will more specifically review work dealing with the modeling of charge transport in conjugated polymers as well as singlet fission and exciton transport in small molecules. In all cases, we will highlight how these processes are sensitive to the relative arrangement of the materials at the nanoscale.