

Supplementary Material

A low-cost and high-yield green preparation method of Graphdiyne and Hydrogen-substituted Graphdiyne and its photocatalytic properties

Zhiliang Jin*[§], Youlin Wu[§]

*School of Chemistry and Chemical Engineering, Ningxia Key Laboratory of Solar Chemical
Conversion Technology, North Minzu University, Yinchuan 750021, P.R.China*

Corresponding author: zl-jin@nwnu.edu.cn (Z.L. Jin); [§] Equal contribution

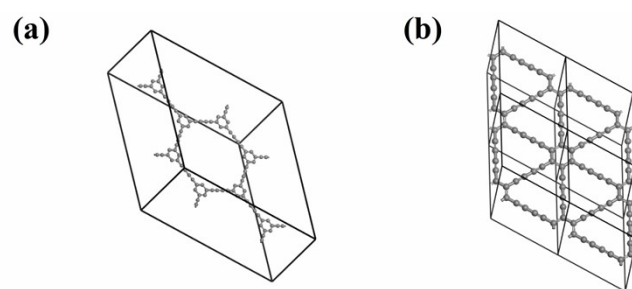


Fig. S1 (a, b) the theoretical computational model of H-GDY and GDY.

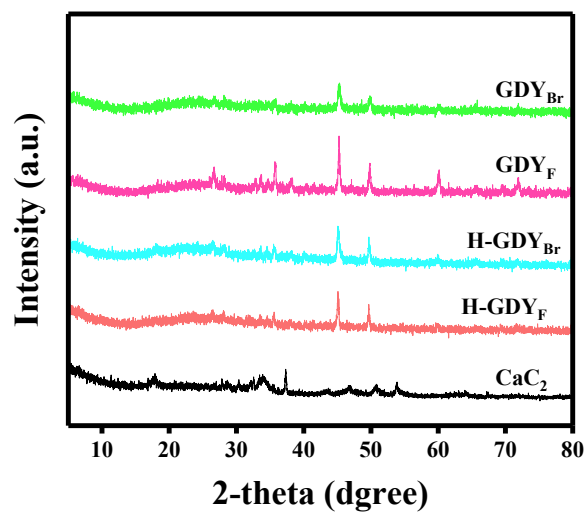


Fig. S2 XRD patterns of CaC₂, H-GDY_F, H-GDY_{Br}, GDY_F, and GDY_{Br}.

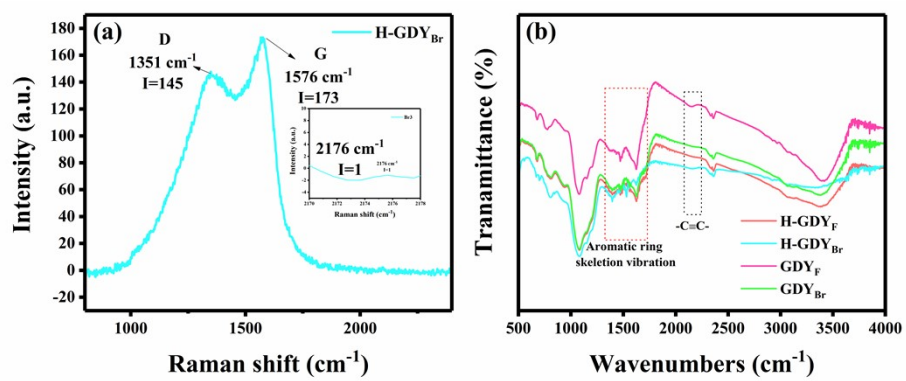


Fig. S3 (a) Raman spectrum of H-GDY_{Br}, (b) FT-IR spectrum of all alkynyl carbon materials.

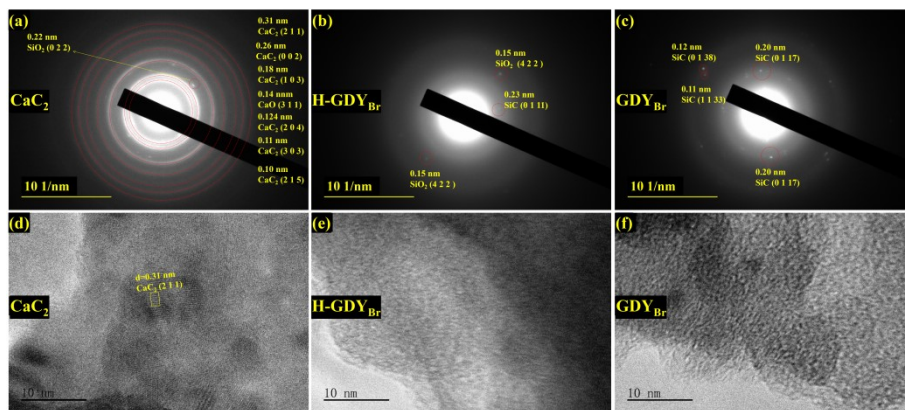


Fig. S4 (a-f) Selected area electron diffraction ring and High magnification TEM images of CaC₂, H-GDY_{Br} and GDY_{Br}.

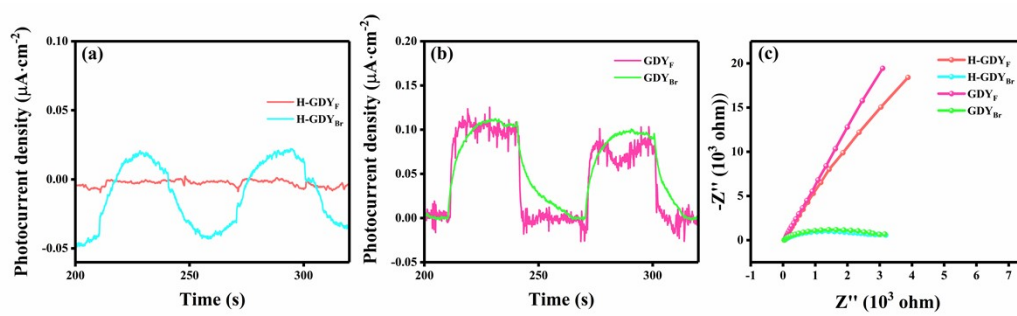


Fig. S5 (a, b) photocurrent response curves, (c) Nyquist plots of electrochemical impedance spectroscopy.

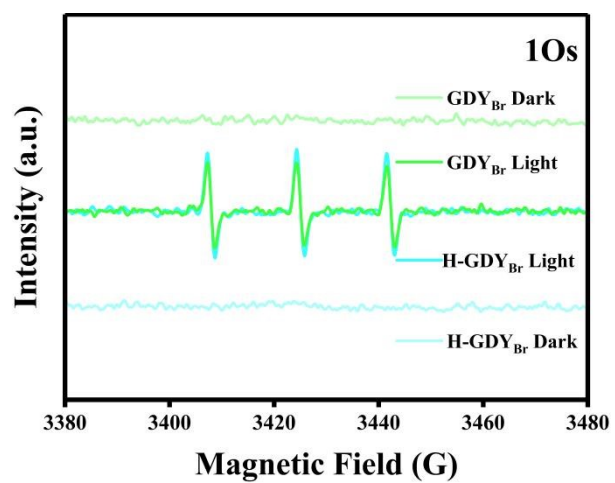


Fig. S6 Electron paramagnetic resonance diagram of 1Os.

Table S1 The difference and yield of various H-GDY and GDY.

Samples	Different halogenated benzene names	Yields (%)
GDY _F	hexafluorobenzene	42.36 %
GDY _{Br}	hexabromobenzene	48.15%
H-GDY _F	1,3,5-Trifluorobenzene	48.15 %
H-GDY _{Br}	1,3,5-Tribromobenzene	51.16%

Table S2. The S_{BET} and aperture test results data of CaC_2 , H-GDY_{Br} and GDY_{Br}.

Samples	S_{BET} (m^2g^{-1})	Pore volume (cm^3g^{-1})	Average pore size (nm)
CaC_2	4.8786	0.0146	9.9221
H- GDY _{Br}	105.4017	0.1702	11.5402
GDY _{Br}	82.1067	0.2247	13.6440