

Benzene Bridged Carbon Nitride for Efficient Photocatalytic Hydrogen Evolution

Junxia Chu[‡], *Wencheng Li*[‡], *Zhijun Cao*, *Xin Bai*, *Dr. Xi Rao*^{*}, *Prof. Shaohui Zheng*^{*}, and *Prof. Yongping Zhang*^{*}

School of Materials and Energy, Southwest University, Chongqing 400715, China

[‡]These authors contributed equally to this work.

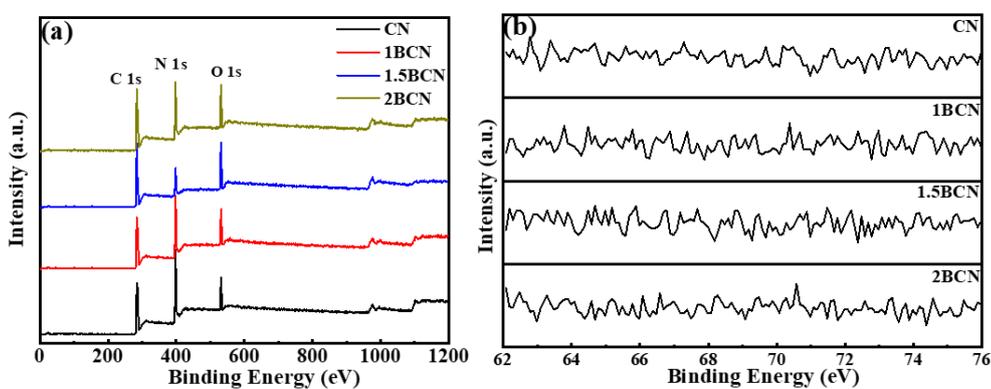


Figure S1. XPS survey (a) and high-resolution Br 1s spectra (b) of CN, and BCN.

Table S1. The Component Ratios of the N 1s Spectra for Different Samples

| samples | binding energy (eV) | peak assignment | atomic percentage |
|---------|---------------------|--------------------------------------------|-------------------|
| CN | 397.8 | sp ² bonded C–N=C | 75.5 |
| | 399.1 | sp ³ bridged N–[C] ₃ | 10.4 |
| | 400.3 | C–NH _x | 14.1 |
| 1BCN | 397.8 | sp ² bonded C–N=C | 73.1 |
| | 399.1 | sp ³ bridged N–[C] ₃ | 15.4 |
| | 400.2 | C–NH _x | 11.5 |
| 1.5BCN | 398.7 | sp ² bonded C–N=C | 73.3 |
| | 399.0 | sp ³ bridged N–[C] ₃ | 15.6 |
| | 400.1 | C–NH _x | 11.1 |
| 2BCN | 397.8 | sp ² bonded C–N=C | 73.4 |
| | 399.1 | sp ³ bridged N–[C] ₃ | 15.8 |
| | 400.5 | C–NH _x | 10.8 |

The calculated density of state (DOS) is shown in Fig. S5. The results show that the valence bands are mainly contributed by N atoms, and the conduction bands are mainly contributed by C atoms. The partial DOS trend of C and N is consistent and the intensity is similar, indicating that the sp² hybridization of C and N atoms takes place, which is mainly the aromatic ring structure with C-N as the skeleton. The introduction of benzene ring has little effect on the density of states.

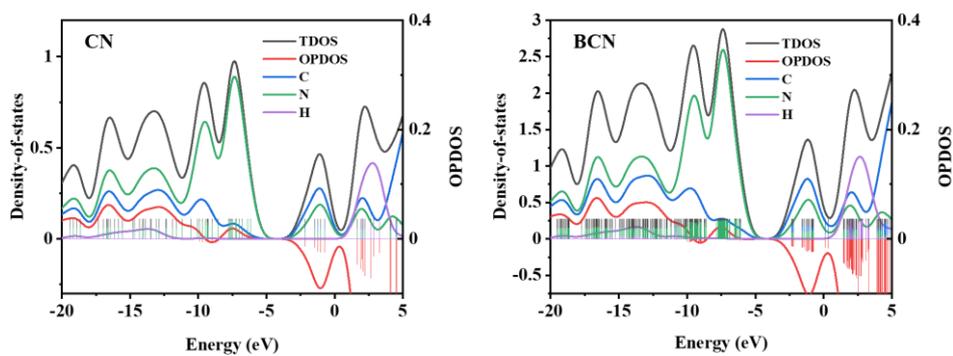


Figure S2. Calculated partial and total density of states (DOS) of CN (a) and BCN (b).

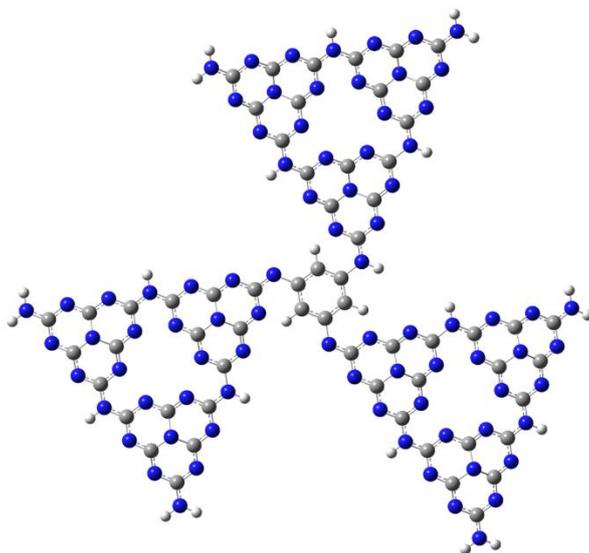


Figure S3. Chemical structure of BCN.

Table S2. The parameters of electron excitation of CN and BCN, obtained with M06-2X/6-311G** theory level

| | Energy level | | | | ΔE_{ST} (eV) | oscillator strengths | dipole moment |
|-----|--------------|--------|--------------|--------|-------------------------|-------------------------|------------------|
| | triplet (eV) | | singlet (eV) | | | | |
| CN | T1 | 3.0226 | S1 | 3.3328 | 0.3102 | 0.0003 | 1.93 D |
| | T2 | 3.0230 | S2 | 3.3572 | 0.3342 | 0.0016 | |
| BCN | T1 | 2.8541 | S1 | 3.5476 | 0.6935 | 0.0029 | 6.95 D |
| | T2 | 2.9177 | S2 | 3.5797 | 0.6620 | 0.0083 | |