Supplementary Information

Catechol sensor based on pristine and transition metal embedded Holey Graphyne:

A First-principle Density Functional Theory Study

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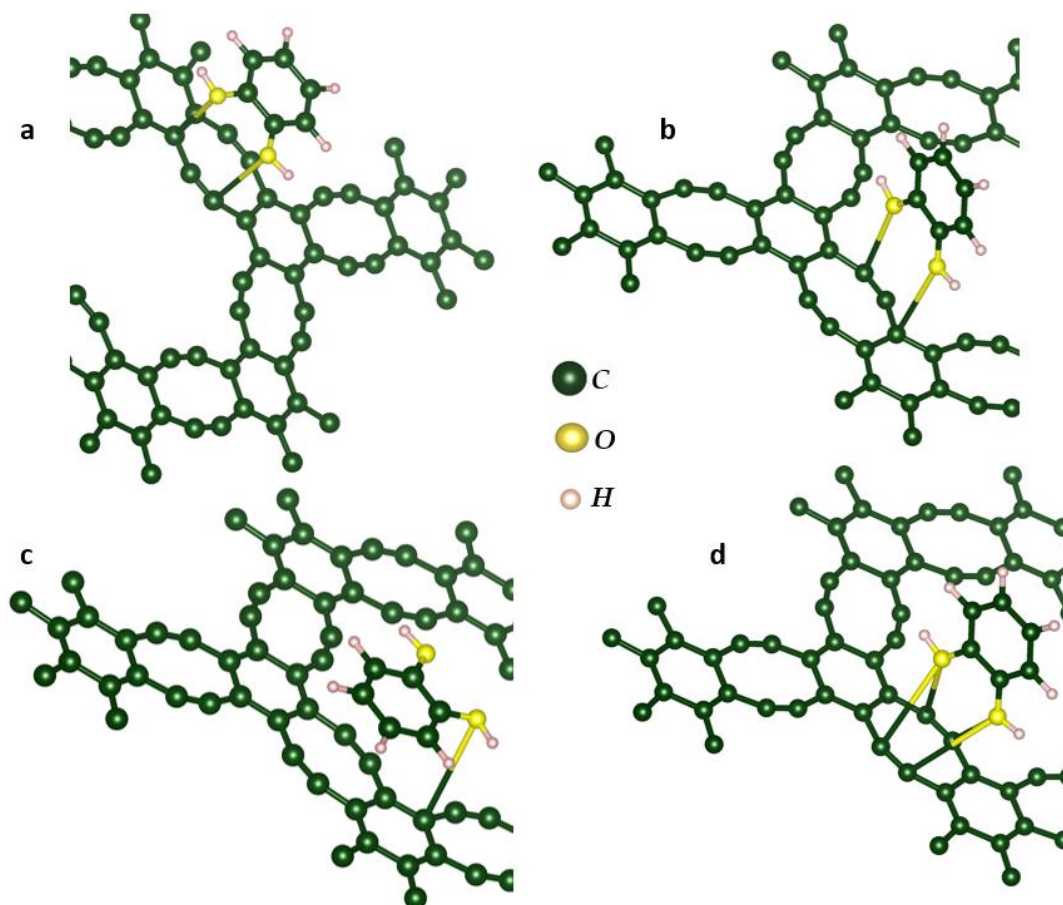*Email: nkkalarikkal@mgu.ac.in, brahma@barc.gov.in

Figure.S1: DFT optimized structures of Cc adsorption vertically above the (a) O site and (b) b4 site and horizontally above the (c) H site and (d) O site.

System	Binding Energy (eV)	Bond distance (d_{C-O}) (Å)
Cc horizontally @ H site	0.61	3.19
Cc vertically @ b4 site	-0.6	3.2
Cc vertically @ H site	-0.59	3.23
Cc horizontally @ O site	-0.5	3.33

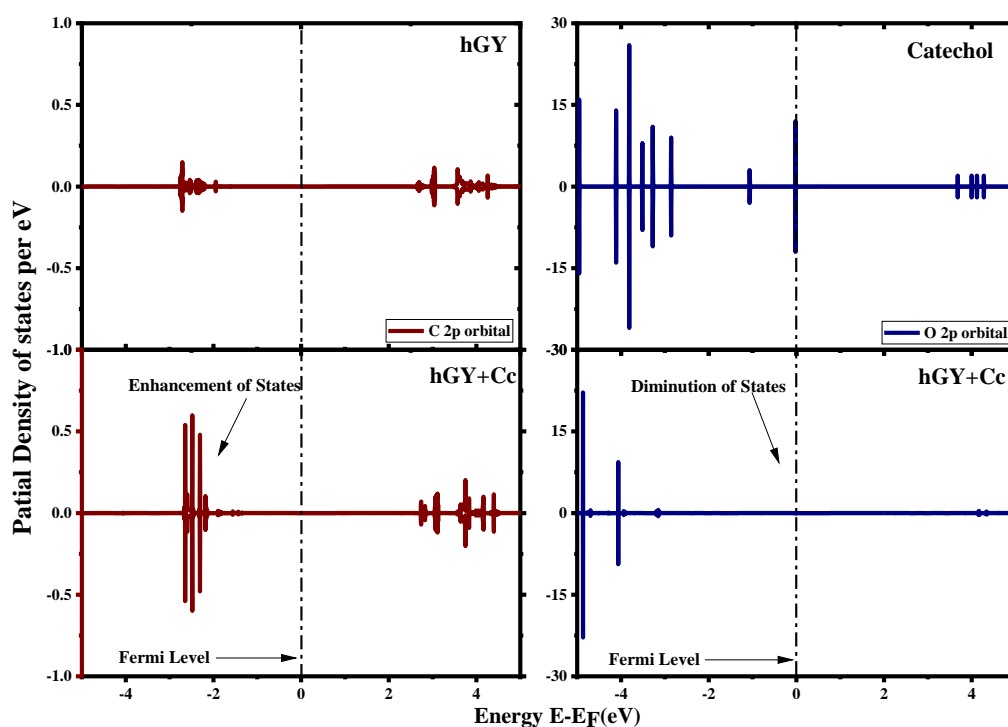Table.S1: Binding energy and distance of Cc molecule adsorbed at various adsorption sites

Figure.S2: Partial Density of states plots: the left panel compares the C *2p* orbitals in hGY to those in Cc adsorbed hGY, whereas the right panel compares the O *2p* of Cc in isolated and hGY+CC system.
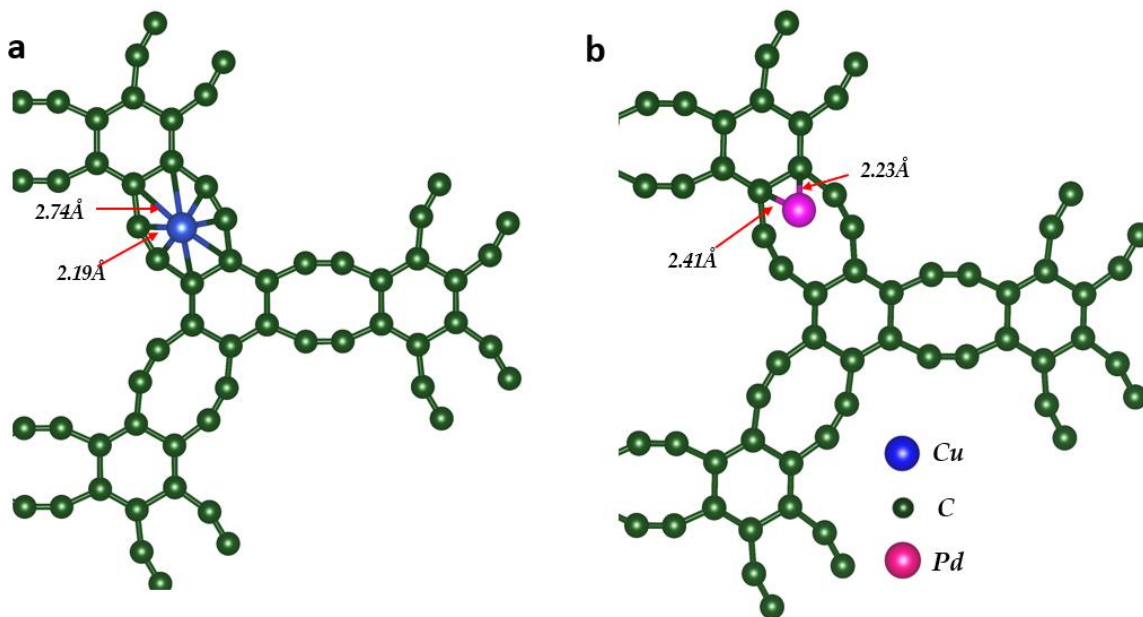
Figure.S3: Top view of most stable adsorption geometries of (a) Cu and (b) Pd embedded hGY monolayer. The bond distance of the TM with the two types of C atoms is also depicted.
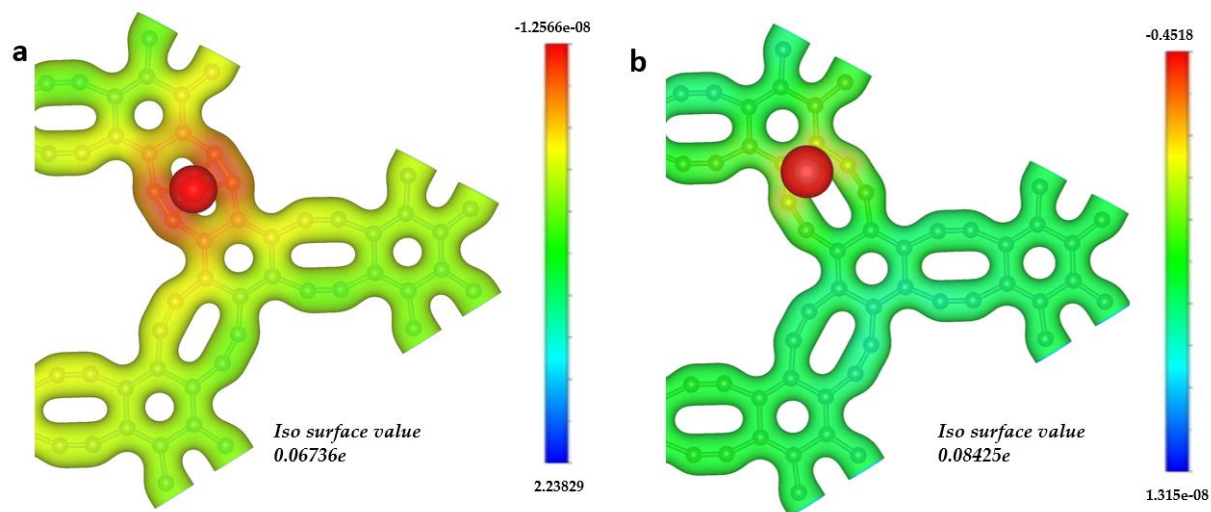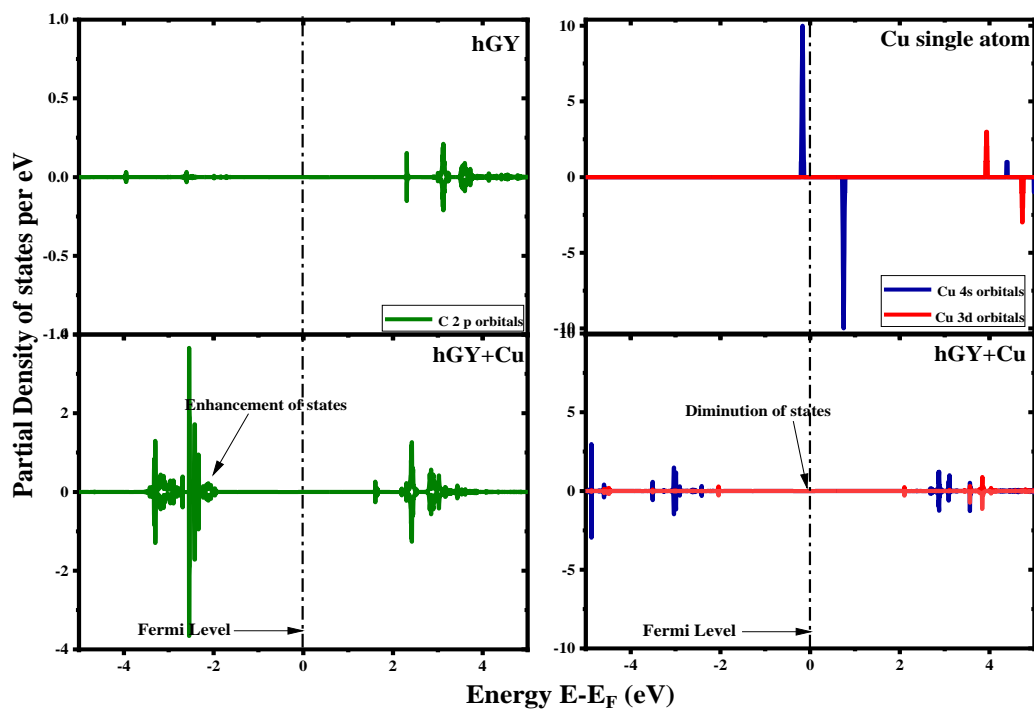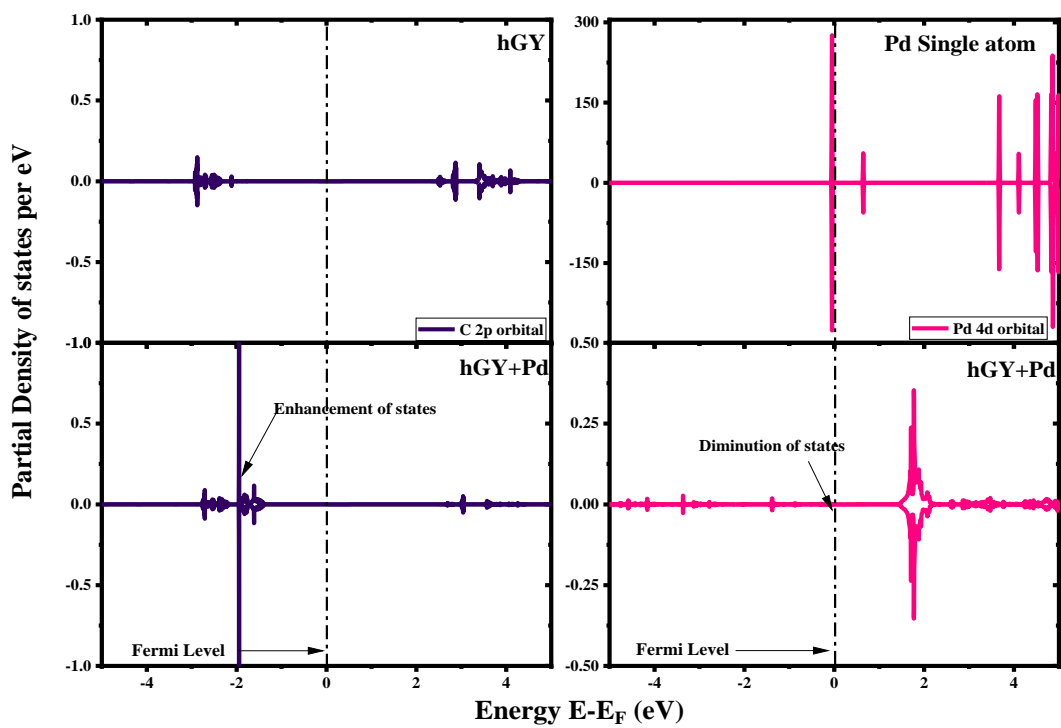

Figure.S4: Charge density difference plot (cdd) of (a) hGY+Cu and (b) hGY+Pd systems. The corresponding iso surface values are indicated in the figure. The green and red colours denote the charge gain and loss, respectively.

a)

b)

Figure.S5: Partial Density of states plots: the left panel compares the C *2p* orbitals in hGY to those in TM embedded hGY, and the right panel compares the valence orbitals of TMs in the isolated atom to that in TM embedded hGY system. (TM= (a) Cu and (b) Pd)
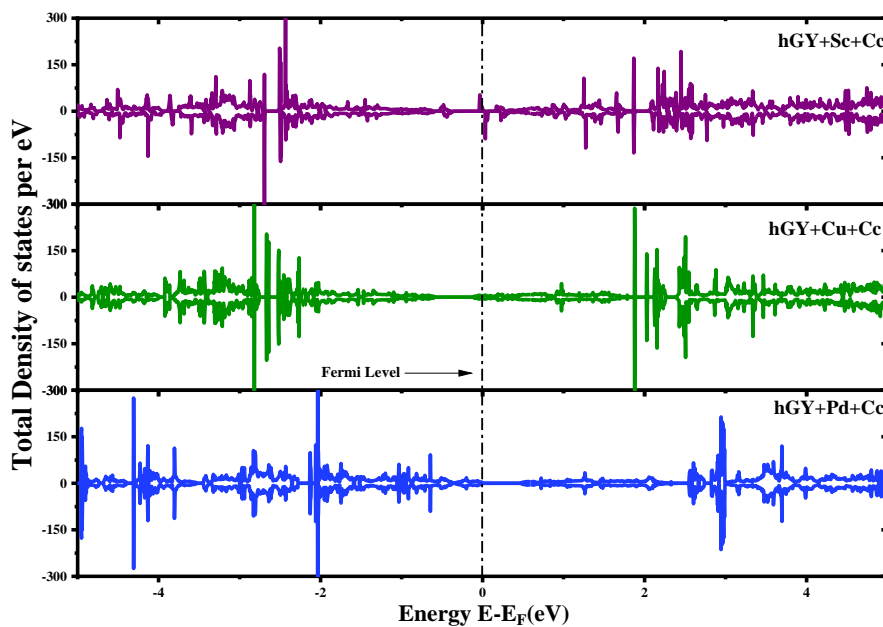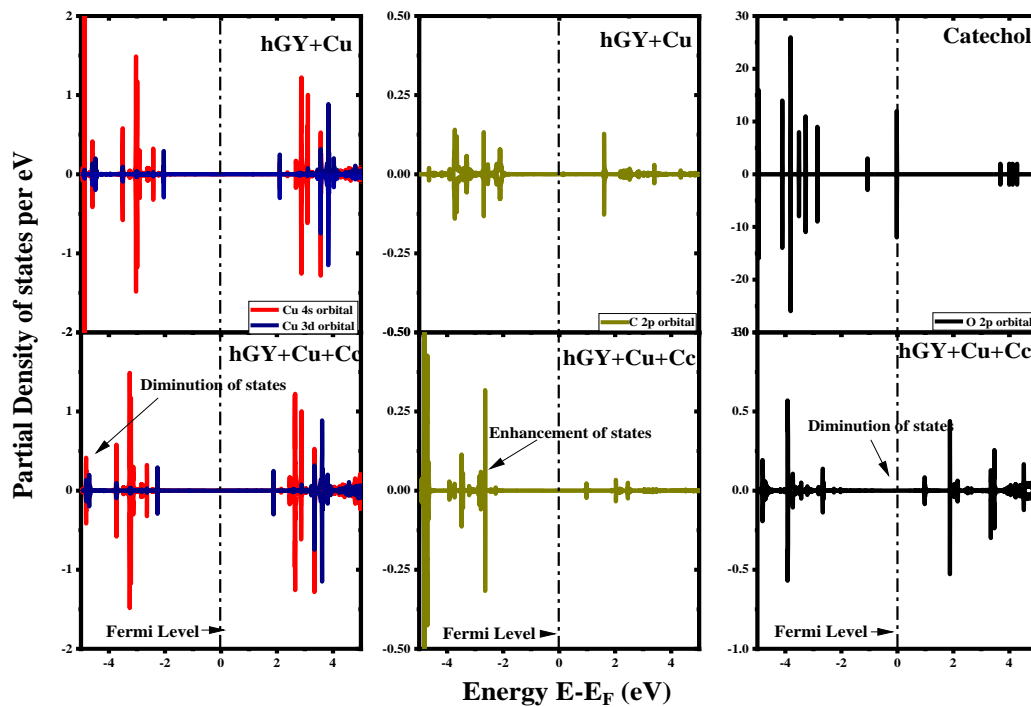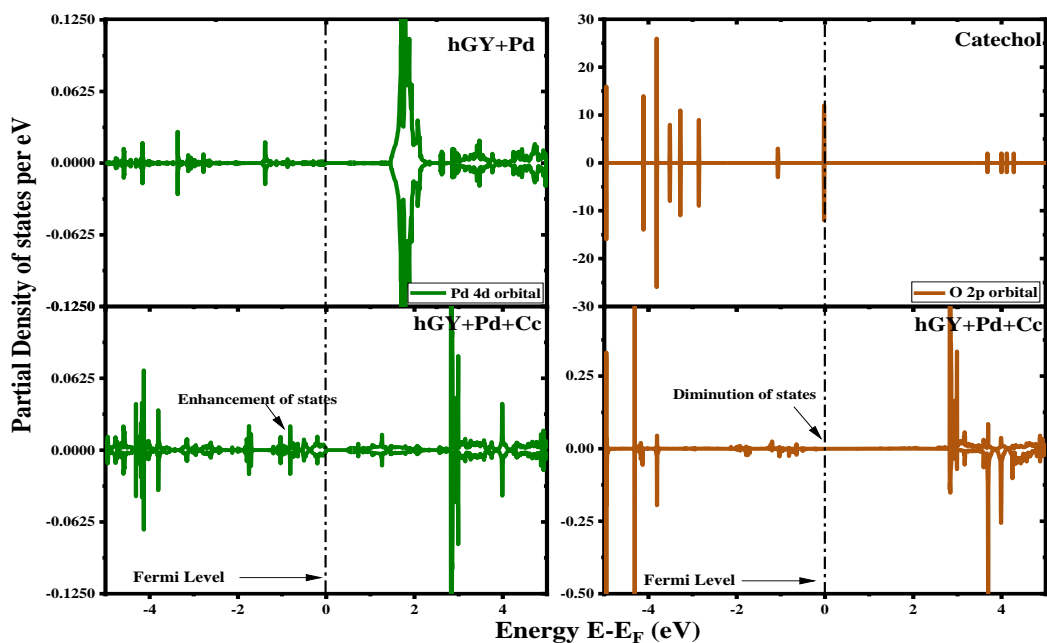

Figure.S6: Total DOS plots of Cc adsorbed TM (Sc, Cu and Pd) embedded hGY system

a)

b)

Figure.S7: Partial density of state plots that compares the (a)Valence orbitals of Cu (left panel), C 2p orbitals of hGY (middle panel) and O 2p orbitals of Cc (right panel) in hGY+Cu and hGY+Cu+Cc systems. (b)4d orbitals of Pd (left panel) and O 2p orbitals of Cc (right panel) in hGY+Pd and hGY+Pd+Cc systems. The Fermi level is denoted by the vertical dotted line and is set to 0 eV.