

Supporting information

Demonstration of the nanosize effect of carbon nanomaterials on the dehydrogenation temperature of ammonia borane

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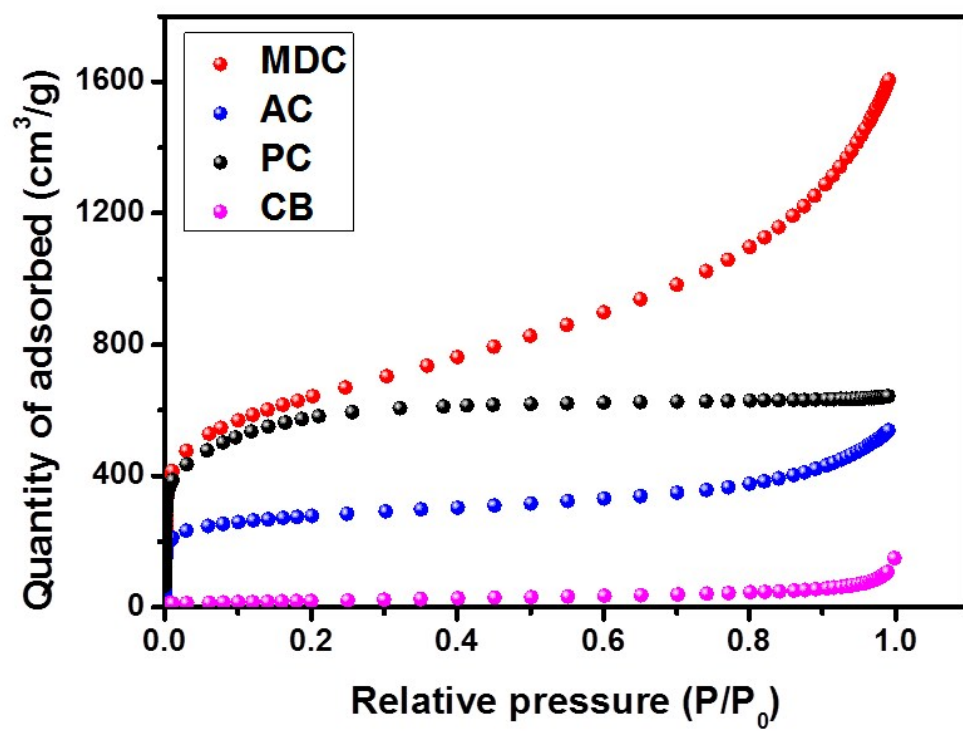
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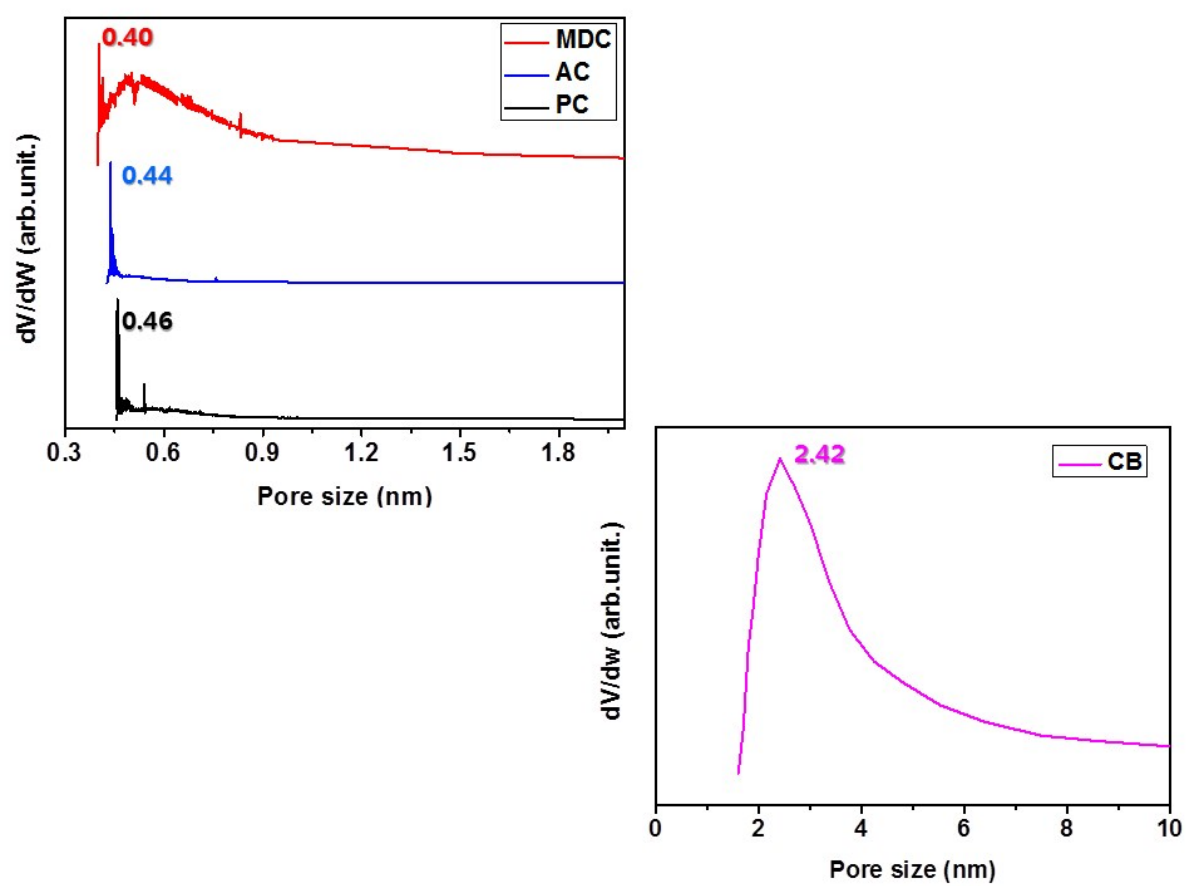
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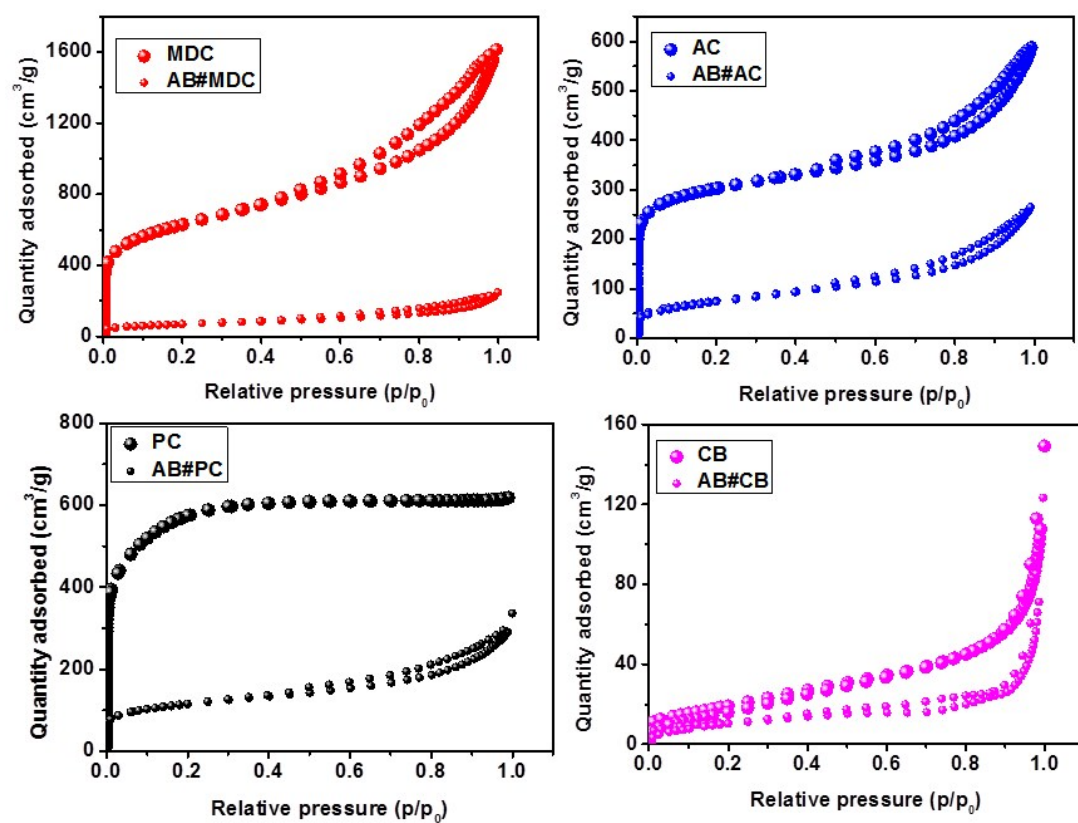
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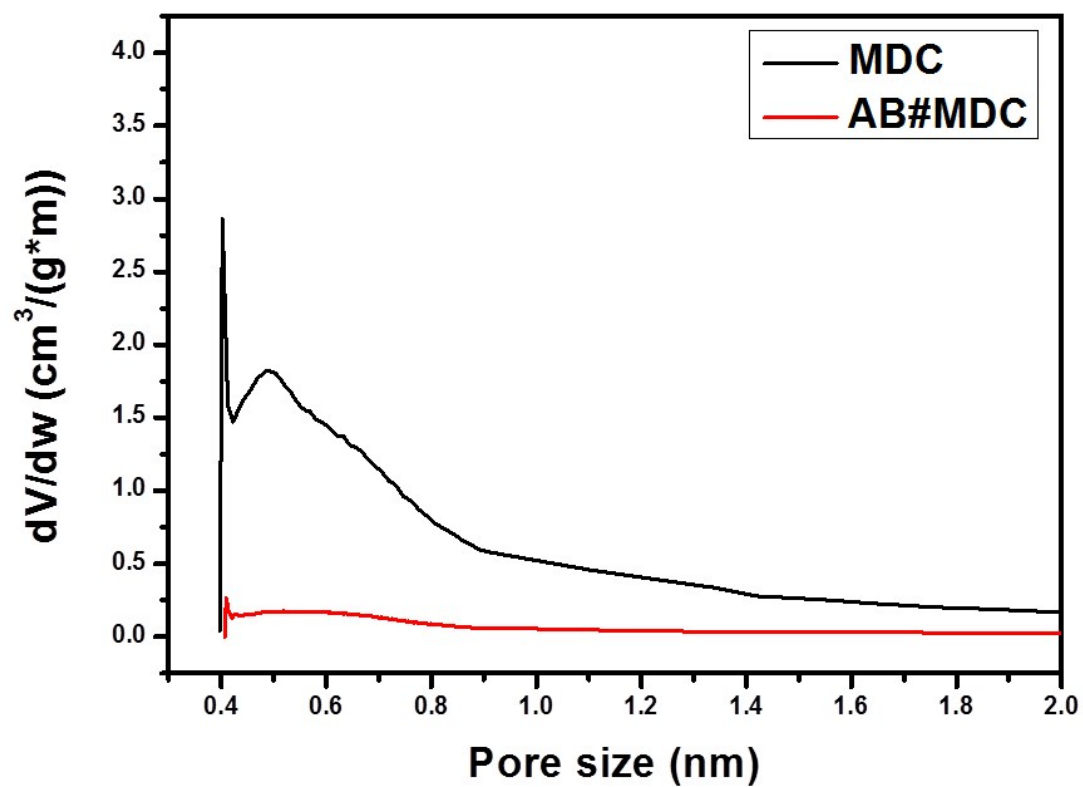
< Figure S1 > N₂ isotherm at 77 K of MDC, AC, PC, and CB



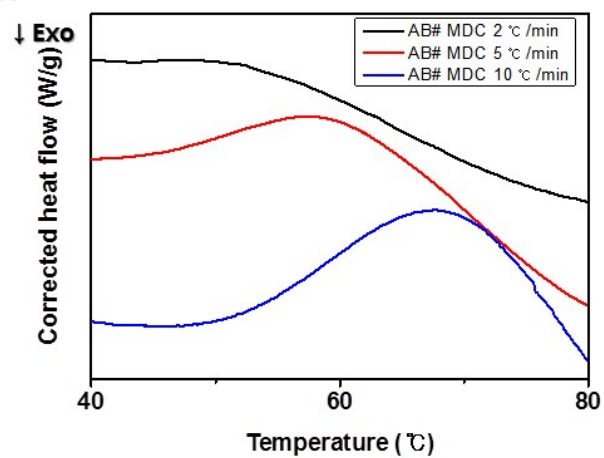
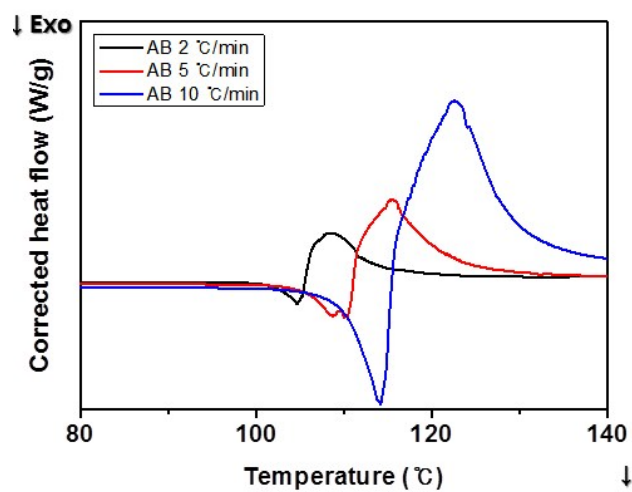
< Figure S2 > The repeated calculation of pore size distribution of MDC, AC, PC and CB



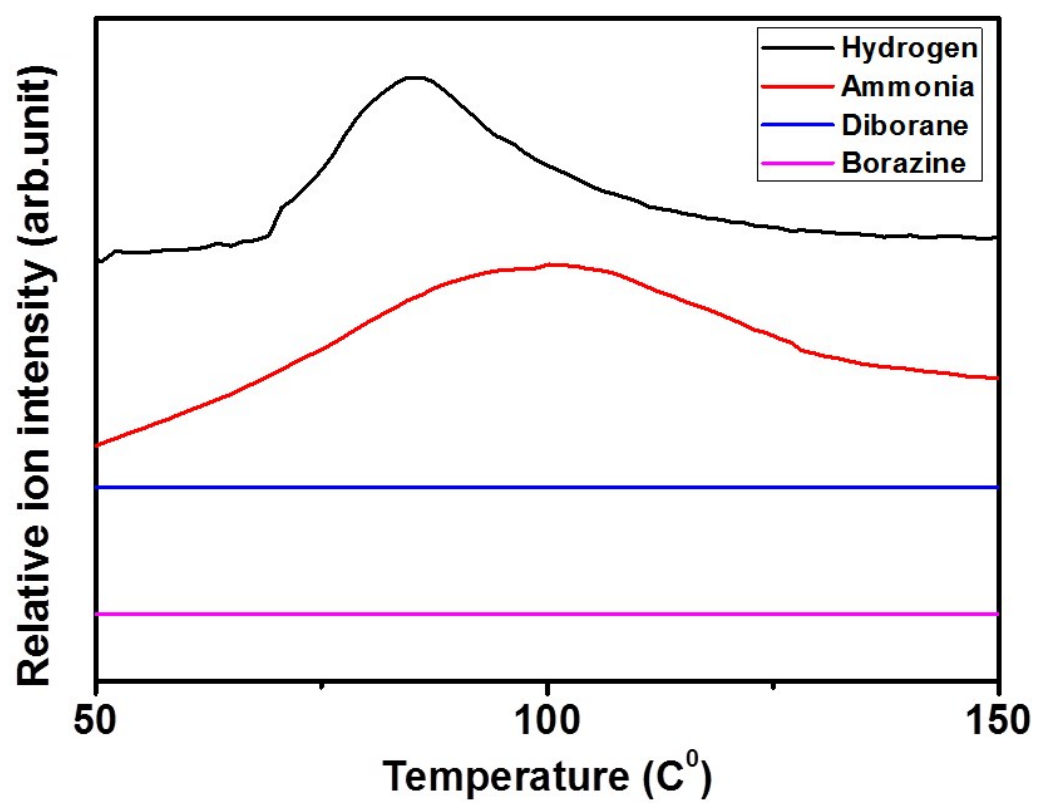
< Figure S3 > Comparison of N₂ isotherm at 77 K of pristine samples and AB infiltrated samples



< Figure S4 > Analysis of pore size distribution of MDC and AB#MDC : the highly decrease of pore volume over the pore size range after the infiltration of AB



< Figure S5 > Heat flow from AB#MDC and pristine AB during heat treatment at different heating rate by DSC



< Figure S6 > TPD-MS profile of AB#MDC for evolved gases

	Pore volume (cm ³ /g)	BET SSA (m ² /g)
MDC	2.49	2222
AB#MDC	0.38	246
AC	0.91	1093
AB#AC	0.41	272
PC	0.96	2014
AB#PC	0.52	394
CB	0.23	73
AB#CB	0.19	37

< Table S1 > Variation of pore volume and BET SSA after the infiltration of AB

Temperature (°C)	Weight of MDC (mg)	Weight of AB (mg)	Detected H ₂ (μmol/ml)	Volume of sample cell (ml)	H ₂ (wt%)
60	x	15	0	100	0
70	x	15	2.10*10 ⁻²	100	2.80*10 ⁻²
80	x	15	2.50*10 ⁻²	100	3.30*10 ⁻²
60	2.5	5	0.91	100	3.60 (2.40)
70	2.5	5	1.43	100	5.70 (3.80)
80	2.5	5	1.78	100	7.1 (4.70)

< Table S2 > Numerical data for calculating H₂ release performance

	AB#MDC	AB+THF
Temperature (°C)	Released H₂ (wt%) $\frac{H_2}{AB} * 100$	Released H₂ (wt%) $\frac{H_2}{AB} * 100$
60	3.6	1.2*10⁻¹
70	5.7	5.2*10⁻¹
80	7.1	1.0

< Table S3 > H₂ desorption performance of AB#MDC and AB solvated in THF

Support	Exp.Temp (°C)	Time (min)	AB based H ₂ density (wt%)	whole sample based H ₂ density(wt%)	Ref
MDC	80	30	7.1	4.7	This work
Microporous carbon	80	30	< 8.0 ^a	< 5.4 ^a	[S1]
Silica aerogel	80	30	0.9	0.5	[S2]
Fe-MIL-53	80	30	< 1.3	< 1.1	[S3]
Li-CMK-3	80	30	< 7 ^a	< 3.5 ^a	[S4]
Li-CMK-3	60	30	< 6 ^a	< 3.0 ^a	
Zn-MOF74	75	30	-	< 4 ^a	[S5]
Zn-MOF74	65	30	-	< 2 ^a	
GO	70	30	< 7.0 ^a	<1.8 ^a	[S6]
GO	80	30	< 9.0 ^a	<2.3 ^a	
MOF-5	75	30	< 5.5	< 0.2	[S7]

< Table S4 > Comparison of the performances of AB infiltrated porous materials within 80 °C

a : calculated value for the same experimental condition, referring to the data in previous studies

References

- [S1] Z. Yang, D. Zhou, B. Chen, Z. Liu, Q. Xia, Y. Zhu and Y. Xia, *J. Mater. Chem. A.*, 2017, 5, 15395-15400.
- [S2] M. Rueda, L. M. Sanz-Moral, J. J. Segovia and Á. Martín, *Microporous Mesoporous Mater.*, 2017, 237, 189-200.
- [S3] G. Srinivas, W. Travis, J. Ford, H. Wu, Z. X. Guo and T. Yildirim, *J. Mater. Chem. A.*, 2013, 1, 4167-4172.
- [S4] L. Li, X. Yao, C. Sun, A. Du, L. Cheng, Z. Zhu, C. Yu, J. Zou, S. C. Smith, P. Wang, H. M. Cheng, R. L. Frost and G. Q. Lu, *Adv. Funct. Mater.*, 2009, 19, 265-271.
- [S5] Srinivas, G., et al., Zn-MOF assisted dehydrogenation of ammonia borane: Enhanced kinetics and clean hydrogen generation. *Int. J. Hydrog. Energy.*, 2012. 37(4): p. 3633-3638.
- [S6] Tang, Z., et al., Graphene oxide based recyclable dehydrogenation of ammonia borane within a hybrid nanostructure. *J. Am. Chem. Soc.*, 2012. 134(12): p. 5464-5467.
- [S7] Li, Z., et al., Improved thermal dehydrogenation of ammonia borane by MOF-5. *RSC Adv.*, 2015. 5(14): p. 10746-10750.