Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Enhanced Hydrogen Storage Kinetics and Air Stability of Nanoconfined $NaAlH_4$ in Graphene Oxide Framework

Hyung Wan Do,[ab] HyeonJi Kim[a] and Eun Seon Cho*[a]

[a]Department of Chemical and Biomolecular Engineering, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Republic of Korea

[b]Current address: KIURI Institute, Yonsei University, Seoul 03722, Republic of Korea

*Corresponding author: escho@kaist.ac.kr

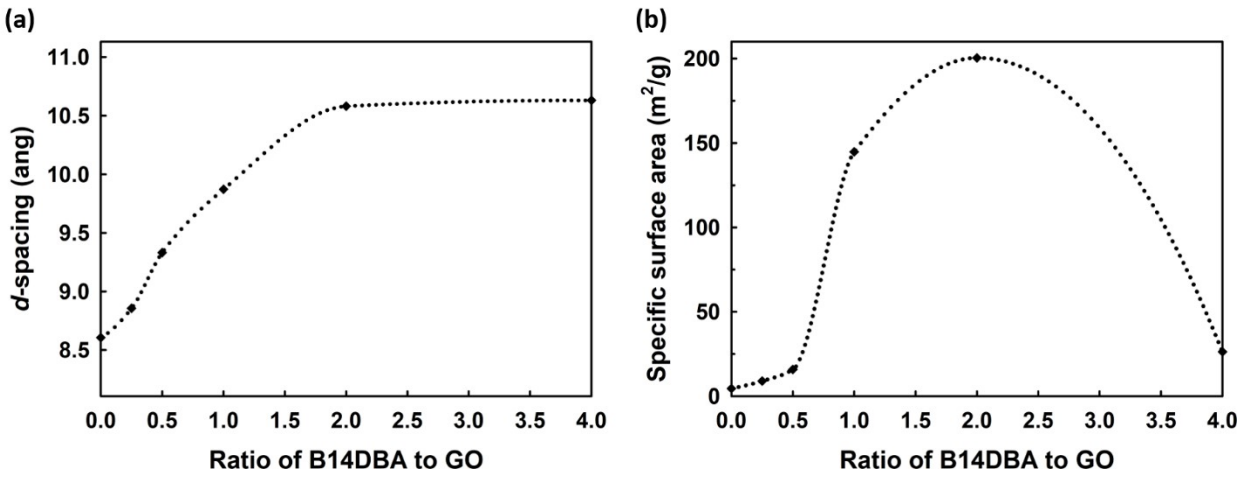

Fig. S1 (a) The *d*-spacing of the prepared GOFs depending on the ratio of B14DBA to GO, calculated from XRD peak analysis. (b) BET specific surface area of GOFs with different ratios of B14DBA to GO, calculated from N_2 adsorption-desorption isotherm measurements.

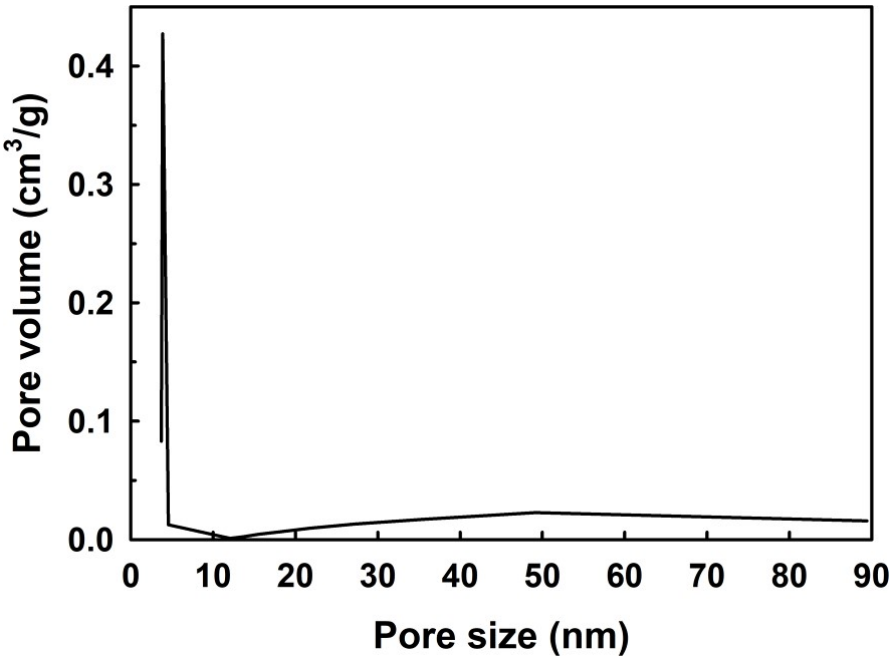

Fig. S2 BJH desorption *dV*/*d*log*D* pore volume vs. pore size for GOF (1:2), showing pore size distribution of the GOF.

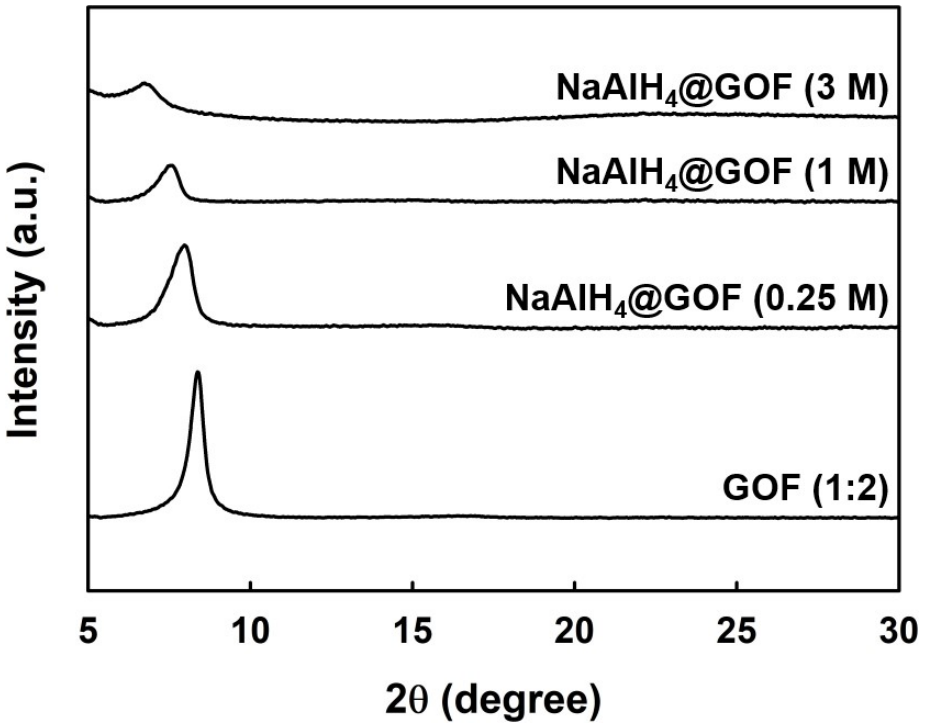

Fig. S3 XRD patterns of GOF (1:2), $NaAlH_4$@GOF (0.25 M), $NaAlH_4$@GOF (1 M), and $NaAlH_4$@GOF (3 M).

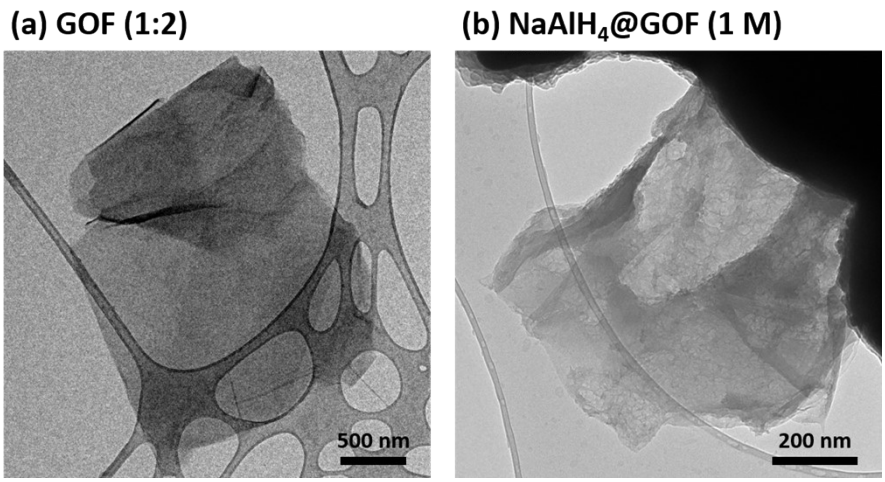

Fig. S4 TEM images of (a) GOF (1:2) and (b) $NaAlH_4$@GOF (1 M). Surface morphology did not show significant changes upon $NaAlH_4$ infiltration.

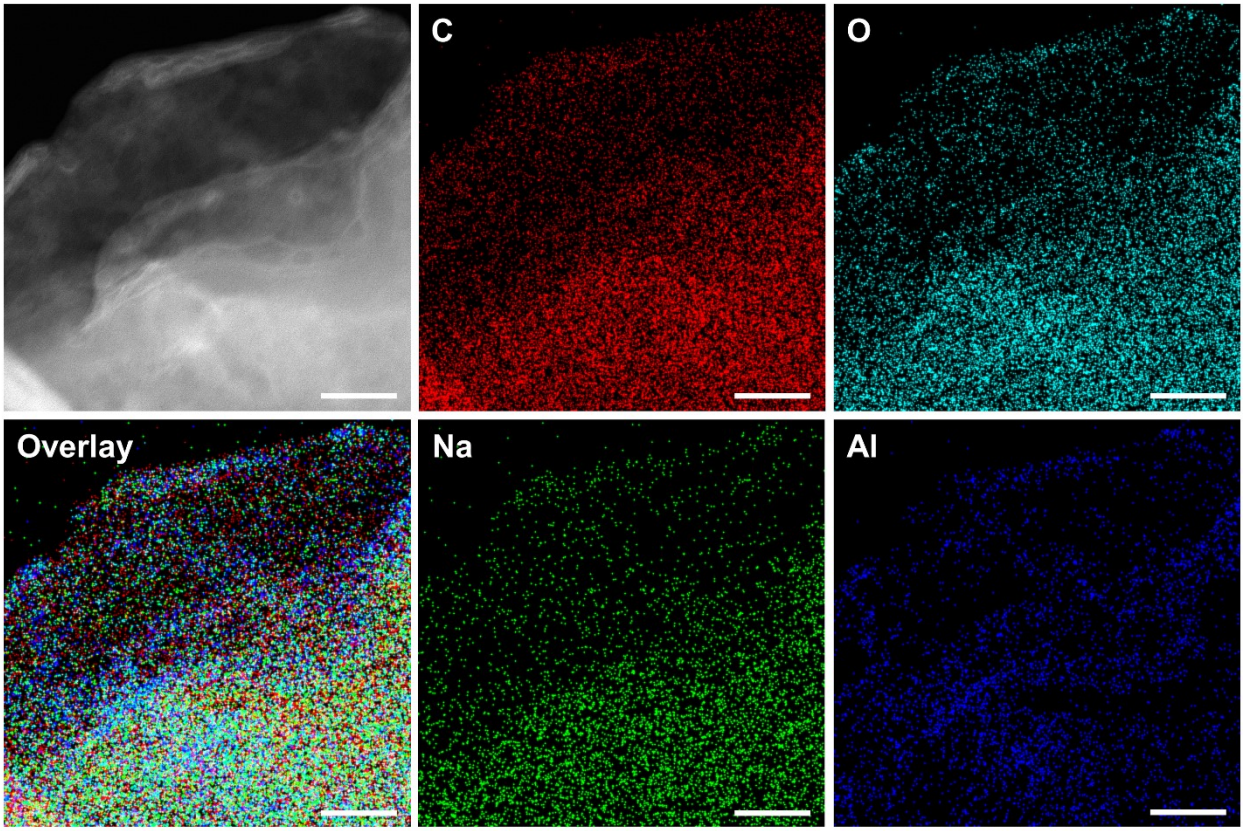

Fig. S5 BF-STEM-EDS images of $NaAlH_4$@GOF (1:2) (all scale bars are 50 nm).

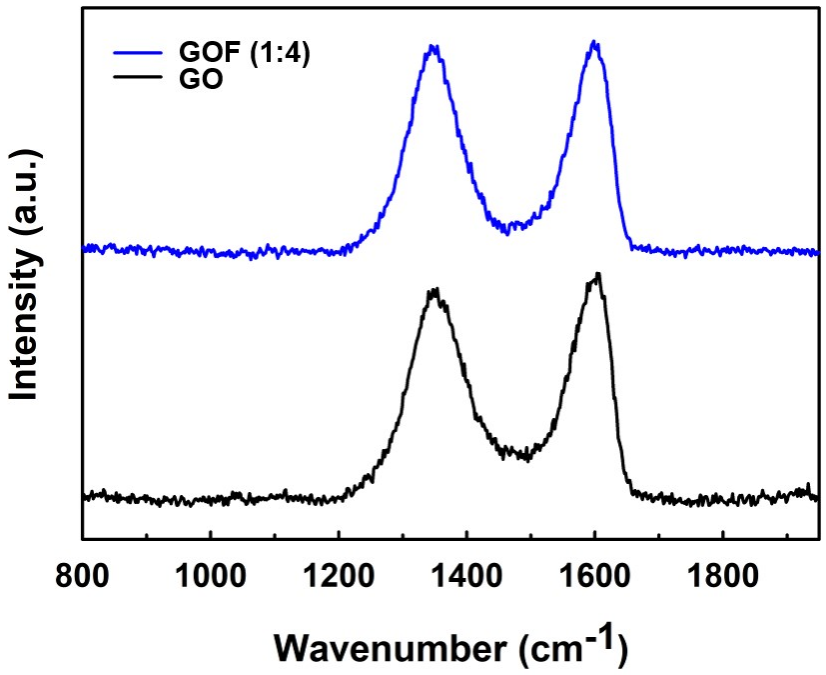

Fig. S6 Raman spectra showing both D-band and G-band of GO and GOF (1:4). The two spectra are nearly identical in peak position and intensity.

Table S1. Summary of activation energies (E_a) for the dehydrogenation of bulk, nanoconfined, and catalyst-doped $NaAlH_4$ from this work and selected previous studies.[1-10]

Modification	Material	E_a, 1st step (kJ/mol)	E_a, 2nd step (kJ/mol)	Reference
-	Undoped $NaAlH_4$	128	159	[1]
	Undoped $NaAlH_4$	118.1	120.7	[2]
Nanoconfined	$NaAlH_4$@GOF	47.13	108.45	This work
	$NaAlH_4$@porous carbon (200 nm)	124.3	-	[1]
	$NaAlH_4$@porous carbon (60 nm)	102.1	-	
	$NaAlH_4$@porous carbon (30 nm)	84.9	-	
	$NaAlH_4$@porous carbon (4 nm)	69.7	-	
	$NaAlH_4$@NPC	75.5	-	[3]
	$NaAlH_4$@CMK-3	66.5	-	
	$NaAlH_4$@CNF	58	-	[4]
	$NaAlH_4$@Cu-BTC	53.3	-	[5]
Catalyst-doped	Ti-doped $NaAlH_4$	79.5	97.1	[2]
	2D Ti_3C_2-doped $NaAlH_4$	87.3	88.1	[6]
	CeO_2@C-doped $NaAlH_4$	90.3	81.7	[7]
	CeB_6-doped $NaAlH_4$	69.3	99.1	[8]
	CeO_2-doped $NaAlH_4$	89.8	101.6	
	CeF_3-doped $NaAlH_4$	111.6	108.9	
Nanoconfined and catalyst-doped	$NaAlH_4$(Ti)@MOF-74(Mg)	57.4	-	[9]
	$NaAlH_4$@CeO_2	76.32	-	[10]
	$NaAlH_4$@N-doped NPC	44.1	-	[3]
	$NaAlH_4$@N-doped CMK-3	45.6	-	

References

1. X. Fan, X. Xiao, J. Shao, L. Zhang, S. Li, H. Ge, Q. Wang and L. Chen, *Nano Energy*, 2013, **2**, 995-1003.
2. G. Sandrock, K. Gross and G. Thomas, *Journal of Alloys and Compounds*, 2002, **339**, 299-308.
3. C. L. Carr, W. Jayawardana, H. Zou, J. L. White, F. El Gabaly, M. S. Conradi, V. Stavila, M. D. Allendorf and E. H. Majzoub, *Chemistry of Materials*, 2018, **30**, 2930-2938.
4. C. P. Baldé, B. P. C. Hereijgers, J. H. Bitter and K. P. de Jong, *Journal of the American Chemical Society*, 2008, **130**, 6761-6765.
5. R. K. Bhakta, S. Maharrey, V. Stavila, A. Highley, T. Alam, E. Majzoub and M. Allendorf, *Physical Chemistry Chemical Physics*, 2012, **14**, 8160-8169.
6. R. Wu, H. Du, Z. Wang, M. Gao, H. Pan and Y. Liu, *Journal of Power Sources*, 2016, **327**, 519-525.
7. X. Zhang, Y. Liu, K. Wang, Y. Li, M. Gao and H. Pan, *ChemSusChem*, 2015, **8**, 4180-4188.
8. X. Fan, X. Xiao, L. Chen, L. Zhang, J. Shao, S. Li, H. Ge and Q. Wang, *Journal of Materials Chemistry A*, 2013, **1**, 9752-9759.
9. V. Stavila, R. K. Bhakta, T. M. Alam, E. H. Majzoub and M. D. Allendorf, *ACS Nano*, 2012, **6**, 9807-9817.
10. Q. Gao, G. Xia and X. Yu, *Nanoscale*, 2017, **9**, 14612-14619.