Interfacial electronic properties in functional organic materials for energy conversion

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Over the past two decades, the science and engineering of organic semiconducting materials have advanced very rapidly, leading to the demonstration and optimization of a range of organics-based solid-state devices, including organic light-emitting diodes, field-effect transistors, photodiodes, and photovoltaic cells. Particularly attractive for organic semiconductors are flexible plastic substrates that can lead to applications and consumer products with lower cost, highly flexible form factors, and light weight. These attributes, combined with the ability to tune the physical properties of organic (macro)molecules by fine tuning their chemical structure, constitute the main drivers boosting research and industrial interest in organic photovoltaics.

Critical to the operation of organic solar cells are the interfaces between (metal or conducting oxide) electrodes and organic layers and between organic layers. In this presentation, we focus on the computational characterization of these interfaces by means of quantum-mechanical calculations and molecular simulations. We are especially interested in gaining an understanding of the electronic and geometric structure of the interfaces, in order to optimize the efficiency of the various optical and electronic processes taking place in the solar cells.