Hybrid inorganic organic systems (HIOS) are promising candidates for future (opto-)electronic devices by taking advantage of the complementary beneficial properties of two different material classes. However, inadequate interfacial energy level alignment is an intrinsic obstacle to superior device function. Hence, to design efficient HIOS devices, understanding and controlling HIOS energy level alignment is a key factor. Employing molecular electron donor or acceptor interlayers to tune the work function ($\phi$) of a metal and thus the energy level alignment relative to an organic semiconductor (OSC) was reported previously [1].

In this contribution the concept is extended to HIOS interfaces comprising ZnO. The $\phi$ and energy level alignment modification caused by deposition of several donor and acceptor molecules onto different ZnO faces is investigated. $\phi$ reductions down to 2.2 eV by using the organometallic donor $[\text{RuCp}^*\text{mes}]_2$ [2] and $\phi$ increases up to 6.4 eV using perfluorinated tetracyanoquinodimethane (F4TCNQ) [3] are demonstrated. For molecular acceptor adsorption, significant adsorption induced upward band bending of up to 0.9 eV is found within ZnO, whereas for donor adsorption no downward bending could be induced. Exploiting the huge $\phi$ modifications of ZnO, upward and downward HIOS energy level readjustments are shown, which realize ultimately low electron- or hole-injection barriers at the HIOS interface. Moreover, by using an OSC whose gap matches that of ZnO, the energy level offsets at the HIOS interface could be eliminated. This enables highly efficient, non-quenched energy transfer across the HIOS interface, which is usually inhibited by unfavorable energy level alignment.

Keywords: ZnO, energy level alignment, energy transfer

References