Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Table **S1**: Energies of the GQD-dopant complexes with a variation in the position of the dopants on QDs. Energies are scaled with respect to the most stable conformation.

QD-dopant Complex	Energy of the structure in Figure 2 (eV)	Energy of the structure in Figure S1 (eV)
GQD-TCNQ	0.00	0.06
GQD-TTF	0.00	0.04
BNQD-TCNQ	0.00	0.05
BNQD-TTF	0.00	0.04

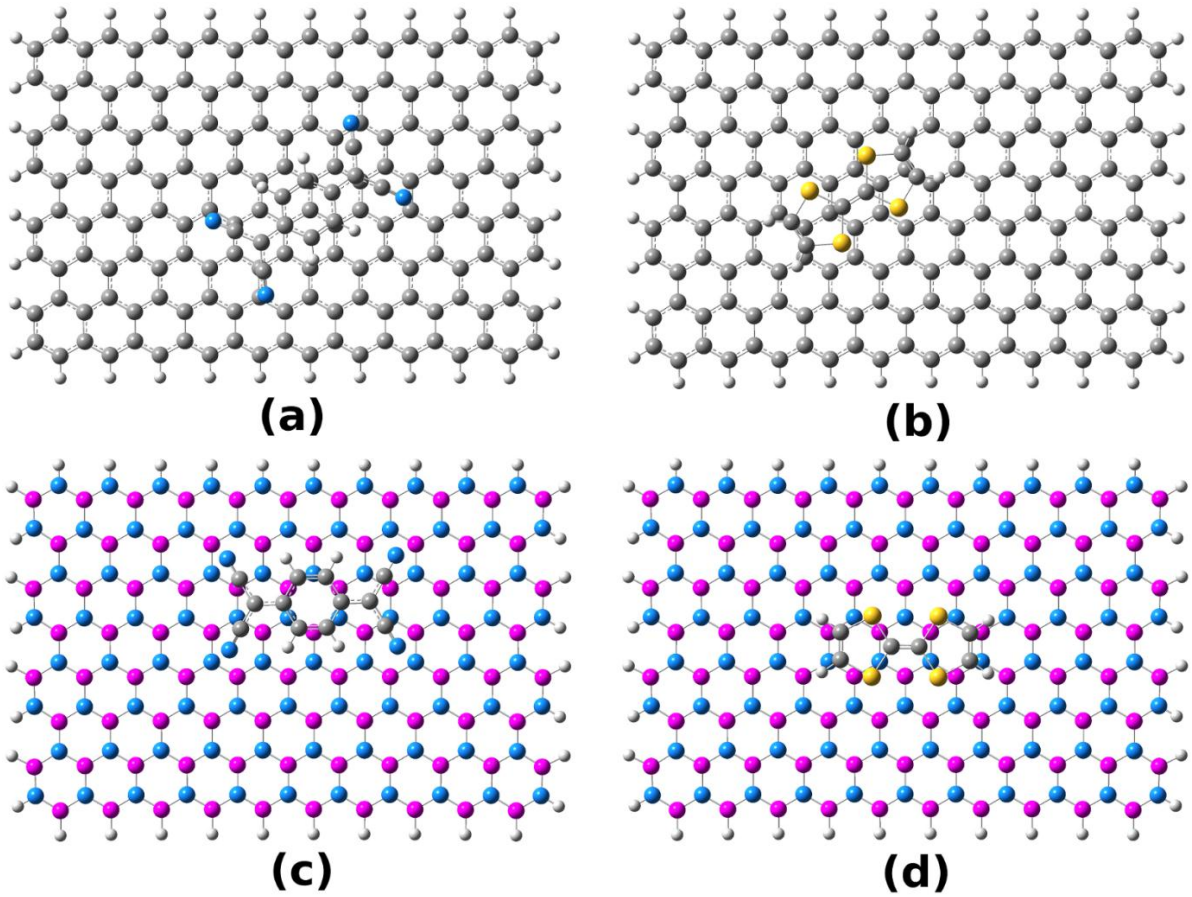

Figure **S1**: (a) TCNQ adsorbed on (21, 8) GQD, (b) TTF adsorbed on (21, 8) GQD, (c) TCNQ adsorbed on (21, 8) GQD and (d) TTF adsorbed on (21, 8) GQD. In this figure, the positions of the TCNQ and TTF on GQD are swapped with their positions on BNQD as in the figure 2, and vice-a-versa for BNQD.

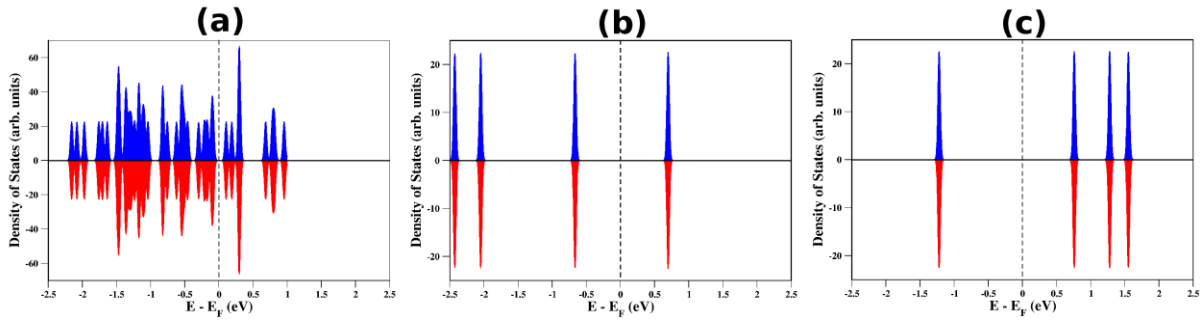

Figure **S2**: DOS plots of (a) (21, 8)-GQD, (b) TCNQ and (c) TTF show all the systems are non-spin-polarized.