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New mechanism for work-function tuning: ZnO surfaces modified by a strong organic electron acceptor YONG XU, OLIVER T. HOFMANN, RINKE PATRICK, MATTHIAS SCHEFFLER, Fritz Haber Institute Berlin, RAPHAEL SCHLESINGER, NORBERT KOCH, Humboldt University Berlin, ANTJE VOLLMER, Helmholtz-Zentrum Berlin — A key task for optimizing optoelectronic devices comprising hybrid inorganic/organic systems is to control the energy level alignment at interfaces. The use of interlayers provides a pathway to solve this challenge. To demonstrate the concept we investigated the polar surfaces of ZnO, modified by the prototypical organic electron acceptor 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ) theoretically and experimentally. DFT-PBE ΔSCF calculations of the O 1s surface core-level shifts combined with XPS measurements suggest that ZnO(000-1)/ZnO(0001) are H/OH covered. Depositing F4TCNQ on these surfaces considerably increases the work function that is shown to be insensitive to the doping level in PBE+vdW. F4TCNQ on ZnO(0001) exhibits an extraordinary high work function due to the appearance of upright adsorption. The PBE+vdW results are in line with the UPS data that shows work-function increases up to 1.4/2.8 eV on ZnO(000-1)/ZnO(0001). In contrast to F4TCNQ on metals, where pronounced bidirectional charge transfer occurs, the charge transfer from ZnO to F4TCNQ is small, pinning the LUMO close to the Fermi level. The polarization of the system, caused by strong charge rearrangement within the adsorbate, is the main mechanism for the large work-function increase.

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