

Electronic Supplementary Information

Catalyzed Eutectic LiBH₄-KBH₄ System Nanoconfined at Low Temperature for Superior Hydrogen Storage Reversibility

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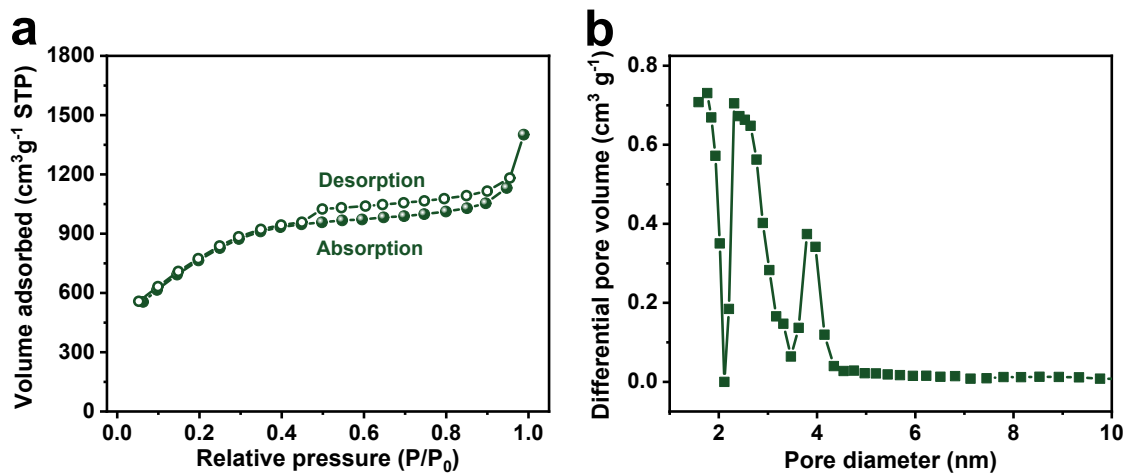


Fig. S1. (a) N₂ sorption isotherms and (b) pore size distributions of the porous carbon scaffold.

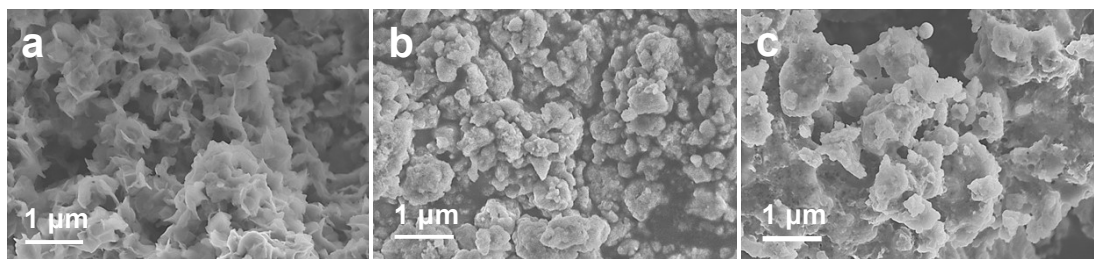


Fig. S2. SEM images of (a) the as-milled pristine LiBH₄, (b) Li/KBH₄ and (c) Li/KBH₄+0.1NiCp₂.

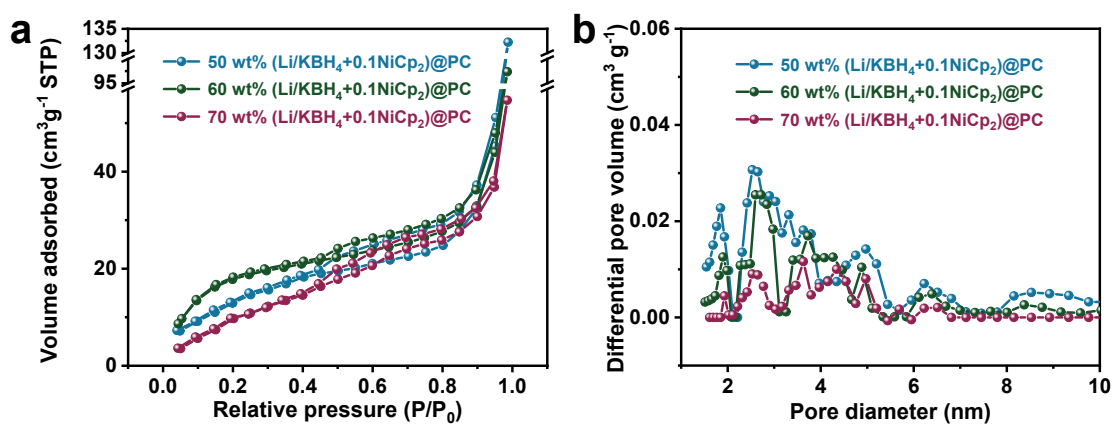


Fig. S3. (a) N₂ sorption isotherms and (b) pore size distributions of the confined systems with different loadings of Li/KBH₄+0.1NiCp₂.

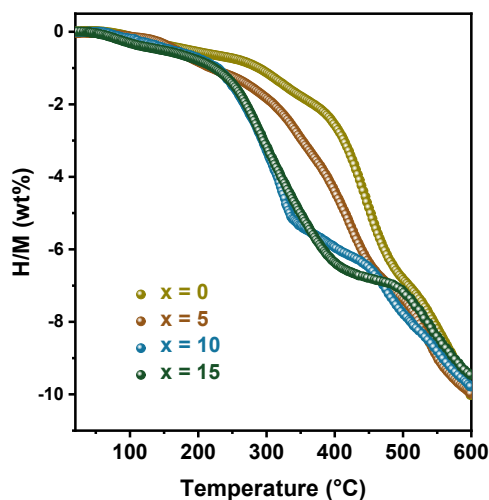


Fig. S4. Dehydrogenation curves of the Li/KBH₄+x wt% NiCp₂ systems with x = 0, 5, 10 and 15.

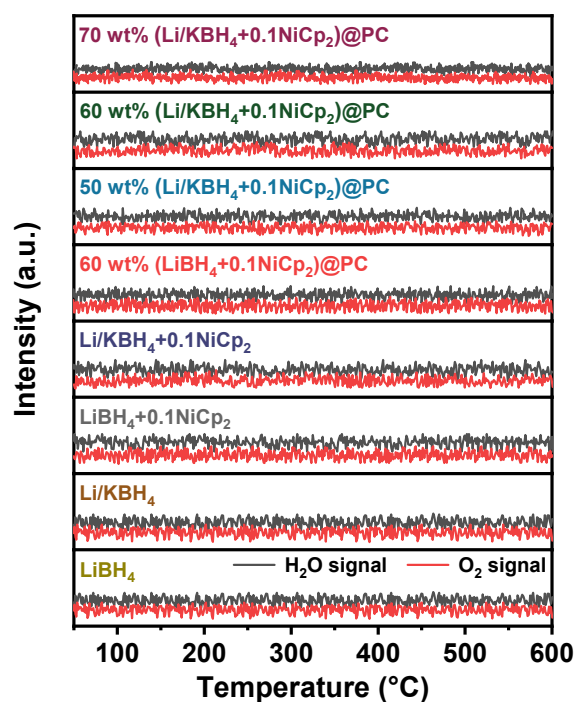


Fig. S5. H₂O and O₂ signals of TPD–MS curves of the confined systems loaded with (Li/KBH₄+0.1NiCp₂), with 60 wt% (LiBH₄+0.1NiCp₂) and the as–milled systems of Li/KBH₄+0.1NiCp₂, LiBH₄+0.1NiCp₂, Li/KBH₄ as well as the pristine LiBH₄.

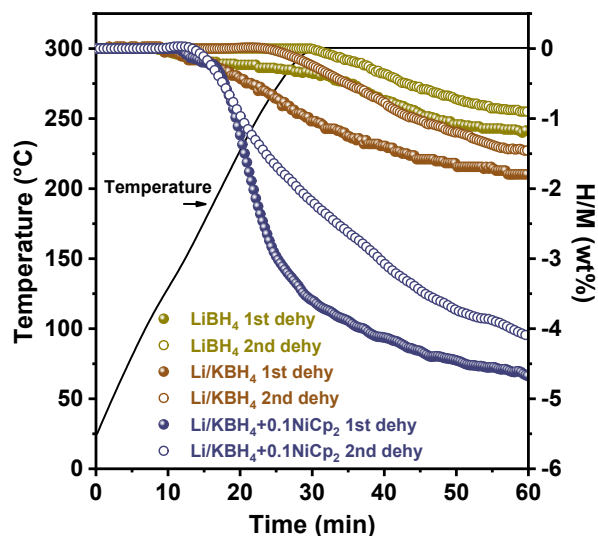


Fig. S6. Isothermal dehydrogenation curves of the as-milled pristine LiBH_4 , Li/KBH_4 and $\text{Li/KBH}_4+0.1\text{NiCp}_2$ at a cyclic regime of dehydrogenation at $300\text{ }^\circ\text{C}$ for 60 min in static vacuum and hydrogenation at $400\text{ }^\circ\text{C}/10\text{ MPa H}_2$ pressure for 120 min.

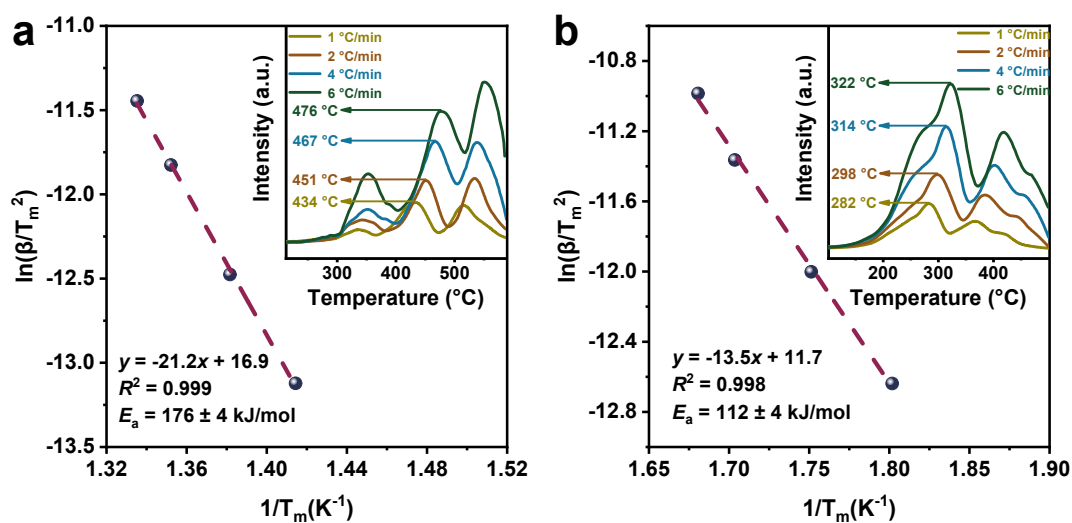


Fig. S7. The Kissinger's plots of the (a) Li/KBH_4 and (b) $\text{Li/KBH}_4+0.1\text{NiCp}_2$ systems. The insets are their TPD-MS curves measured at different heating rates.

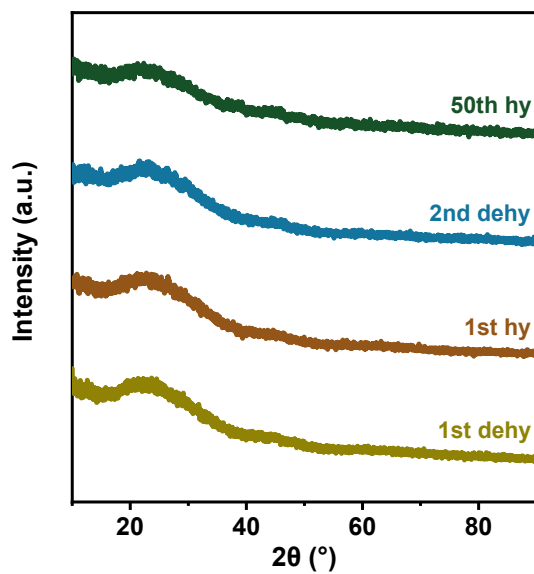


Fig. S8. XRD patterns the confined system with 60 wt% (Li/KBH₄+0.1NiCp₂) at different dehydrogenation (dehy) and hydrogenation (hy) states.

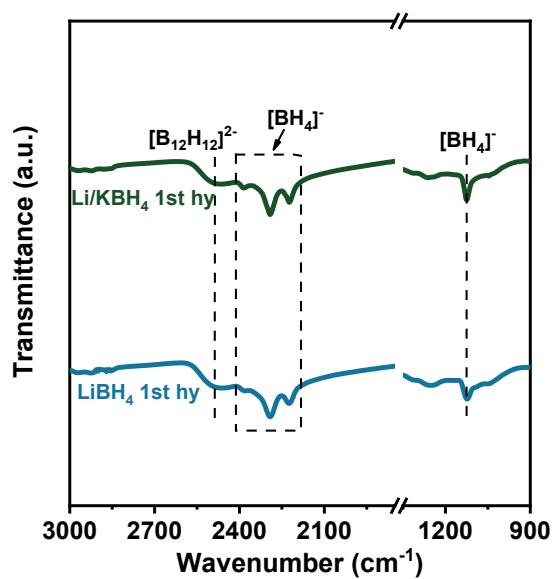


Fig. S9. FTIR spectra of the Li/KBH₄ and LiBH₄ at their initial hydrogenation (hy) states.

Table S1. The cyclic dehydrogenation capacities of the confined system with 60 wt% (Li/KBH₄+0.1NiCp₂).

Cycle number	1	2	3	4	5	6	7	8	9	10
Capacity (wt%)	7.00	6.70	6.68	6.67	6.67	6.67	6.66	6.66	6.66	6.65
Cycle number	11	12	13	14	15	16	17	18	19	20
Capacity (wt%)	6.65	6.66	6.65	6.64	6.64	6.64	6.65	6.64	6.63	6.63
Cycle number	21	22	23	24	25	26	27	28	29	30
Capacity (wt%)	6.64	6.65	6.65	6.64	6.64	6.64	6.63	6.63	6.63	6.63
Cycle number	31	32	33	34	35	36	37	38	39	40
Capacity (wt%)	6.64	6.64	6.64	6.63	6.63	6.63	6.64	6.65	6.65	6.64
Cycle number	41	42	43	44	45	46	47	48	49	50
Capacity (wt%)	6.64	6.64	6.63	6.62	6.62	6.63	6.63	6.62	6.62	6.62