

Supplementary information

Supported ammonia borane decomposition through enhanced homopolar B-B coupling

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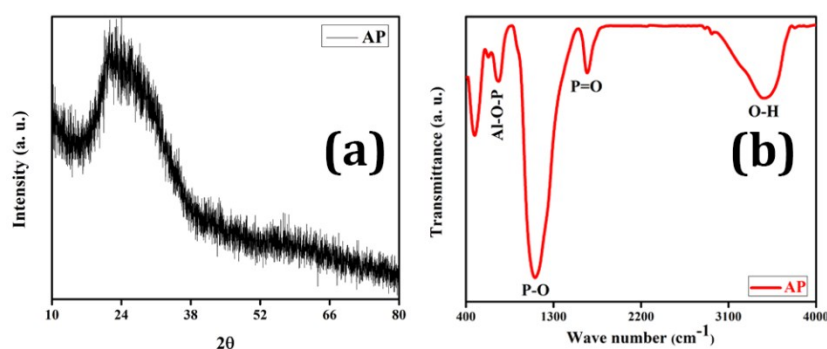


Figure S1: (a) XRD and (b) FTIR of the synthesized AlPO_4 support material

Table S1: FTIR frequencies for synthesized Aluminium phosphate (AP)

Bonding Vibration	Vibrational frequency (cm^{-1})
Al-O-P Vibrations	494, 732
P-O stretching	1111
P=O stretching	1645

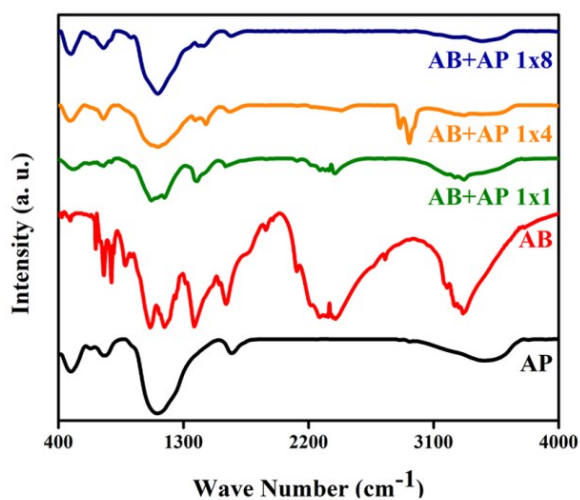


Figure S2: FTIR spectra of AB+AP samples

Table S2: FTIR vibrational frequencies of AB¹

Vibrational frequencies (cm ⁻¹)	FTIR Peak Annotation
603	NBH Rocking
968	¹¹ B-N Stretching (A ₁)
987	¹⁰ B-N Stretching (A ₁)
1175	BH ₃ deformation (A ₁)
1186	BH ₃ deformation (E)
1377	Unassigned
1396	Unassigned
1608	NH ₃ deformation
2340	Sym. B-H stretching (A ₁)
2415	Assym. B-H stretching (E)
3177	Unassigned suggested (overtone)
3337	Sym. N-H Stretching(A ₁)
3386	Asym. N-H stretching (E)

Table S3: AUC comparison of peaks observed in ¹¹B spectra of pure AB and AB+AP 1×1

	Pure AB@10 (%)	AB+AP(1×1)@10 (%)
Peak 1 (30 ppm)	82.17	61.17
Peak 2 (24 ppm)	6.26	21.54
Peak 3 (6.4 ppm)	11.56	17.28

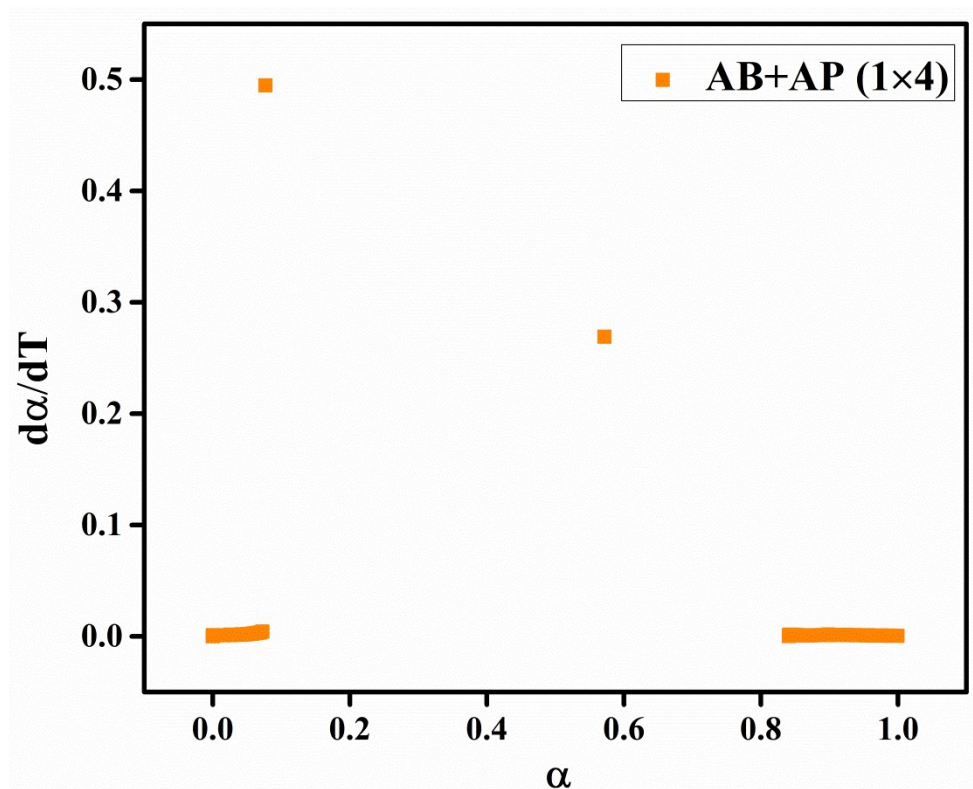


Figure S3: Kinetic data for AB+AP(1×4)@10 thermal decomposition

Table S4: Avrami Erofe'ev model fitting parameters

	n	k	$Adj. R^2$
Pure AB	5 ± 5.76	0.016 ± 0.015	0.42
AB+AP (1×1)	4.67 ± 0.58	0.044 ± 0.00513	0.925
AB+AP (1×4)	2.308 ± 0.156	0.059 ± 0.0033	0.921

References

1. Xie, S., Song, Y. & Liu, Z. In situ high-pressure study of ammonia borane by Raman and IR spectroscopy. *Can. J. Chem.* **87**, 1235–1247 (2009).