

Supplementary material

Metal Decorated γ -Graphyne as Drug transporting agent For Mercaptopurine chemotherapy drug: A DFT study

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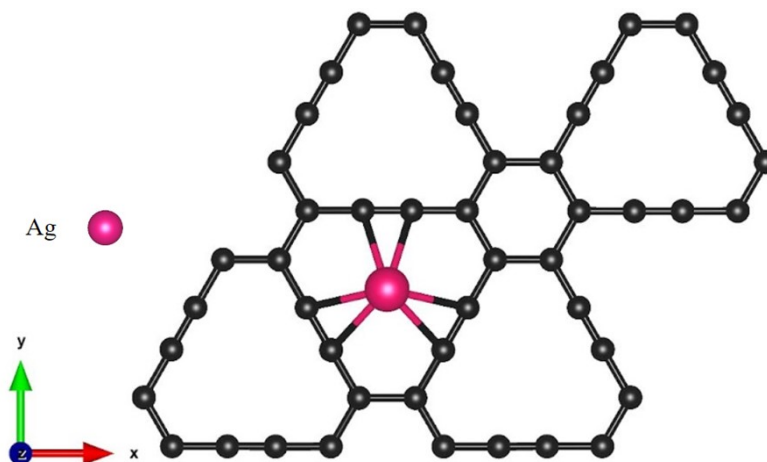


Figure S. 1. Geometrically optimized structure of Ag-decorated GYN.

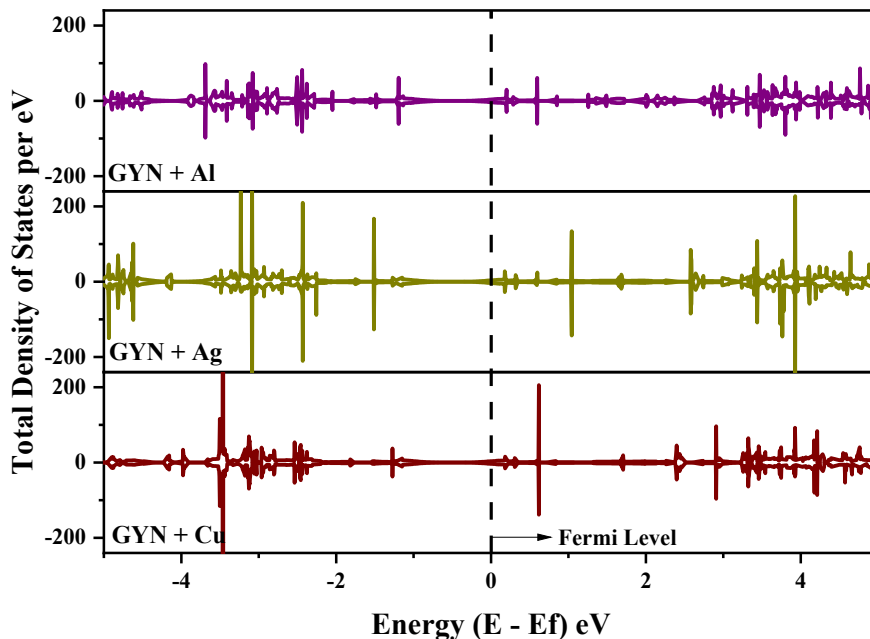


Figure S. 2. TDOS plots of GYN + Al, GYN + Ag, and GYN + Cu systems.

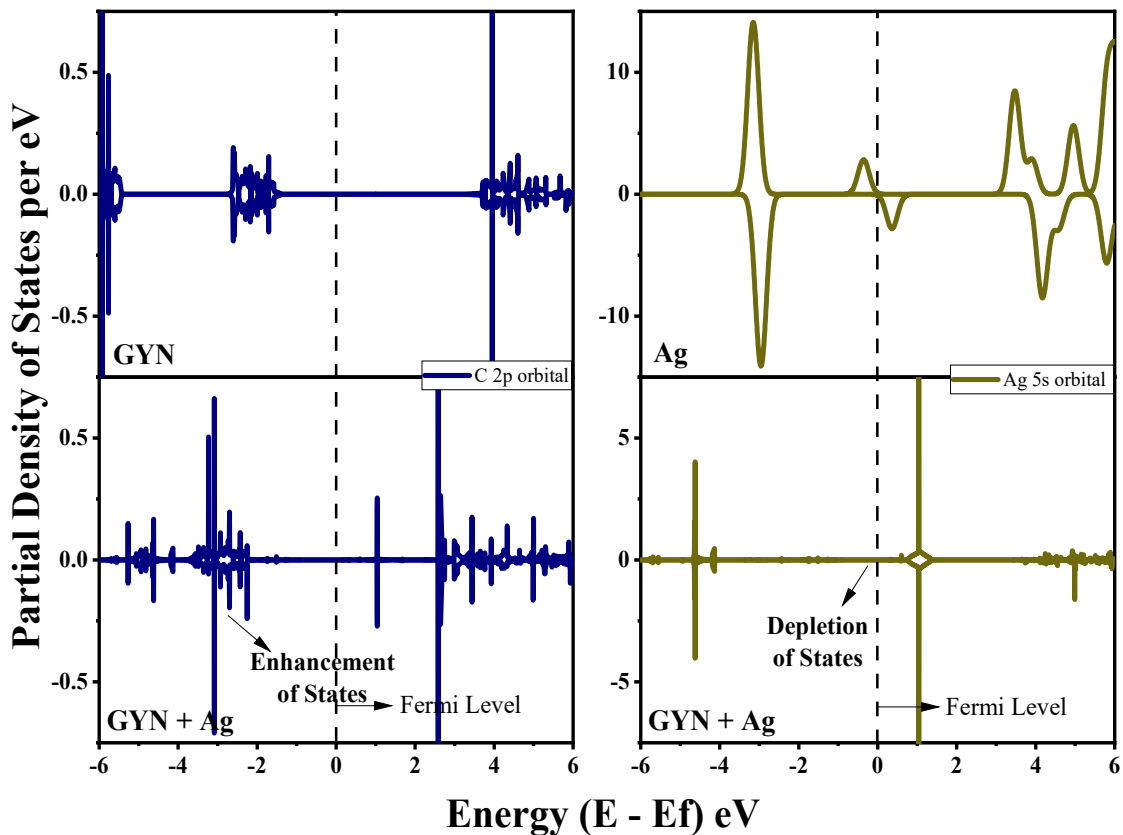


Figure S. 3. Compares the PDOS of $2p$ orbital of the C atom in pristine and Ag-decorated GYN (left segment). Meanwhile, the valence $5s$ orbital of the Ag is compared with that of the single metal atom in its isolated state in the right segment.

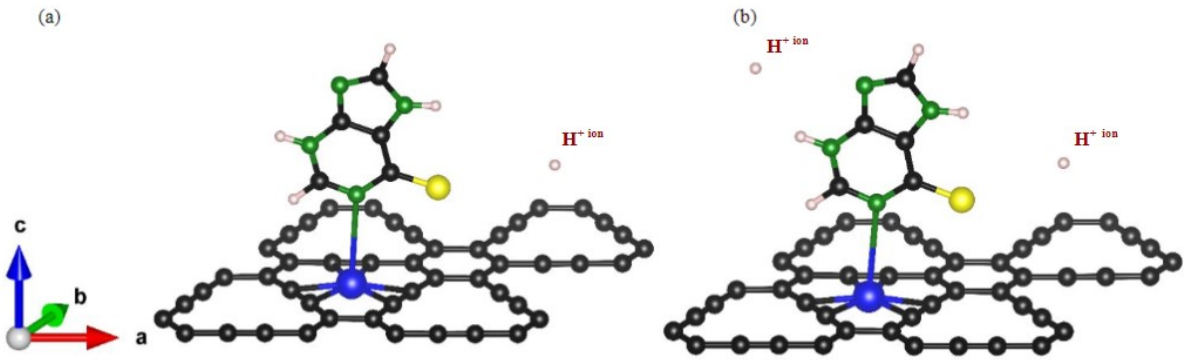


Figure S. 4. The AIMDs images of (a) Al and (b) Cu decorated GYN system at 400K

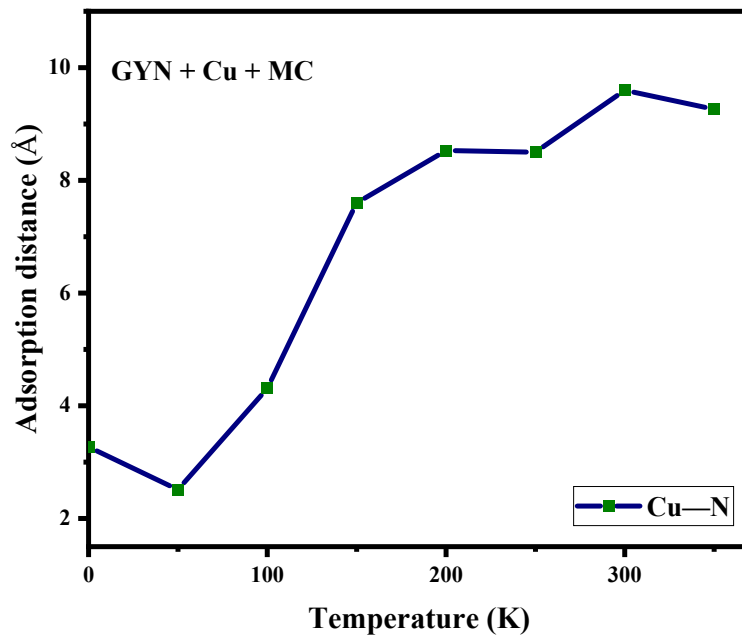


Figure S. 5. Adsorption distance versus temperature plot of MC adsorbed Cu decorated GYN system in the acidic pH environment.