Supporting Information

Design of a photocatalyst combining graphdiyne-Cu/$NiCrO_3$ with Cu as an interfacial charge transfer bridge and its photocatalytic hydrogen evolution

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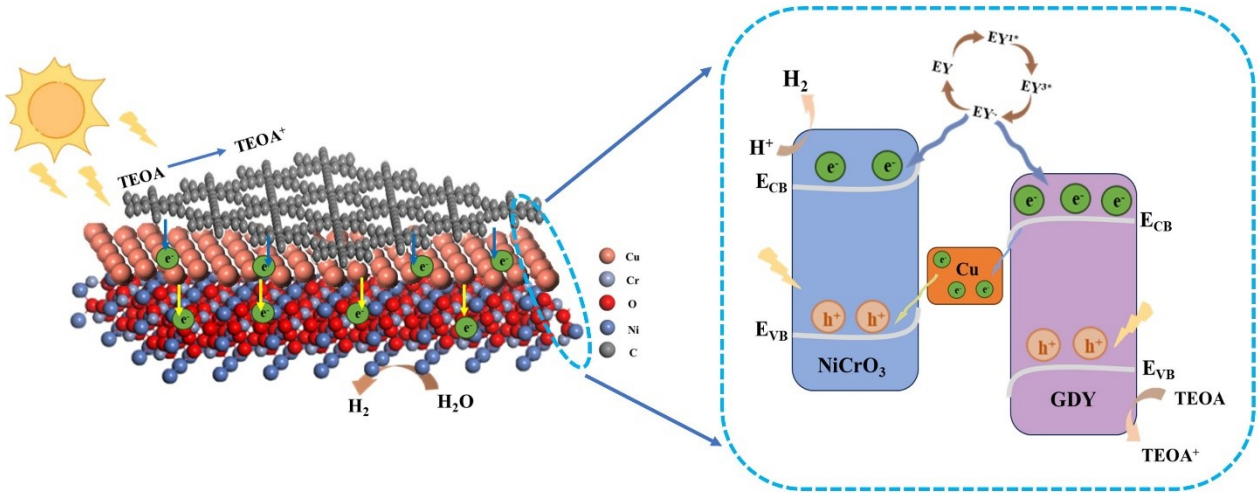

Section S1 Density Functional Theory

The CASPTE module within the Material Studio software suite was used to perform theoretical calculations for all samples in the study. The GGA method using the PBE functional was utilized to investigate the subtle atomic interactions involved in the exchange functional process. During the stage of structural optimization, a plane-wave basis set with an energy threshold of 450 eV was exploited. Ionic relaxation was conducted with the convergence criteria set at a conventional energy of 1×10^{-5} electron volts and force of 0.01 eV Å. Additionally, to reduce interactions between adjacent layers, a vacuum layer of 15.0 Å was included.

Section S2: Characterizations

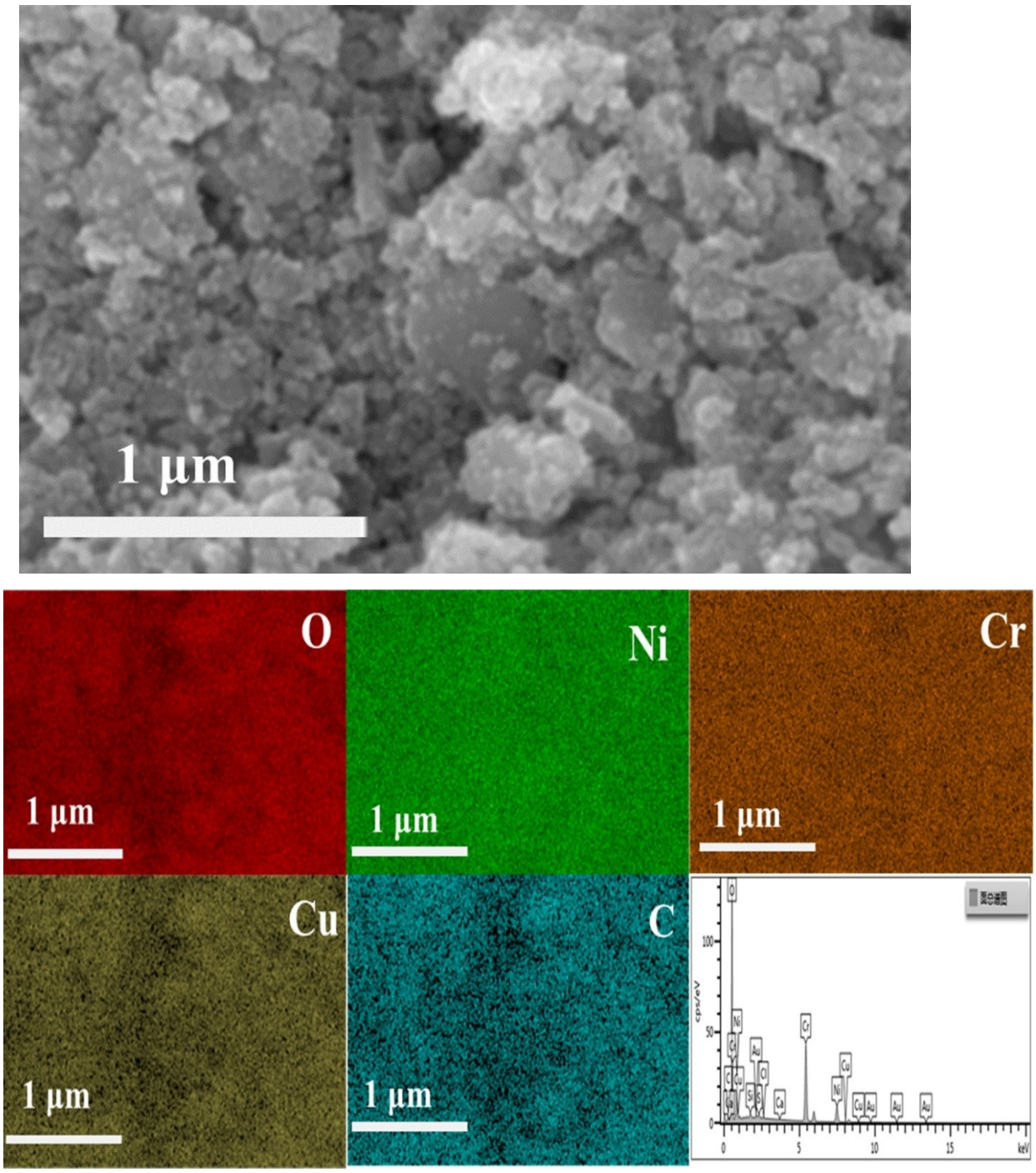

Fig. S1 (a) the EDS of GCNC20

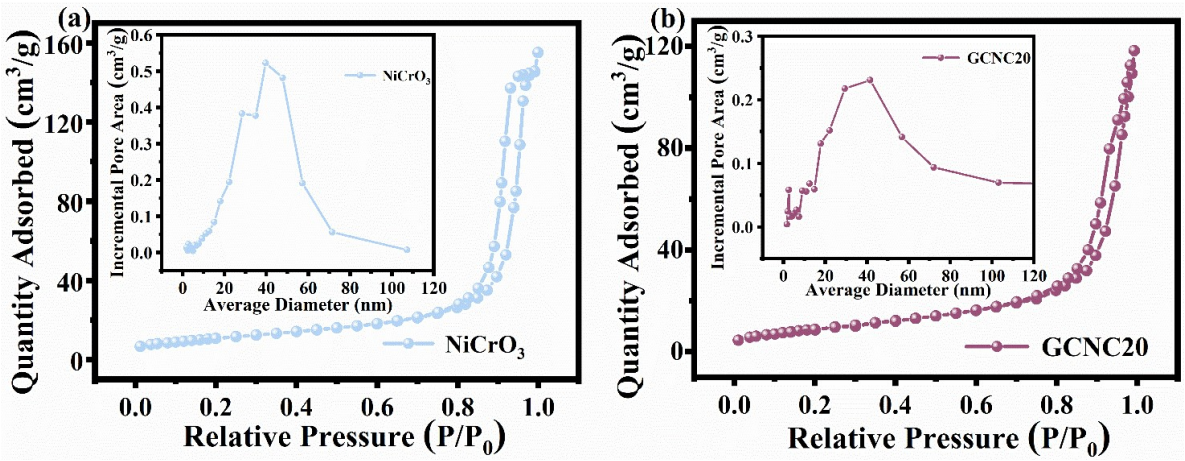

Fig. S2 (a, b) N_2 isothermal adsorption curves of $NiCrO_3$ and GCNC20.

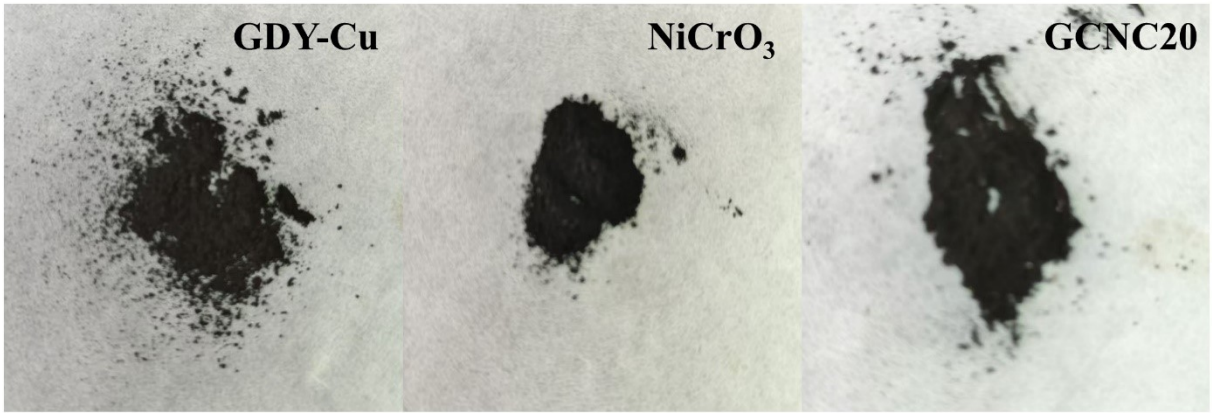

Fig. S3 colors of GDY-Cu, NiCrO3, and GCNC20.

Table S1 the S_{BET}, Pore volume and average pore size of $NiCrO_3$ and GCNC20.

Samples	S_{BET} [m^2 g^{-1}]	Pore volume [cm^3 g^{-1}]	Average pore size [nm]
$NiCrO_3$	39.28	0.23	23.24
GCNC20	33.68	0.18	21.73

Table S2 the content of each element in GCNC20

element	wt %
C	4.67
O	35.89
Cr	37.06
Ni	20.64
Cu	0.51