Peripheral and Structural Effects on the Band Gap of Acceptor-Donor Type Conducting Polymers Containing Pendant Bisfulleroid Groups

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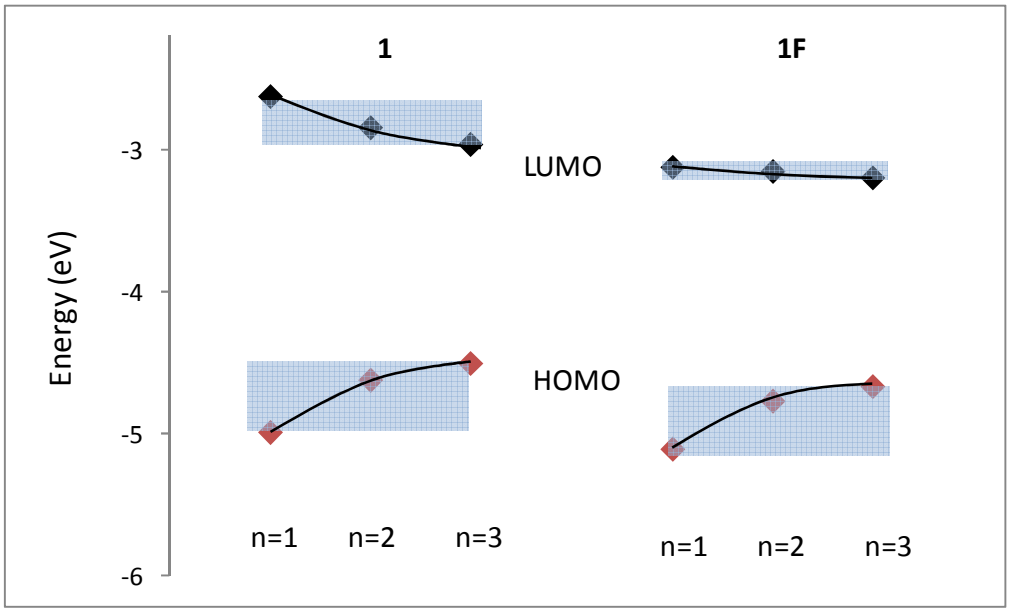

Figure 1S Change in the HOMO and LUMO levels by the extension of the conjugation in the derivatives of **1** and **1F**.

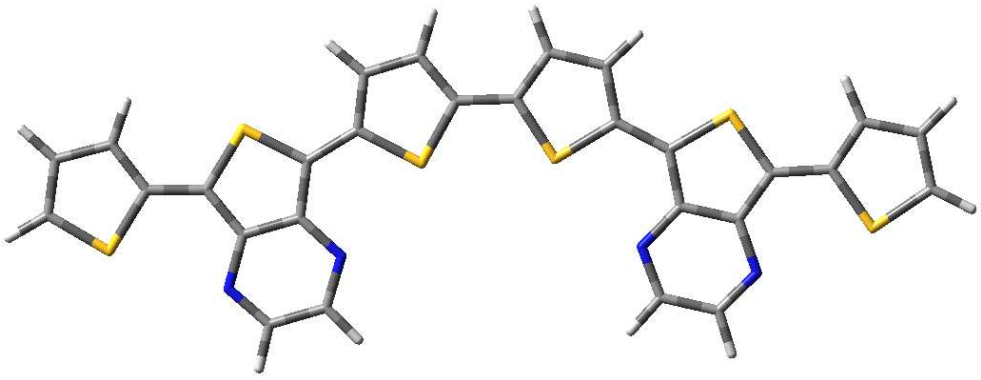

Figure 2S. MPW1B95/6-31G* optimized structure for the dimer of thiophene-thienopyrazine-thiophene where dihedral angle is 0°.

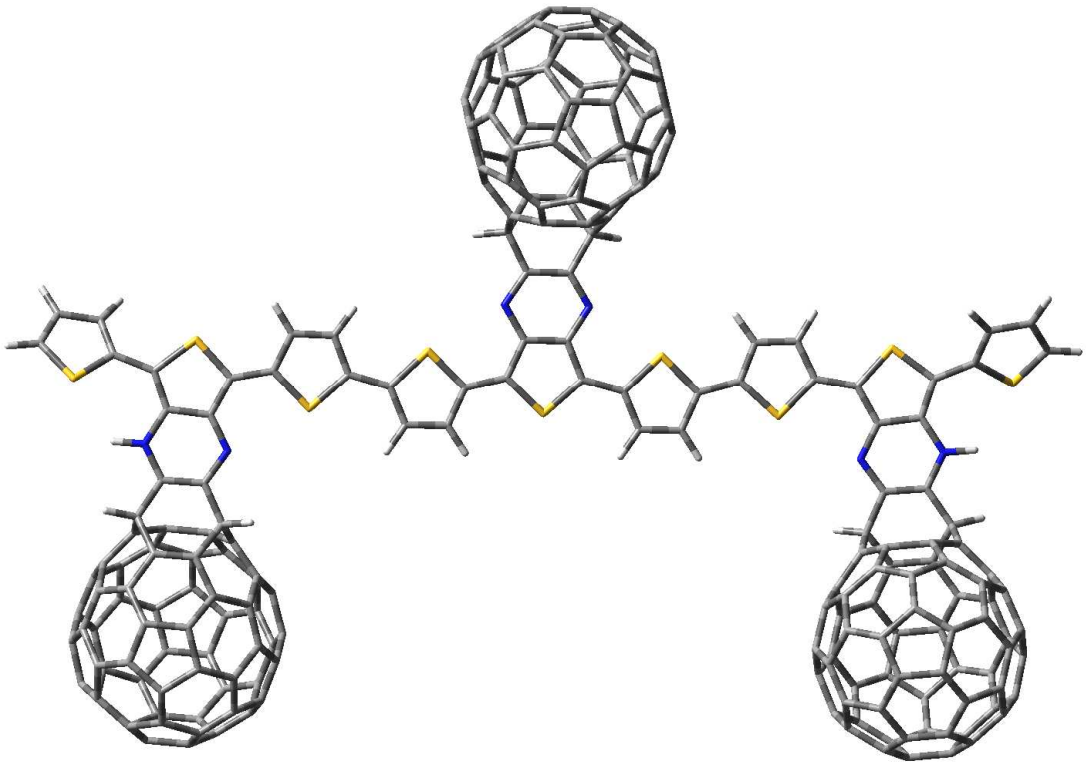

Figure 3S MPW1B95/6-31G* optimized structure of the protonated trimer of **1F**

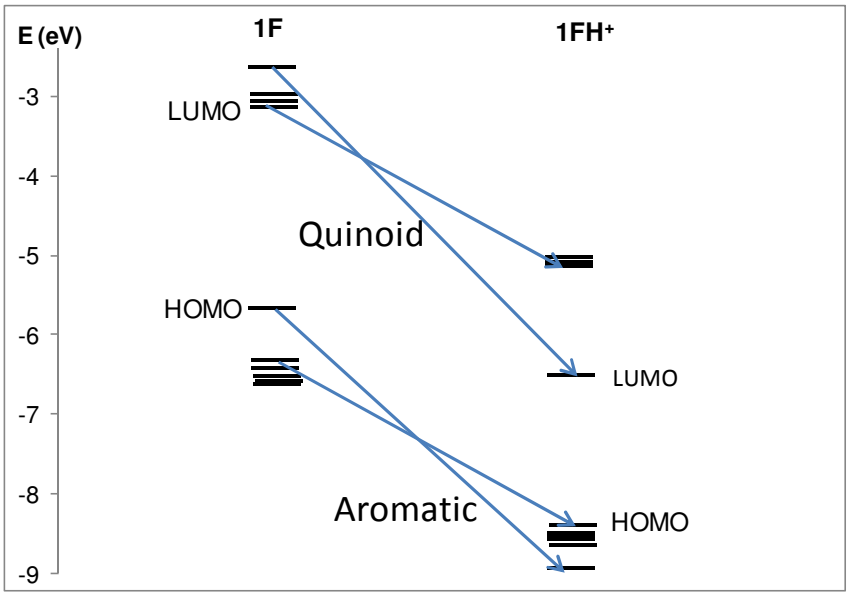

Figure 4S. Change in the orbital energy levels by protonation (MPW1B95/6-31G*)