

Supporting Information

Phosphor-doped hexagonal-boron nitride nanosheets as effective acid-base bifunctional catalyst for one-pot deacetalization-Knoevenagel cascade reaction

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Keywords: *phosphor doping, boron nitride, acid-base catalysis, one-pot cascade reaction*

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1.Supporting tables

Table S1 The inter-planer distance and thickness of single sheet of *h*-BN and BNP samples.

sample	inter-planer distance (nm)	Thickness of single sheet (nm)
<i>h</i> -BN	0.33	2.26
BNP-E-2.1	0.37	1.30
BNP-E-1.4	0.35	1.50
BNP-E-2.8	0.35	1.40

Bragg equation and Scherrer equation were used to calculate the inter-planer distance and the thickness of single sheet, respectively. Bragg equation is described as Equation (1), and Scherrer equation is shown as equation (2).

$$2d_{hkl}\sin\theta_{hkl} = n\lambda \quad (1)$$

$$D_{hkl} = \frac{K\lambda}{\beta\cos\theta} \quad (2)$$

Where, ϑ is the Bragg angle, with the unit of degree. d_{hkl} and D_{hkl} represents inter-planer distance and the thickness of single sheet with the unit of nm, respectively. K is the dimensionless shape factor, with a typical value of 1. λ is the X-ray wavelength of 0.154 nm, and β represents the full width at half maximum (FWHM).

Table S2. The atomic percentage of BNP-2.8 sample.

Element	B	N	P	C	O
Atomic percentage%	10.56	21.44	11.15	18.28	38.56

Table S3. The catalytic performances of BNP immobilized on cordierite in deacetalization-Knoevenagel cascade reaction.

Reaction time, h	Conversion of 1, %	Yield of 2, %	Yield of 3, %	TON*, mol.h ⁻¹ .g ⁻¹	TOF*, h ⁻¹
0	0	0	0		
2	60.21	35.61	24.60	153.76	26.52
4	77.62	28.39	49.23		

Reaction conditions: Benzaldehyde dimethyl acetal (2.5mmol), Malononitrile (3mmol), toluene 20ml. BNP immobilized on cordierite catalyst 0.3 g, reaction temperature 80°C, in oil bath for 24 hours. *TON and TOF were calculated according to the data at reaction time 2 hours. The amount of the dominant acid active site N₃P-OH was estimated by the atom content and the ratio of N₃P-OH and N₂P=O revealed by XPS result.

Table S4. The specific surface area (BET) of the BNP catalysts.

Sample	BNP-1.4	BNP-2.1	BNP-2.8
Specific Surface area (BET) , m ² /g	18.90	20.92	28.73

2.Supporting figures

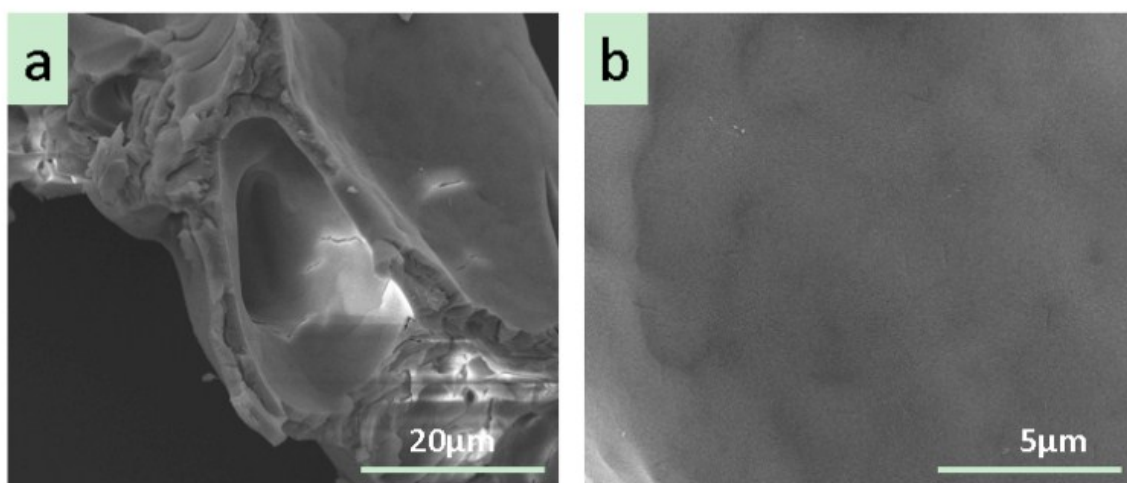


Fig. S1. SEM images of *h*-BN.

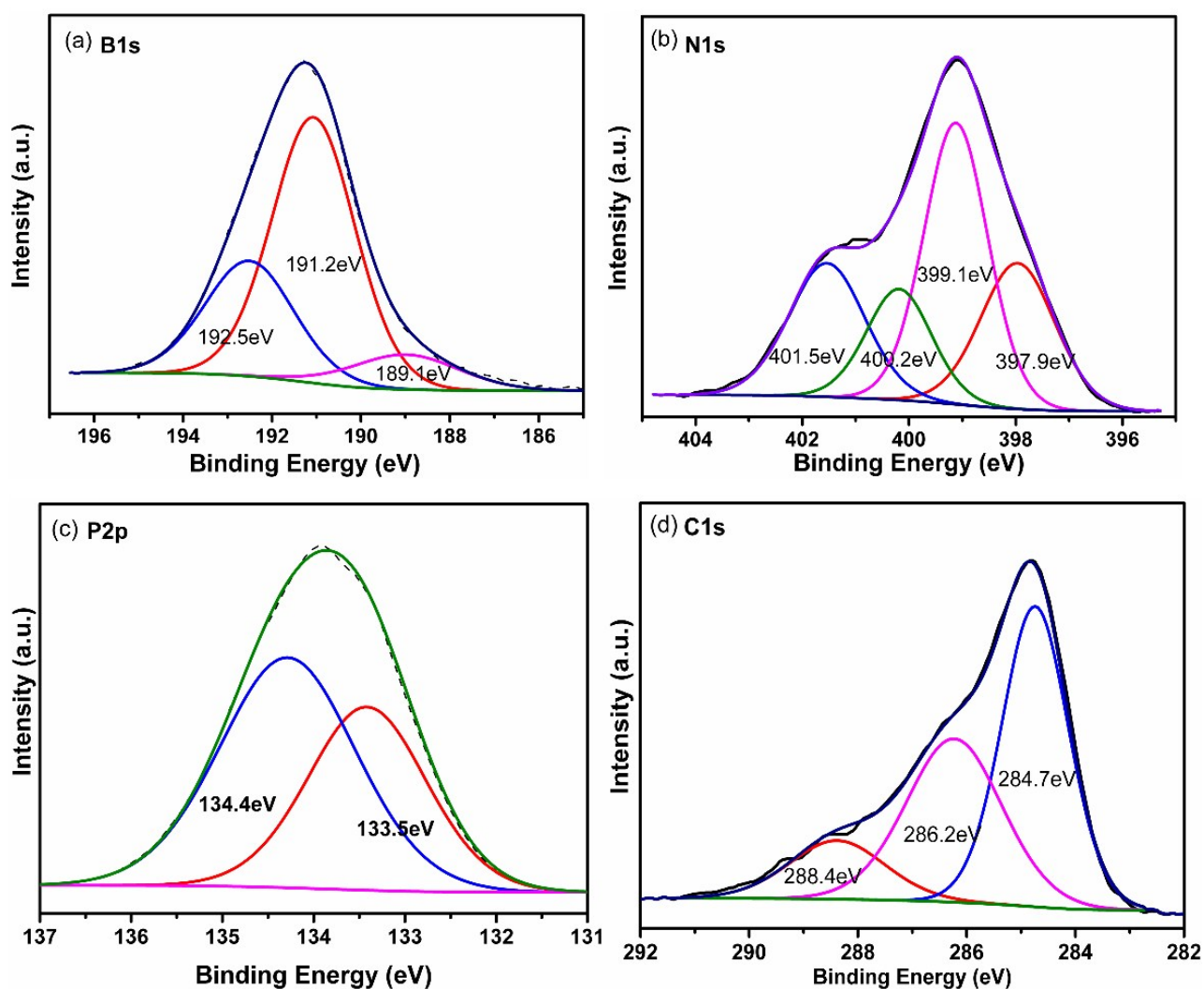


Fig. S2. The XPS spectra of BNP-2.8 sample B1s (a), N1s (b), P2p (c) and C1s(d).

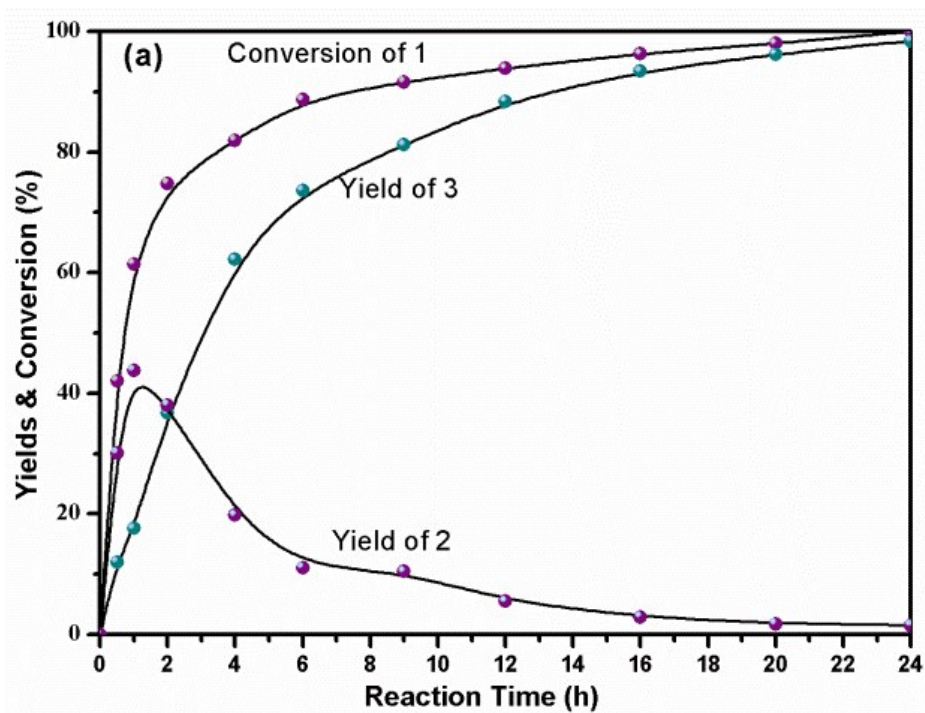


Fig.S3. The kinetics of one-pot deacetalization-Knoevenagel cascade reaction over BNP-2.1 sample

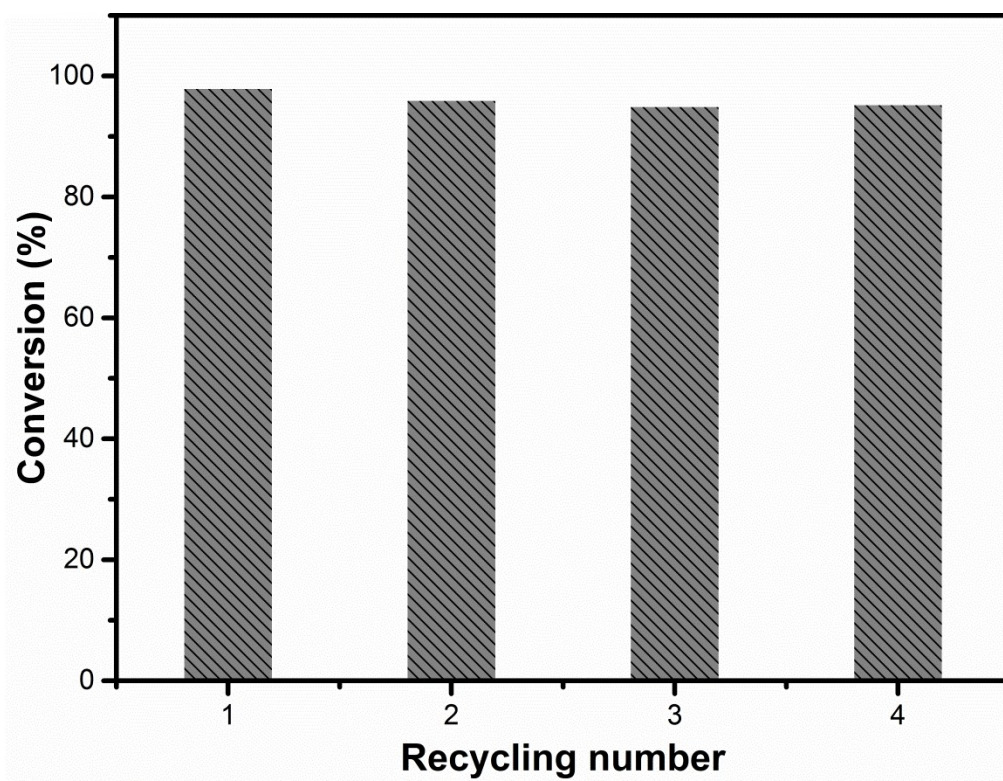


Fig.S4. The Reusability of BNP-2.1 sample with scaled-up reactant amount.

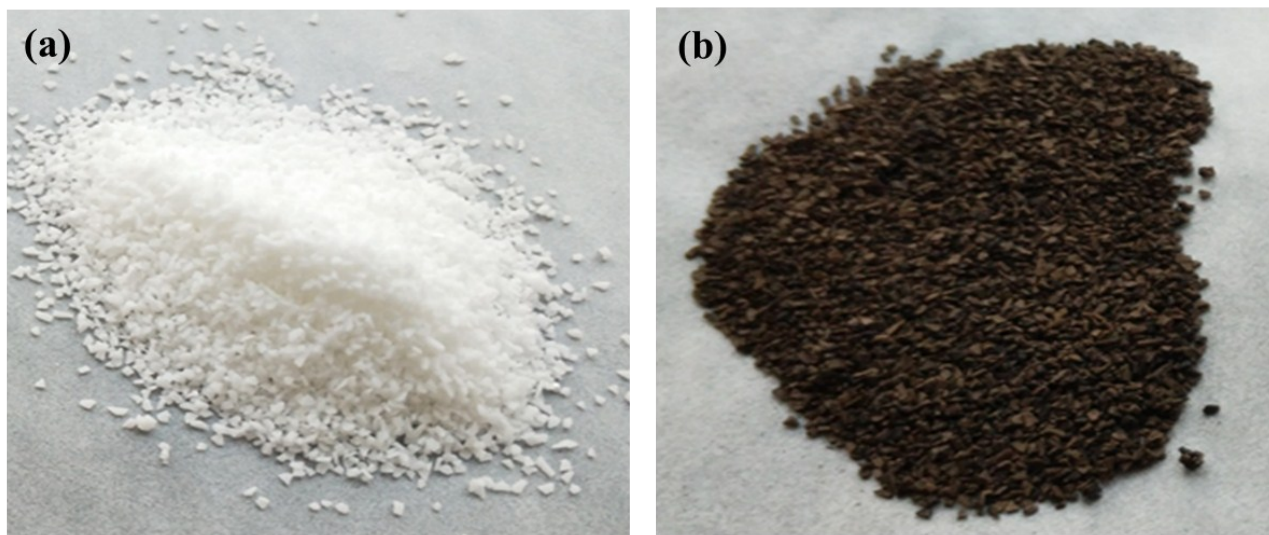


Fig. S5. Photo of (a) cordierite particles with 40-60 mesh and that (b) after BNP-2.1 immobilized thereon.