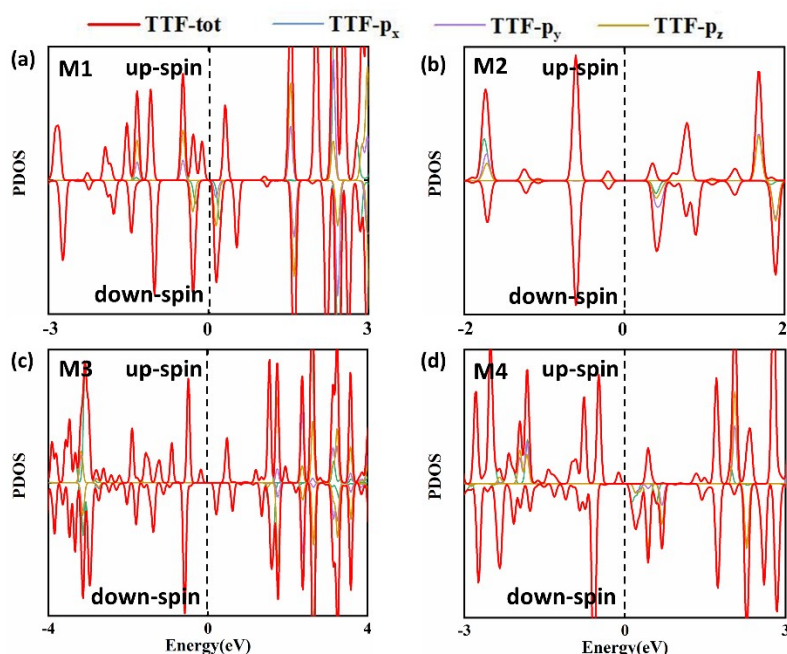


## Supplementary Material

S-Figure 1 gives the calculated the orbital-projected densities of states (PDOS) by HSE06 using Gamma kpoint. We found that M1, M2, M3 and M4 all exhibit semiconductor properties. For M1, M3, M4, the up-spin DOS peaks near to the Fermi level may shift and across the Fermi level, and thus these systems would exhibit half-metallic properties at small bias voltages. Nevertheless, compared to M1, M3, M4, the up-spin state of M2 is far from the Fermi level and that may uncross the Fermi level at small bias voltage. The results are similar to our conclusions under small bias voltages.



S1. The orbital-projected densities of states (PDOS) of TTF in ZGNRs-TTF-ZGNRs devices obtained from HSE calculation.