Supporting Information

Dispersing Agglomerated $Zn_4In_2S_7$ on g-C_3N_4 Nanosheets to Form 2D/2D S-Scheme Heterojunction for Highly Selective Photocatalytic Cleavage of Lignin Models

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S1. Quantification of the reaction.

$$\text{Conversion of PP-ol (\%)} = \frac{peak\ area\ of\ reacted\ PP-ol}{peak\ area\ of\ PP-ol\ input} \times 100\%$$

$$\text{Yield of PP-one (\%)} = \frac{moles\ of\ PP-one\ formed}{moles\ of\ PP-ol\ input} \times 100\%$$

Unless otherwise specified, yields of other products (AP, Phol, BBE, PF) were calculated by the same way as that for PP-one employing the moles of the specific products. At the same time, The moles of products and by-products are calculated by the fitted moles-peak area standard curve formula (Fig. S1).

S2. Theoretical computation method.

The density functional theory (DFT) calculations of work function (WF) were performed using the Quantum Espresso with the Perdewe Burkee Ernzerhof (PBE) functional [1,2]. The Kohn-Sham one-electron valence states were expanded in a plane

wave basis set with a kinetic energy cutoff of 450 eV. The surface was simulated by the slab model, and a larger than 15 Å of vacuum layer was used to eliminate the interaction between periodic images. The work function was evaluated according to Equation (1):

$$WF = E_{vac} - E_f \qquad (1)$$

where WF, E_{vac}, and E_f represent work function, vacuum level, and Fermi level, respectively.

Table S1
Summary of energetic properties for CN and ZIS.

Catalysts	E_g/eV	E_{fb}/eV vs.Ag/AgCl	E_{fb}/eV vs.NHE	E_{cb}/eV	E_{vb}/eV
CN	2.91	-1.33	-1.13	-1.23	1.68
ZIS	2.47	-0.62	-0.42	-0.52	1.95

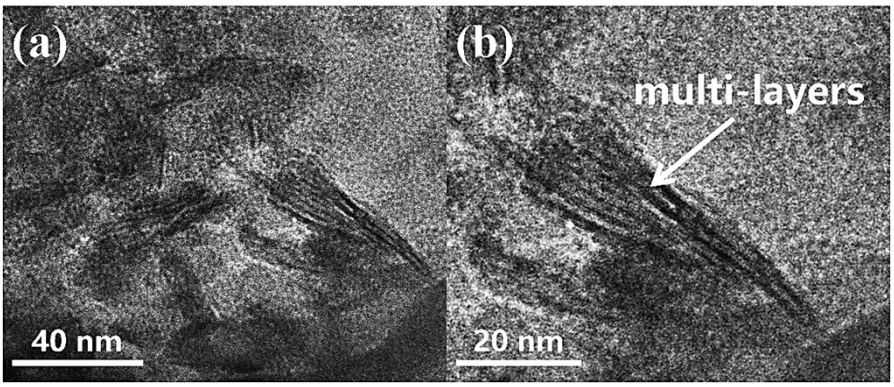
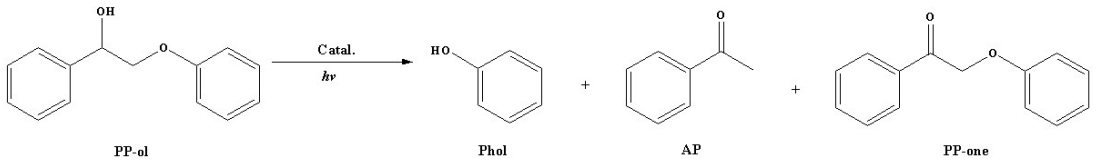
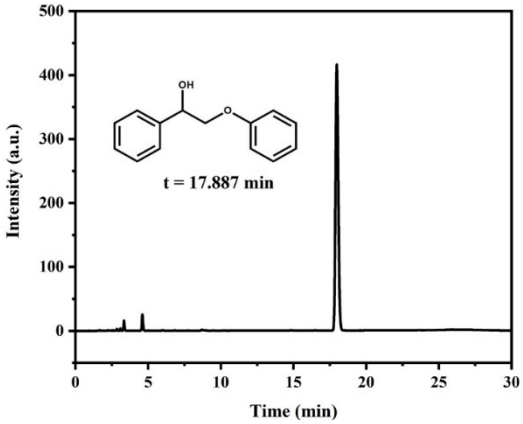
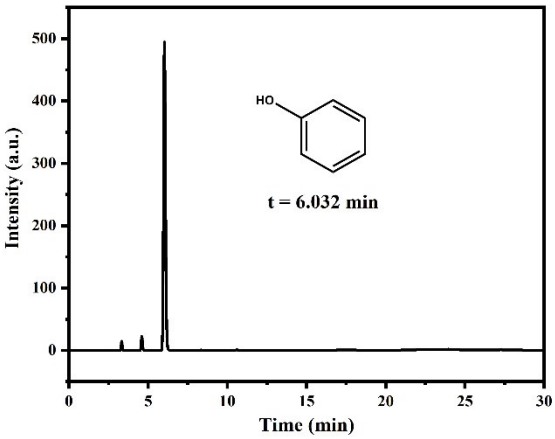
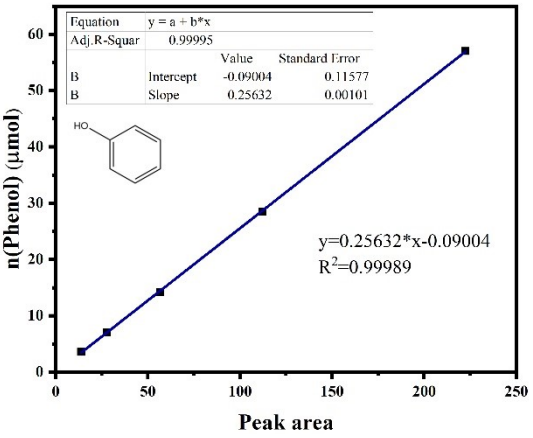


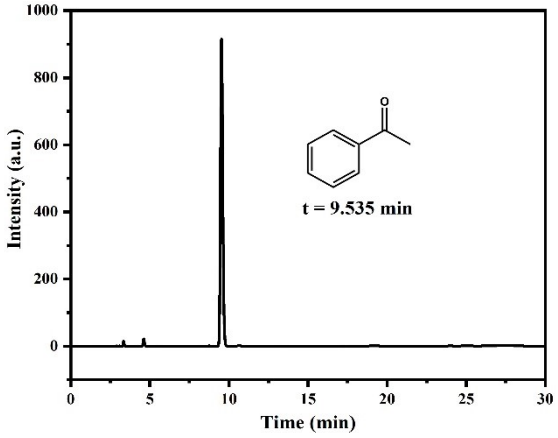
Fig. S1. TEM images of $Zn_4In_2S_7$.

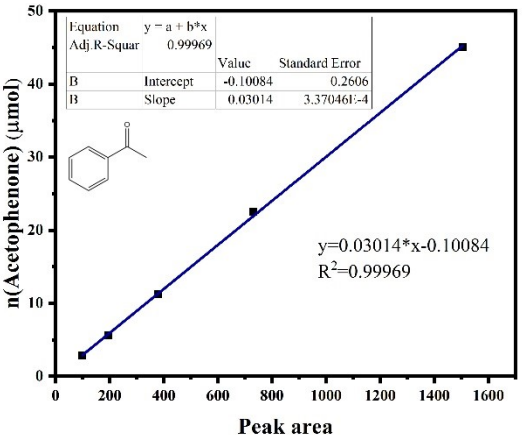

OH
O
Catal.
hv
HO
+
O
+
O
O
PP-ol
Phol
AP
PP-one


OH
O
t = 17.887 min
Intensity (a.u.)
Time (min)


HO
t = 6.032 min
Intensity (a.u.)
Time (min)


Equation y = a + b*x
Adj.R-Squar 0.99995
Value Standard Error
B Intercept -0.09004 0.11577
B Slope 0.25632 0.00101
HO
y=0.25632*x-0.09004
R2=0.99989
n(Phenol) (μmol)
Peak area


O
t = 9.535 min
Intensity (a.u.)
Time (min)


Equation y = a + b*x
Adj.R-Squar 0.99969
Value Standard Error
B Intercept -0.10084 0.2606
B Slope 0.03014 3.37046E-4
O
y=0.03014*x-0.10084
R2=0.99969
n(Acetophenone) (μmol)
Peak area

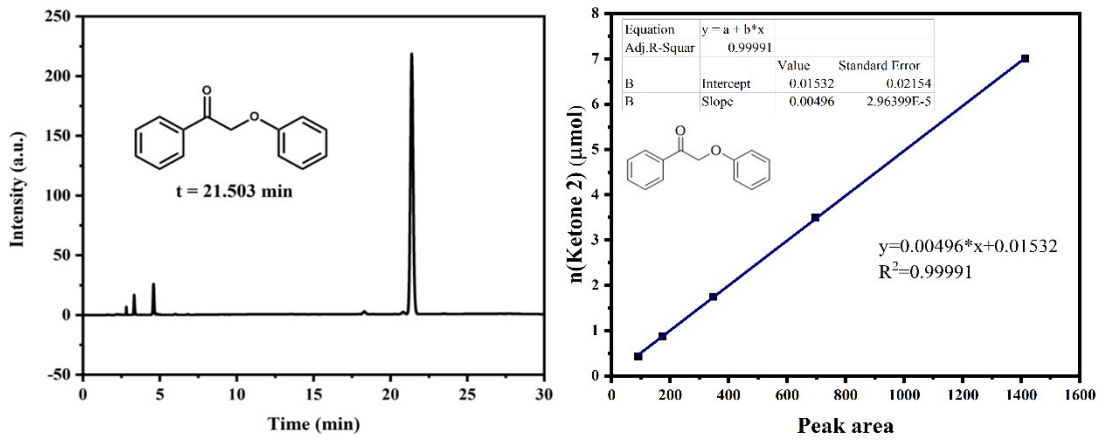


Fig. S2. HPLC spectra and quantitative analysis of PP-ol and its C-O bond breaking products.

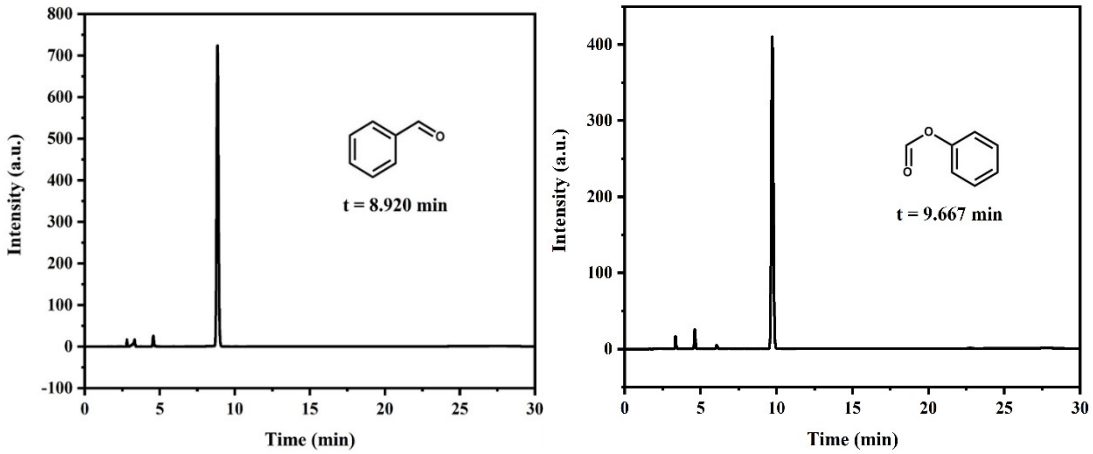


Fig. S3. HPLC spectra of the by-products of broken PP-ol C-C bond.

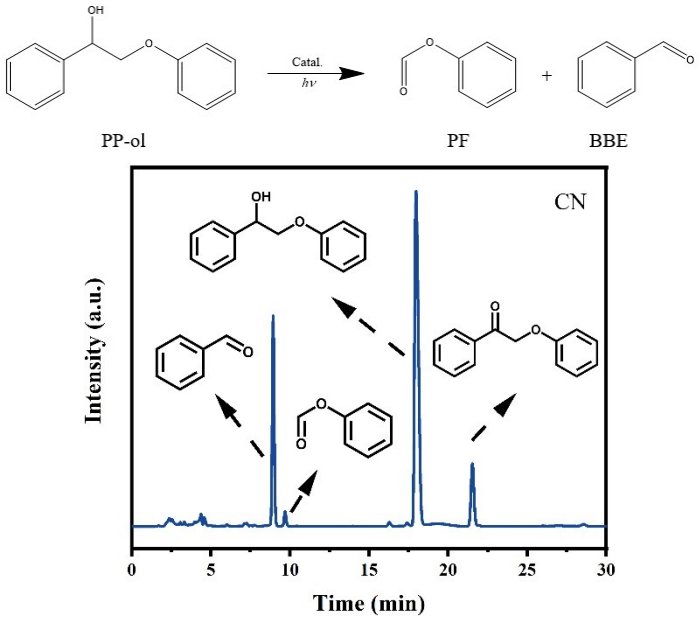


Fig. S4. The by-products that break the C-C bond of PP-ol.

Table S2

Adsorption of pp-ol by CN and ZCN materials after 3h.

Catalyst	CN	ZIS	ZCN-100	ZCN-200	ZCN-300	ZCN-400
Adsorption capacity (%)	3.4	2.2	2.6	2.1	2.5	2.2

References

[1] P. Giannozzi, S. Baroni and N. Bonini, *J. Phys.: Condens. Matter*, 2009, **21**, 395502.

[2] J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865–3868.