Energy and charge transfer in hybrid transition metal dichalcogenides/2D perovskite heterostructures (MX_2/$(PEA)_2PbI_4$)

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Van der Waals heterostructures are currently the focus of intense investigation, this is essentially due to the unprecedented flexibility offered by the total relaxation of lattice matching requirements, and their new and exotic properties compared to the individual layers. I will present the results of the experimental and theoretical studies of the novel hybrid transition metal dichalcogenide/2D perovskite heterostructures. I will discuss the first DFT calculations of a WS_2/PEA_2PbI_4 heterostructure ensemble, which reveal a novel band alignment, where direct electron transfer is blocked by the organic spacer of the 2D perovskite. In contrast, the valence band forms a cascade from WS_2 through the PEA to the PbI_4 layer allowing hole transfer. These predictions are supported by optical spectroscopy studies, which provide compelling evidence for both charge transfer, and non-radiative transfer of the excitation (energy transfer) between the layers. Next, I will demonstrate a long lived interlayer exciton formed in $MoSe_2$/PEA_2PbI_4 system. Our results show that TMD/2D perovskite heterostructures provide a flexible and convenient way to engineer the band alignment.