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Frontiers of controlling energy levels at interfaces

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The alignment of electron energy levels at interfaces between semiconductors, dielectrics, and electrodes determines the function and efficiency of all electronic and optoelectronic devices. Reliable guidelines for predicting the level alignment for a given material combination and methods to adjust the intrinsic energy landscape are needed to enable efficient engineering approaches. These are sufficiently understood for established electronic materials, e.g., Si, but for the increasing number of emerging materials, e.g., organic and 2D semiconductors, perovskites, this is work in progress. The intrinsic level alignment and the underlying mechanisms at interfaces between organic and inorganic semiconductors are discussed first. Next, methods to alter the level alignment are introduced, which all base on proper charge density rearrangement at a heterojunction. As interface modification agents we use molecular electron acceptors and donors, as well as molecular photochromic switches that add a dynamic aspect and allow device multifunctionality. For 2D semiconductors surface transfer doping with molecular acceptors/donors transpires as viable method to locally tune the Fermi-level position in the energy gap. The fundamental electronic properties of a prototypical 1D interface between intrinsic and p-doped 2D semiconductor regions are derived from local (scanning probe) and area-averaged (photoemission) spectroscopy experiments. Future research opportunities for attaining unsurpassed interface control through charge density management are discussed.