

Facile Synthesis of Hydrogen-Substituted Graphdiyne Powder via Dehalogenative Homocoupling Reaction

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| Catalyst | Lewis bases | Condition | Product obtained or not |
|----------|-------------------|--------------------------|---------------------------|
| CuI | Et ₃ N | Toluene/heating | Y |
| CuI | Pyridine | Toluene/heating | Y |
| CuI | DMSO | Toluene/heating | Y |
| CuI | THF | Toluene/heating | N |
| CuI | DMF | Toluene/heating | Y |
| CuI | DMAC | Toluene/heating | N |
| CuI | Et ₃ N | Toluene | N |
| CuI | Pyridine | Toluene | N |
| CuI | Pyridine | NaOH(a.q.) | N |
| None | Et ₃ N | Toluene/heating overtime | A few black powder (CPCM) |
| None | Pyridine | Toluene/heating overtime | A few black powder (CPCM) |
| CuI | None | Toluene/heating | N |

Table S1. Experiment of the reaction condition to obtain HsGDY powder. The Reactant only contains tBEP, heating temperature up to 80 °C and reaction takes longer at lower heating temperature. All experiment is performed under nitrogen atmosphere.

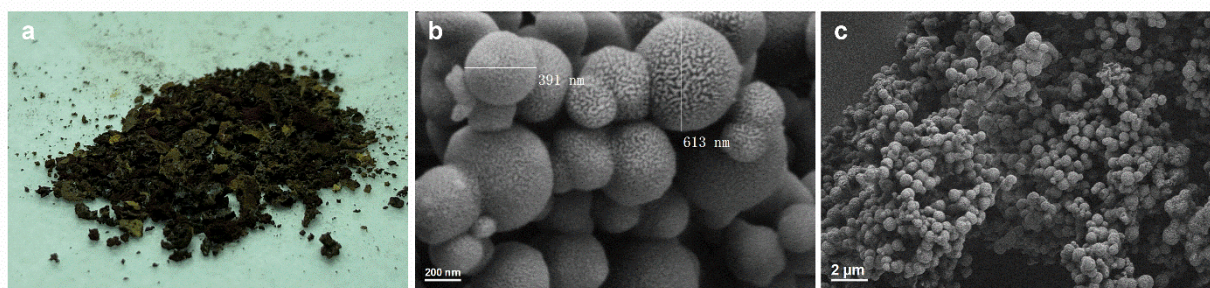


Figure S1. The photograph (a) and SEM images (b,c) of CPCM

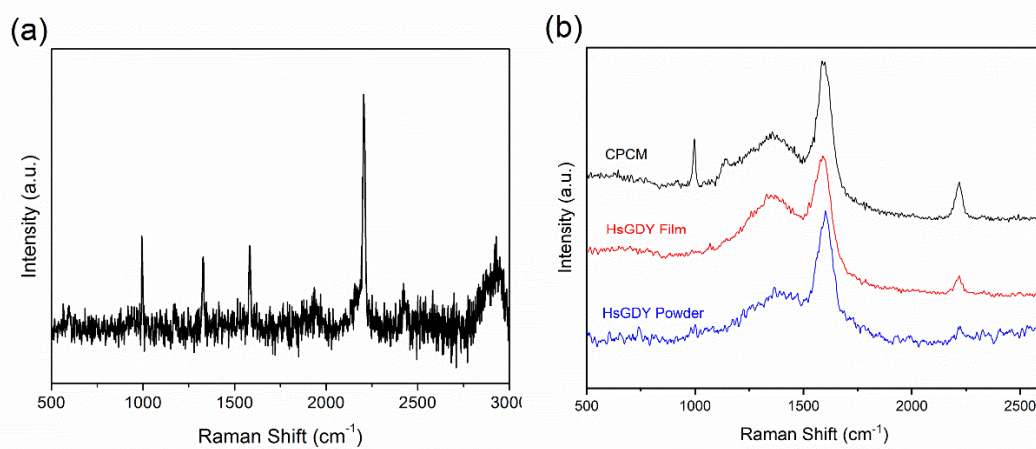


Figure S2. (a) Raman spectrum of tBEP monomer. (b) Raman spectrum of CPCM and HsGDY film.

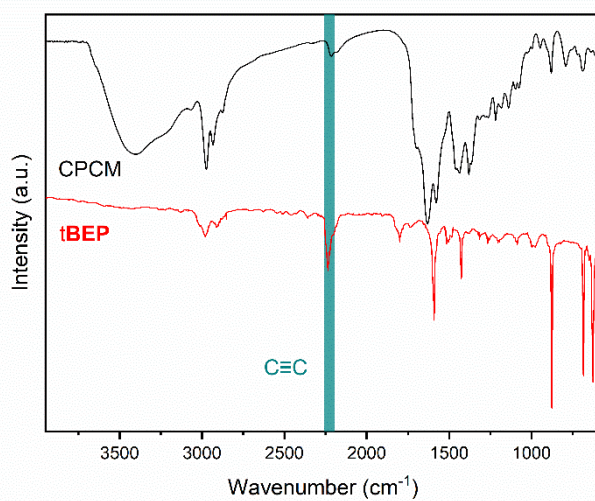


Figure S3. FT-IR spectrum of CPCM and tBEP.

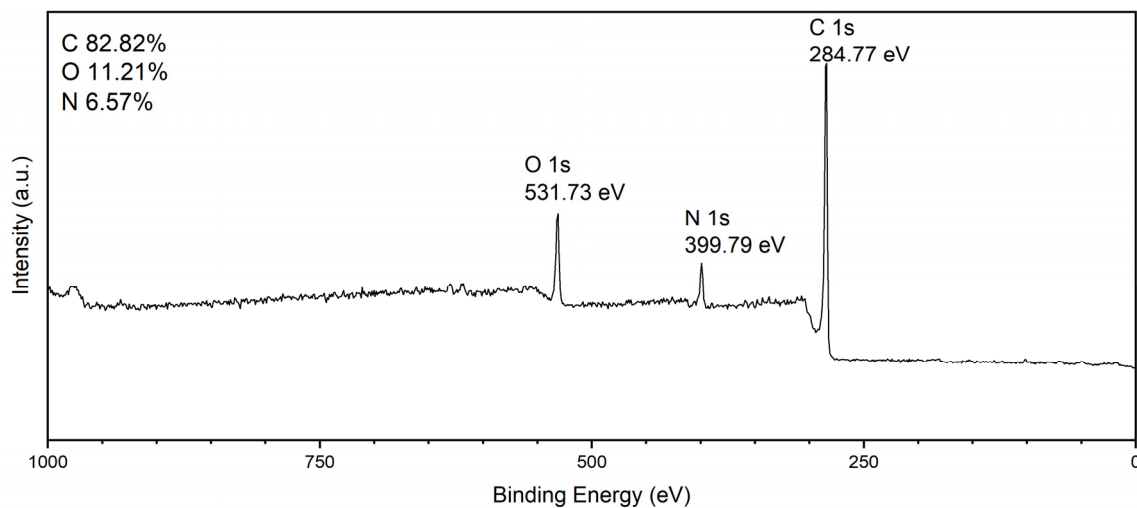


Figure S4. XPS total spectrum of HsGDY powder.

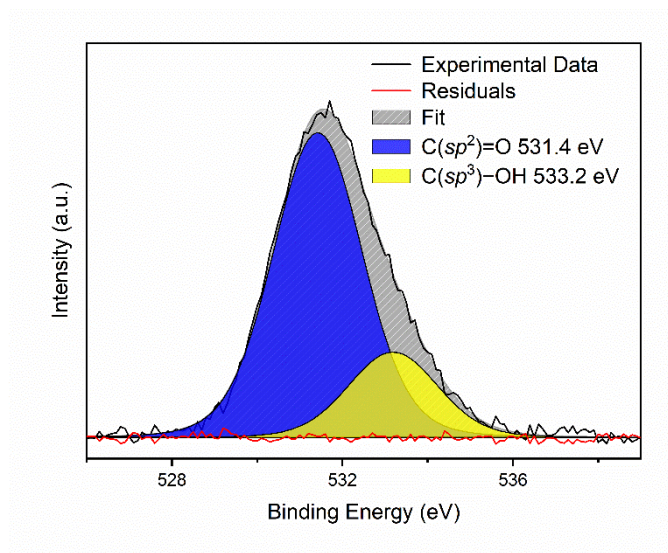


Figure S5. XPS high resolution of O 1s spectrum of HsGDY powder.

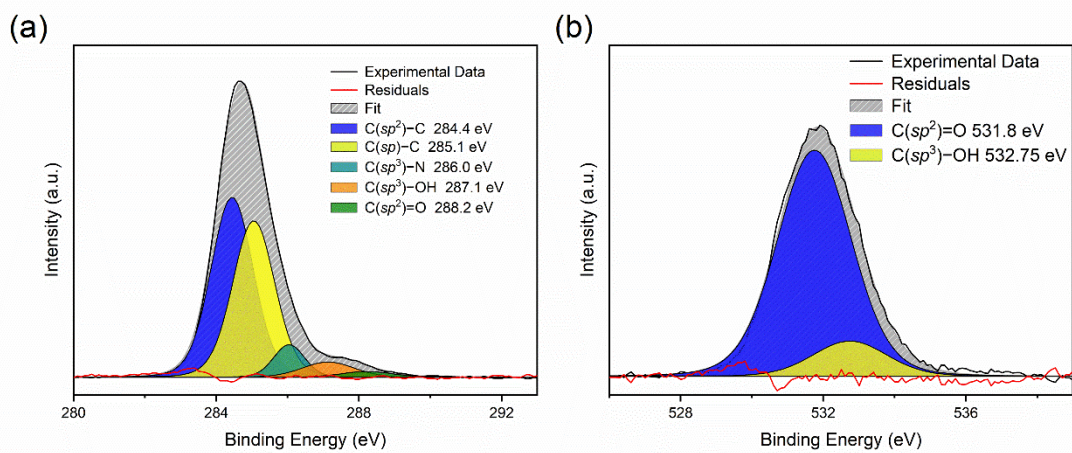


Figure S6. XPS high resolution of (a) C 1s and (b) O 1s spectrum of CPCML.

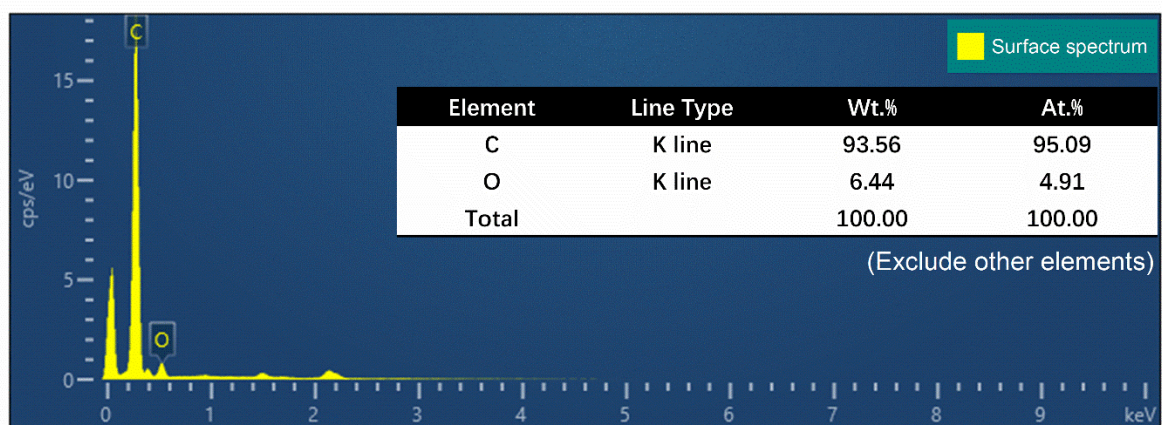


Figure S7. EDS analysis of HsGDY powder.

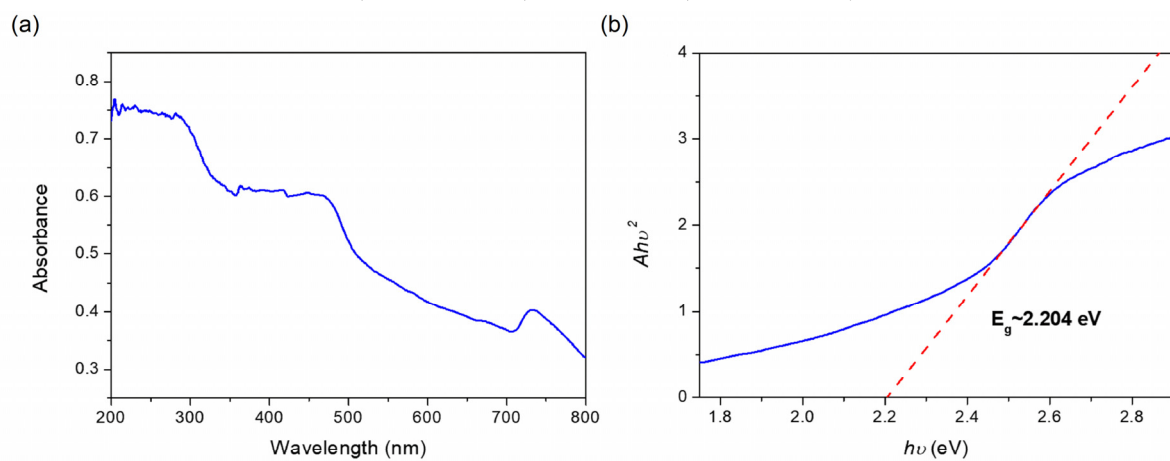


Figure S8. (a) The UV-visible spectrophotometry of HsGDY film (b) Determination of optical band gap of HsGDY film from the Tauc plot.