Fig. S1 Transmission spectrum of M10-H at 1.0 V. Energy window imposed by the bias is shown in a box in the abscissa.

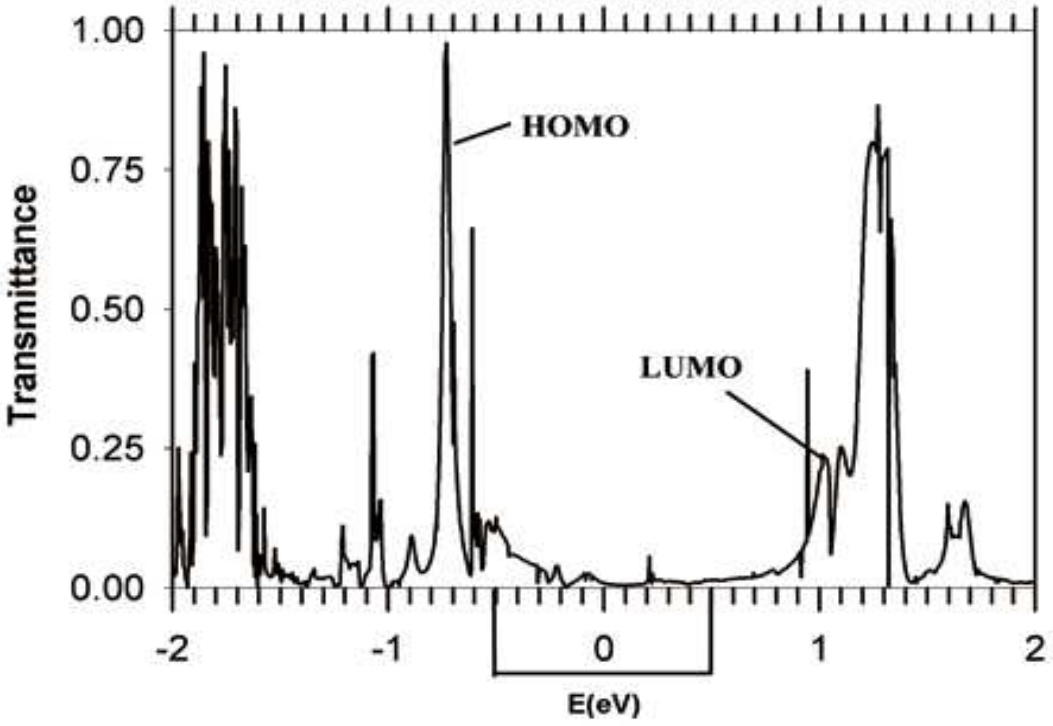

Fig. S2 Voltage drop across regions in Fig. 2 for M10-H at 1.0 V.

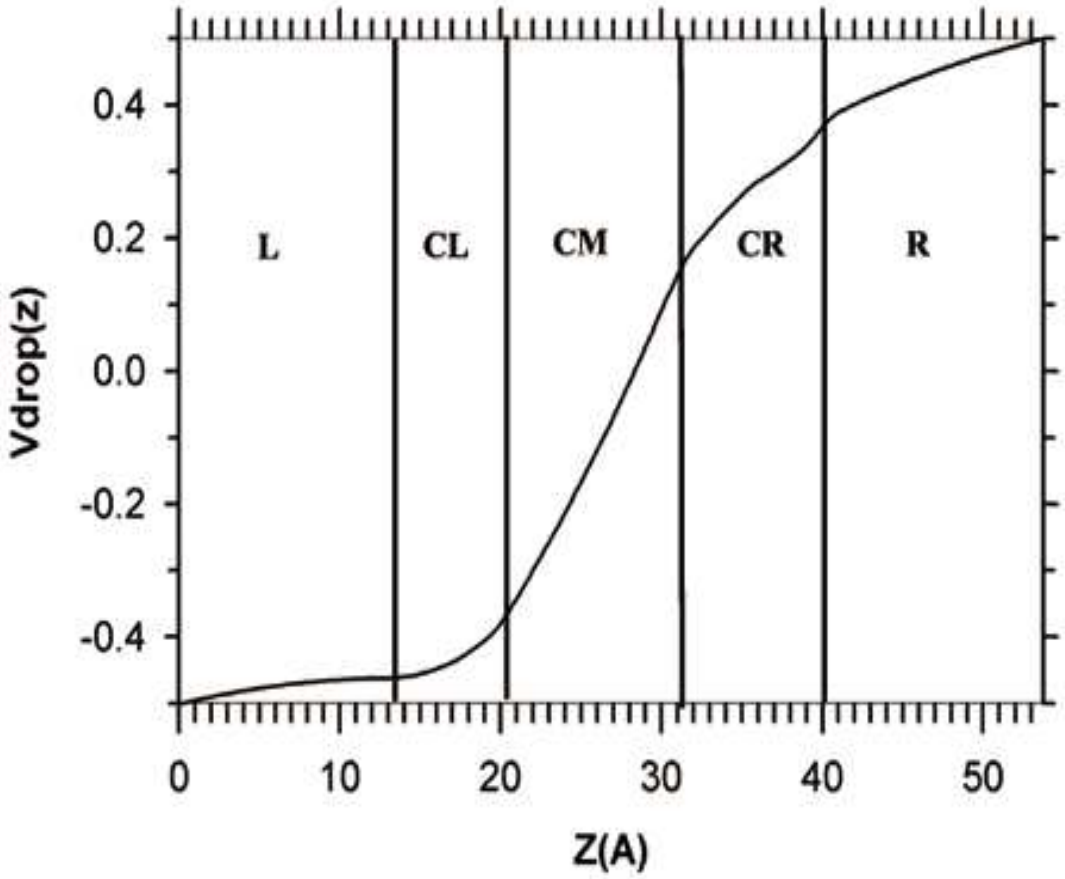

Fig. S3 Transmission spectrum of M10-H at 1.5 V. Energy window imposed by the bias is shown in a box in the abscissa.

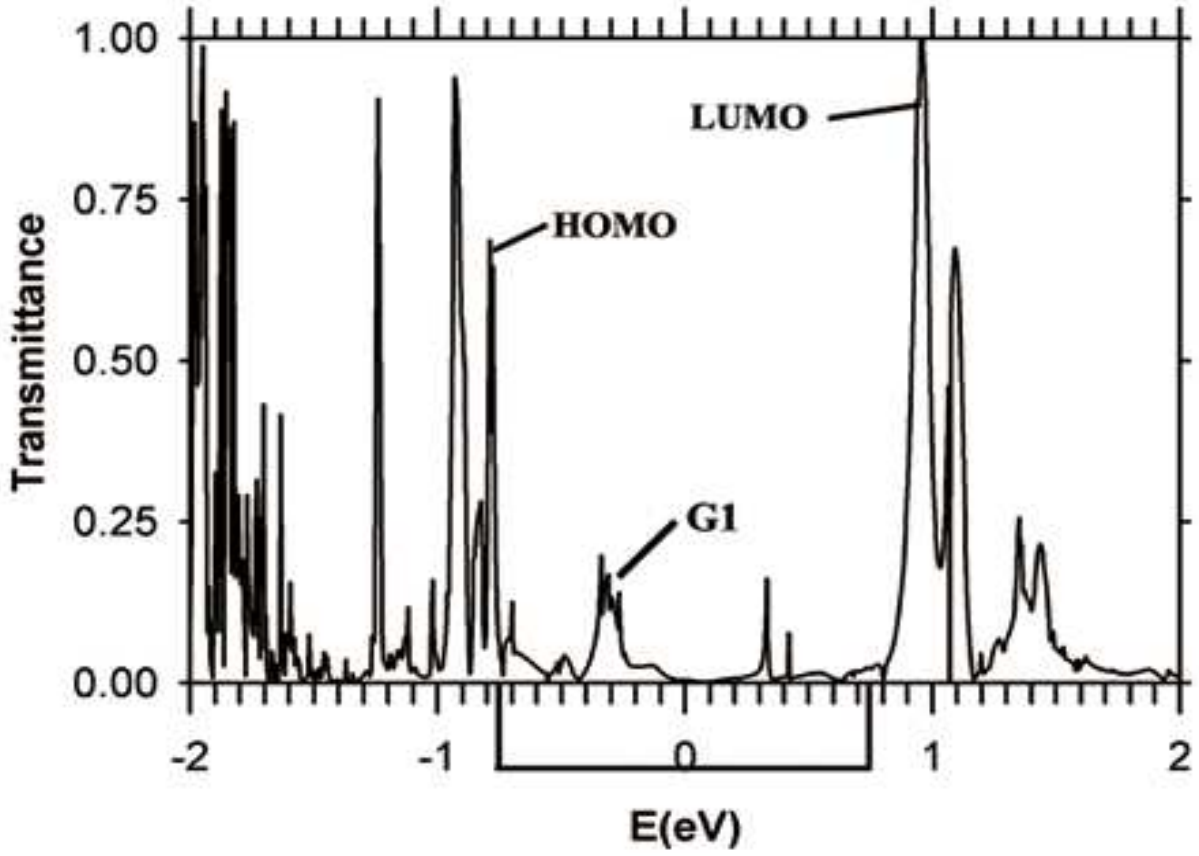

Fig. S4 Transmission spectrum of M10-H at 1.4 V. Energy window imposed by the bias is shown in a box in the abscissa.

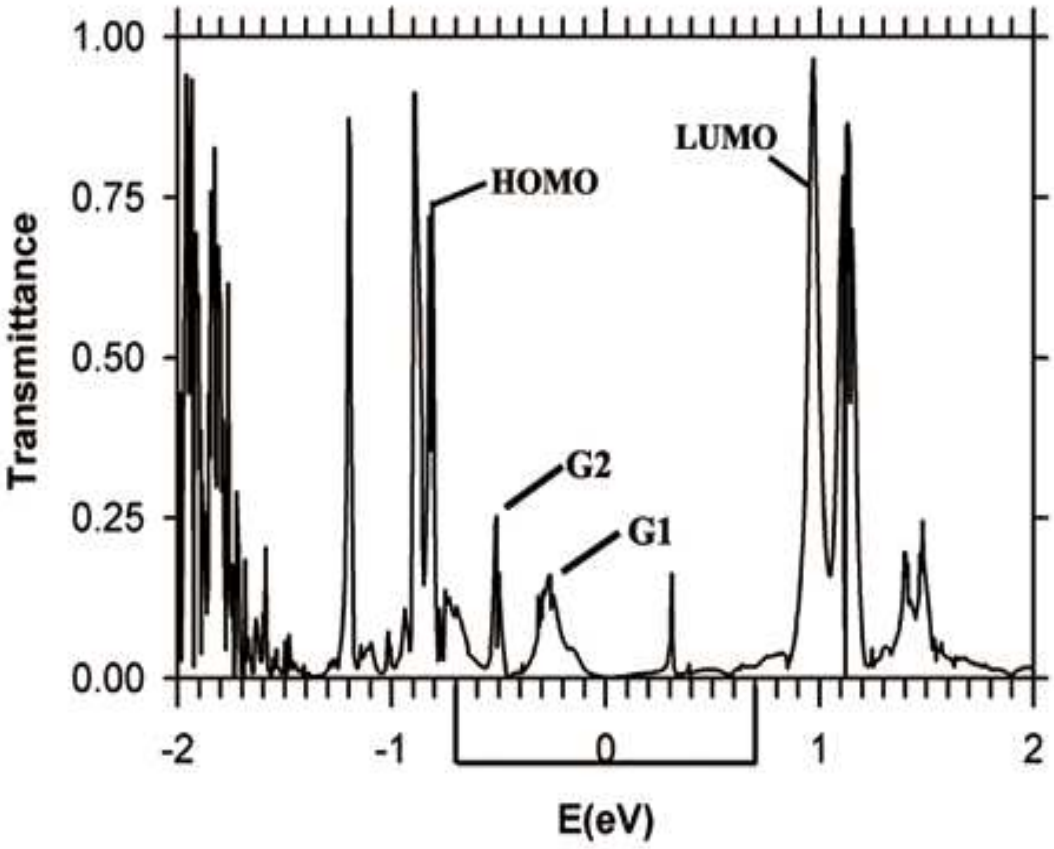

Fig. S5 Projected density of states (PDOS) of M10-H onto the molecular region at 1.4 V.

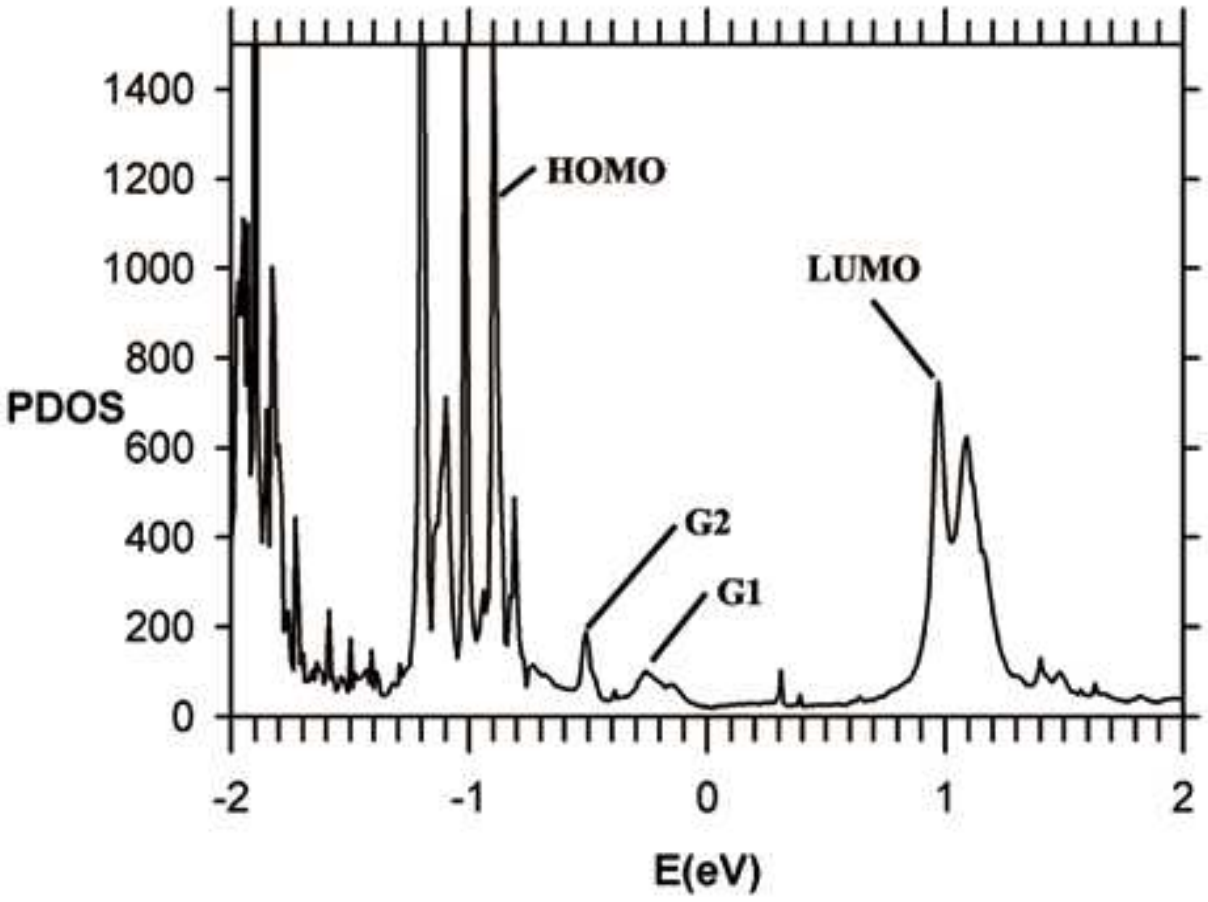

Fig. S6 Projected density of states (PDOS) of M10-H onto the surface of the CL region at 1.4 V.

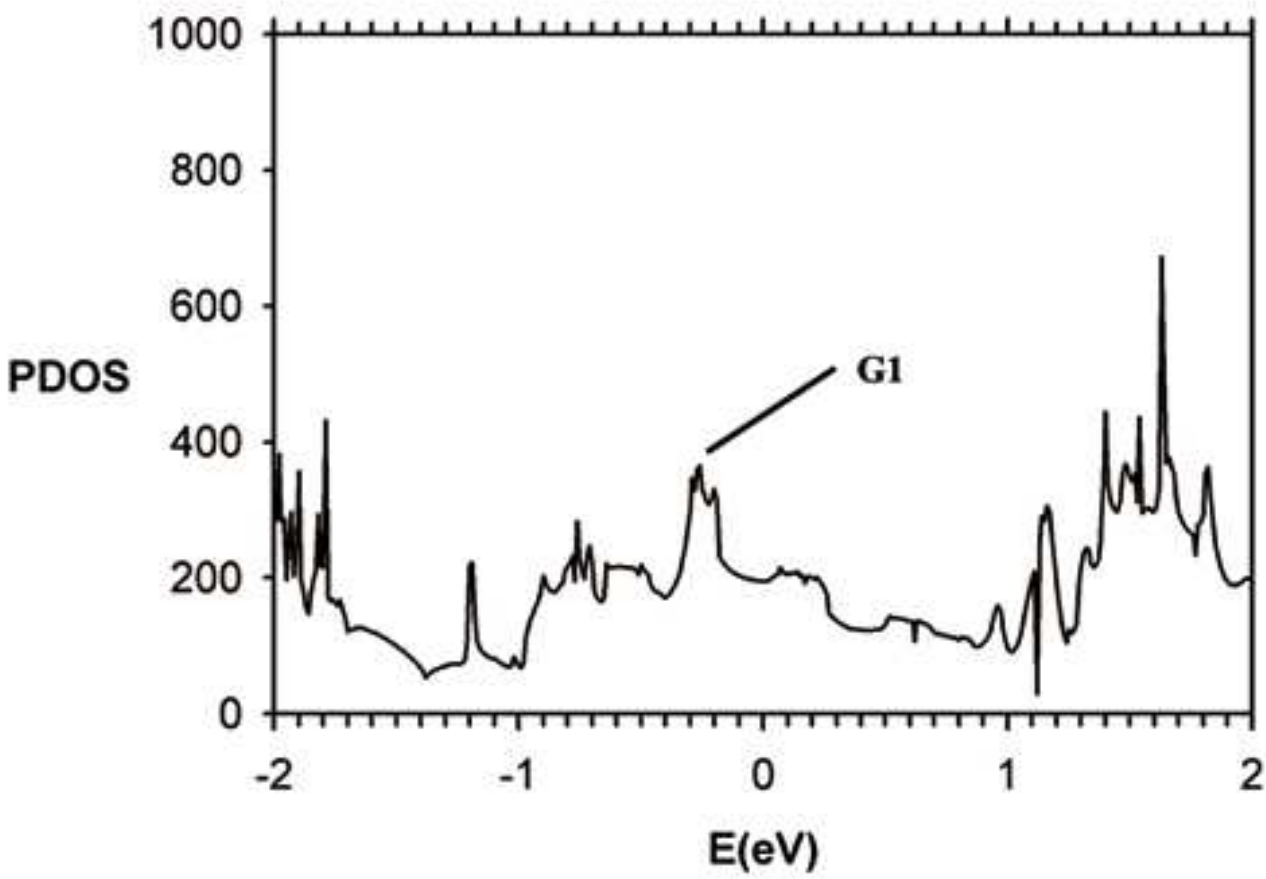

Fig. S7 Projected density of states (PDOS) of M10-H onto the surface of the CR region at 1.4 V.

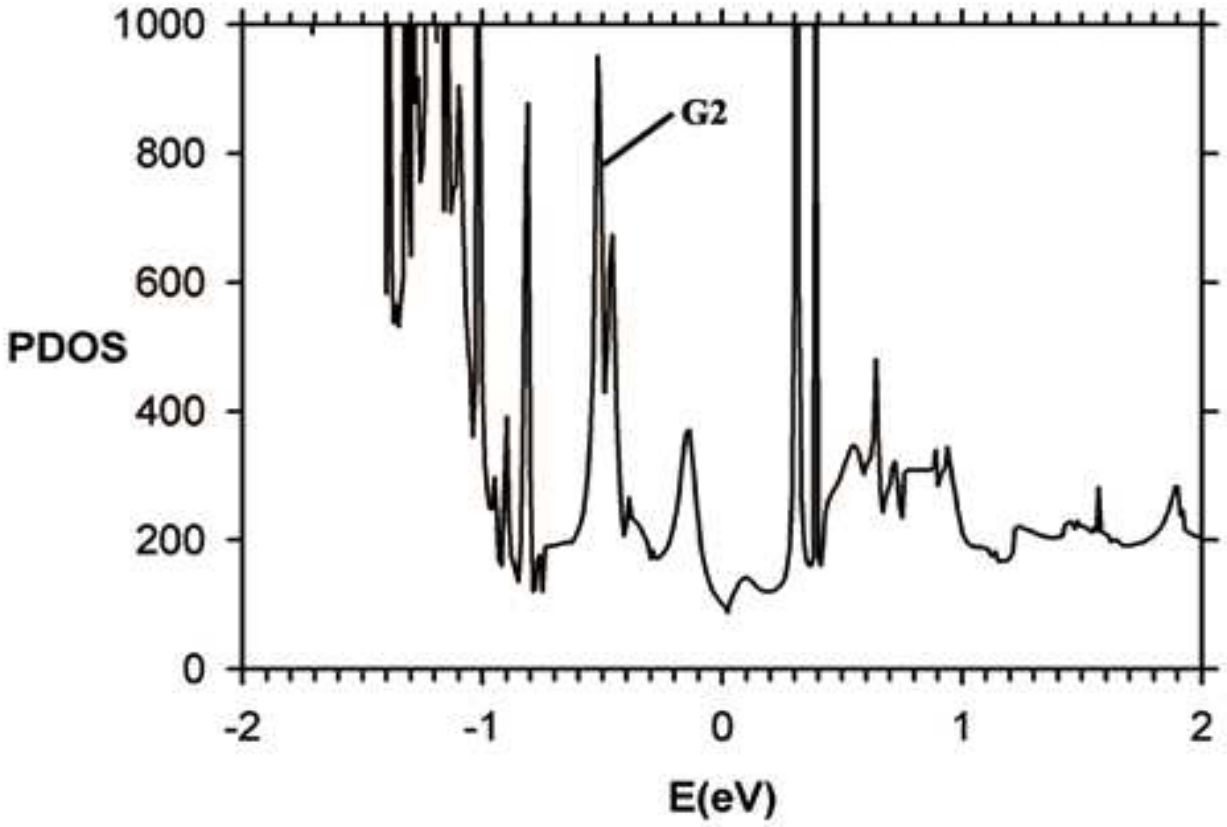

Fig. S8 Transmission spectrum of M10-H at 2.3 V. Energy window imposed by the bias is shown in a box in the abscissa.

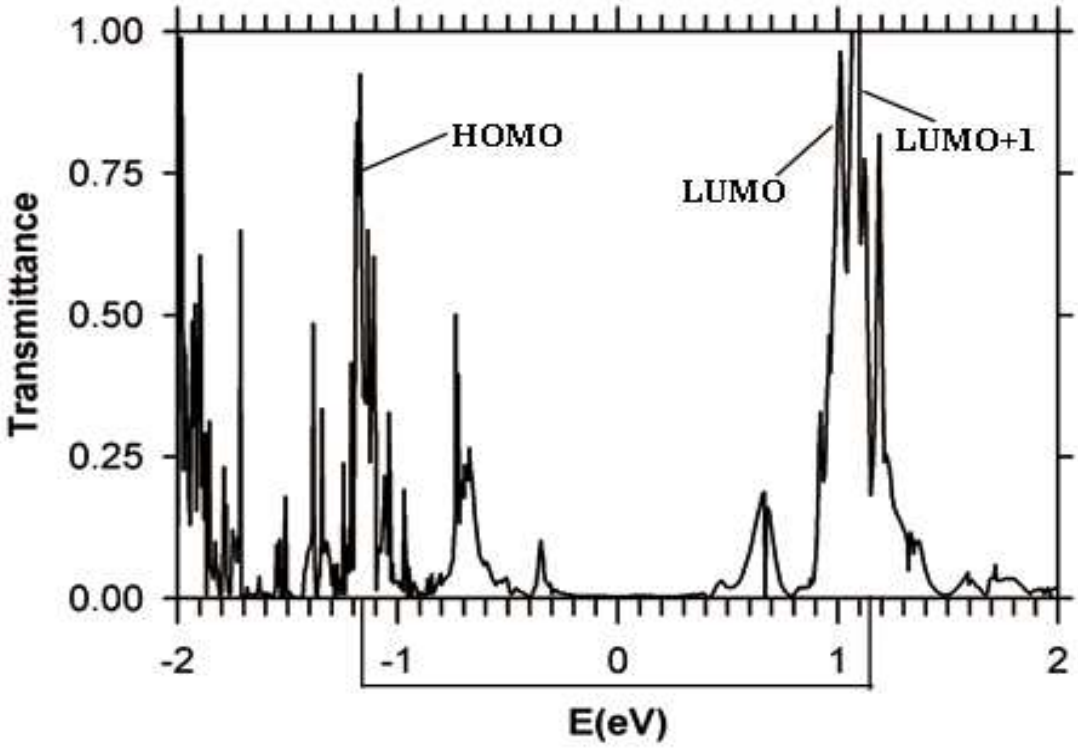

Fig. S9 Projected density of states (PDOS) of M10-Cl3 onto the surface of the CR region -2.4 V.

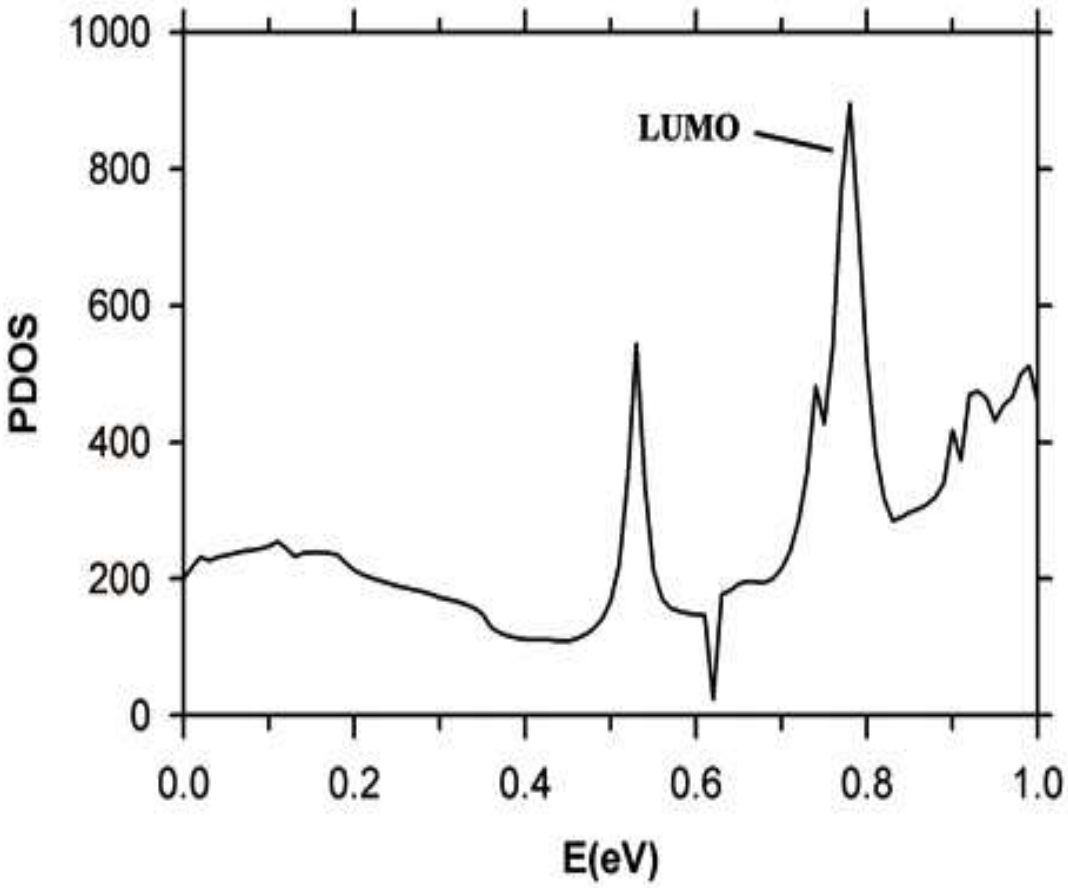
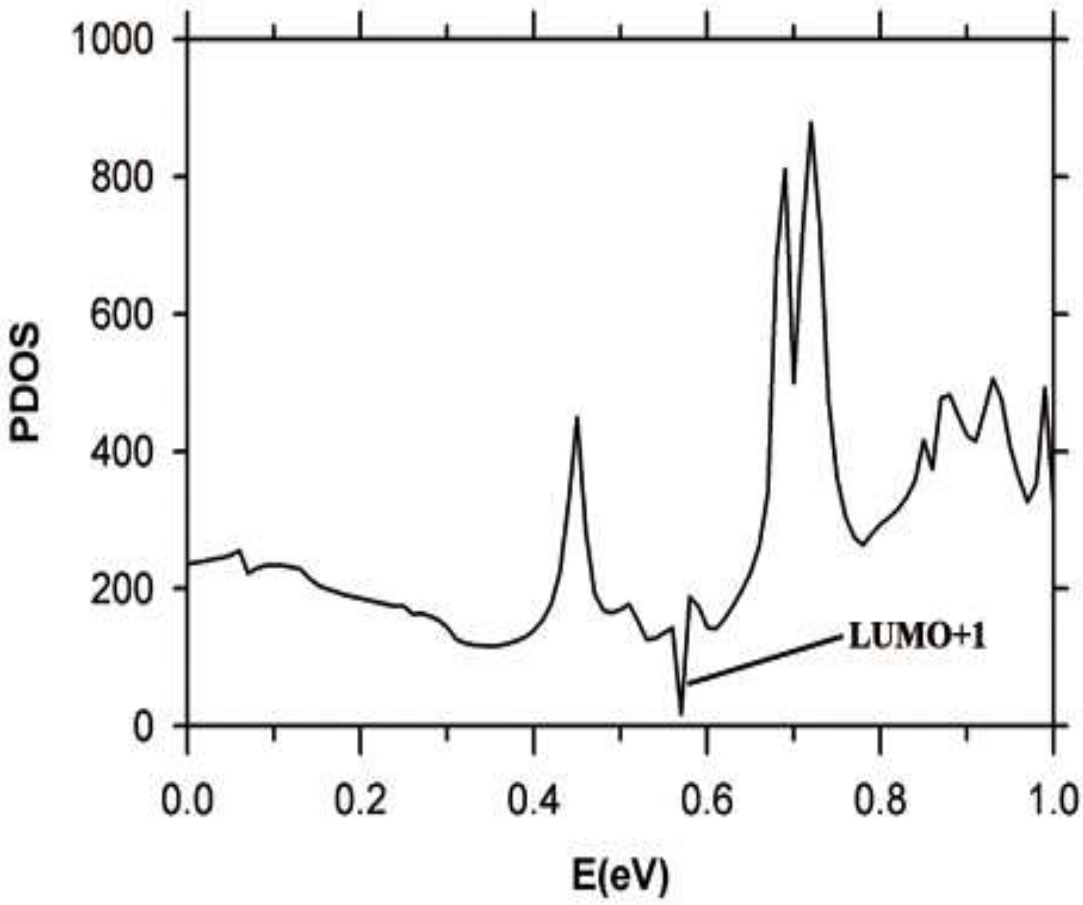
Fig. S10 Projected density of states (PDOS) of M10-Cl3 onto the surface of the CR region at -2.5 V.