

Supplementary Information

In-situ preparation of pseudo-graphite domains in hard carbon via molecular engineering towards high-performance Na-ion batteries

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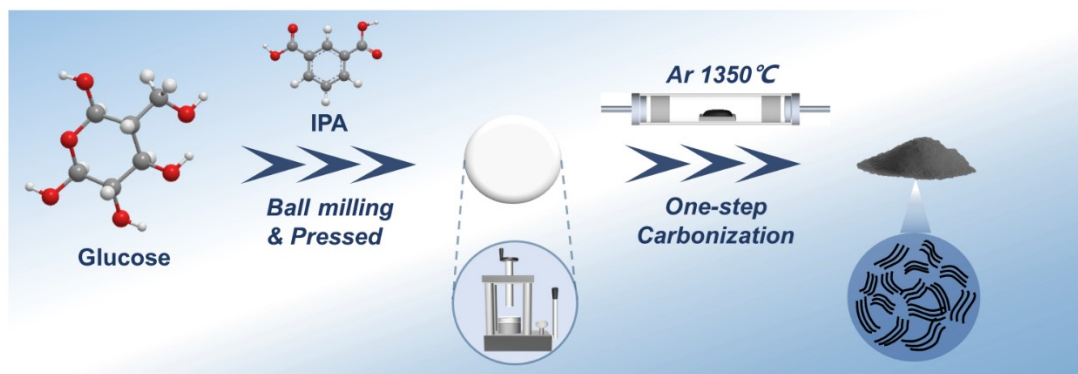


Figure S1. A specific procedure for the synthesis of hard carbon

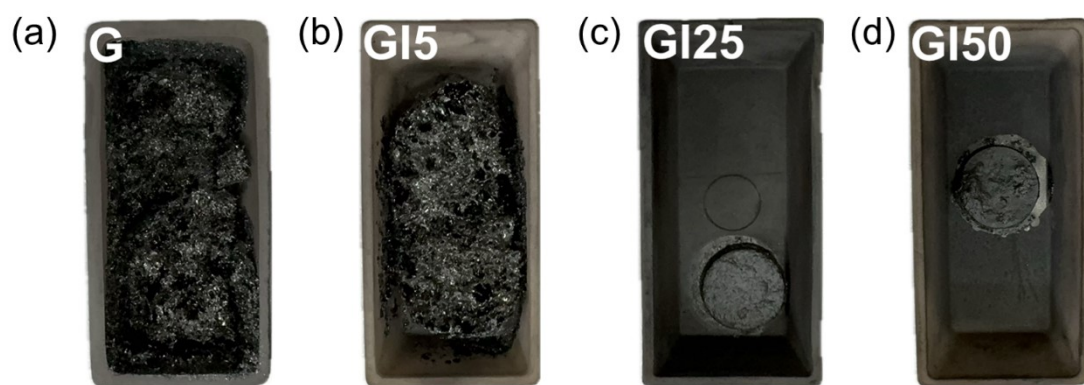


Figure S2. The photographs of hard carbon: (a) G, (b) GI5, (c) GI25 and (d) GI50.

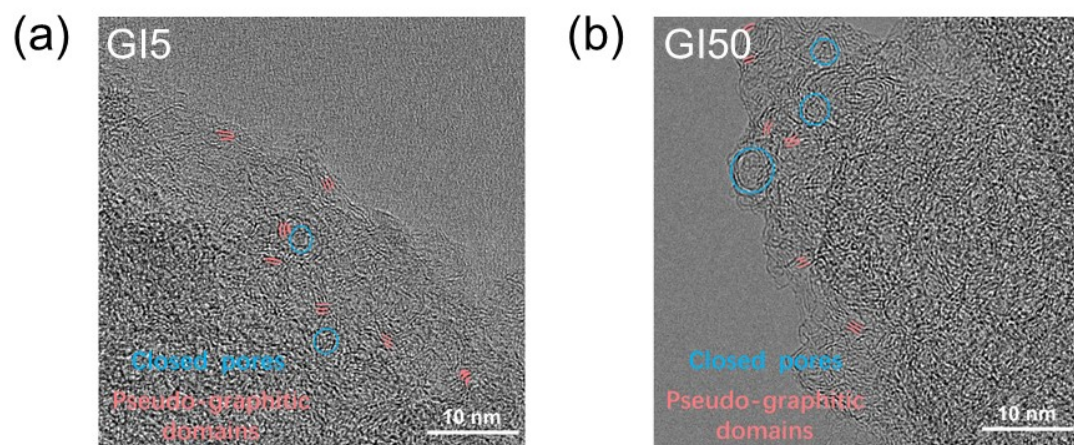


Figure S3. TEM image of (a) GI5 and (b) GI25.

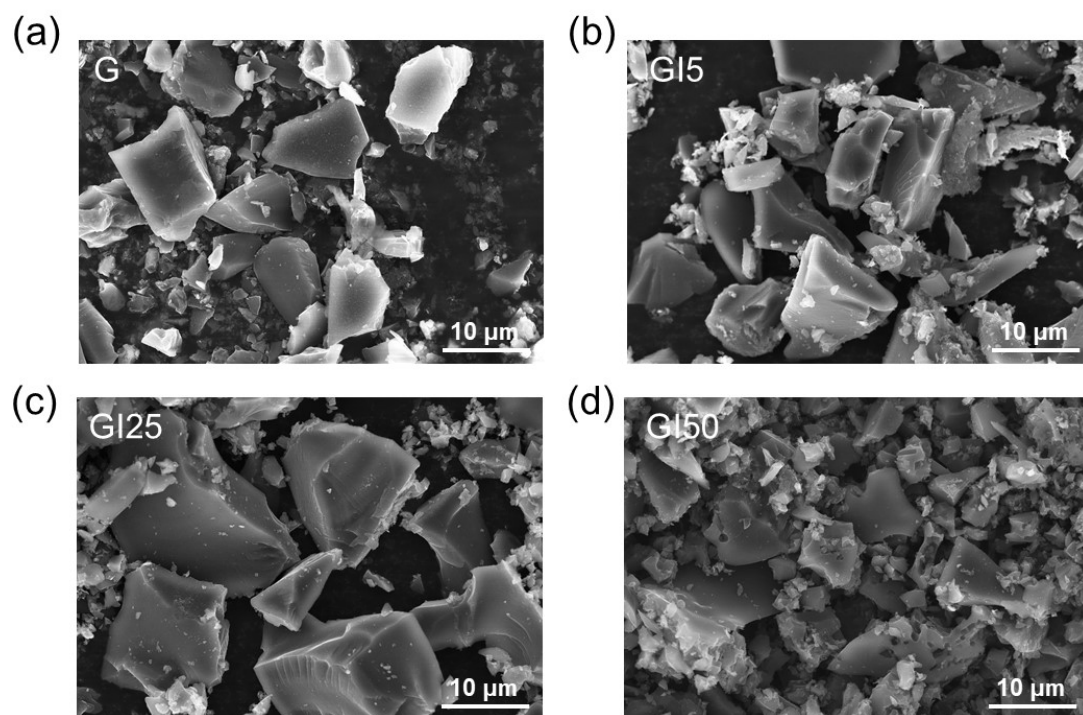


Figure S4. SEM images of (a) G, (b) GI5, (c) GI25 and (d) GI50.

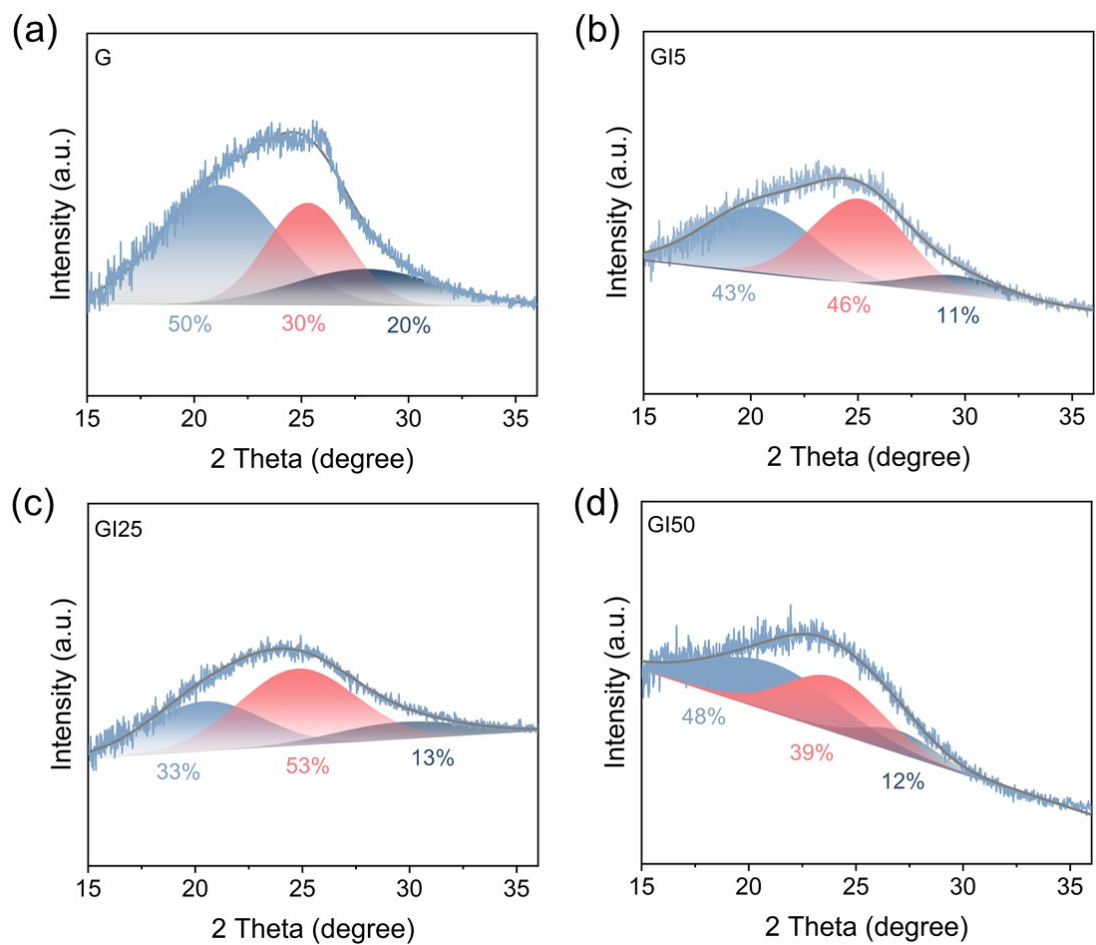


Figure S5. Fitted (002) peaks of (a) G, (b) GI5, (c) GI25 and (d) GI50.

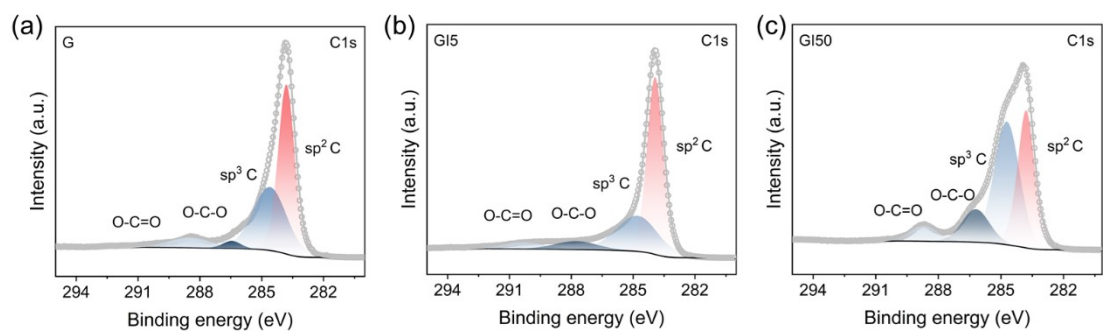


Figure S6. C 1s XPS spectra of (a) G, (b) GI5 and (c) GI50.

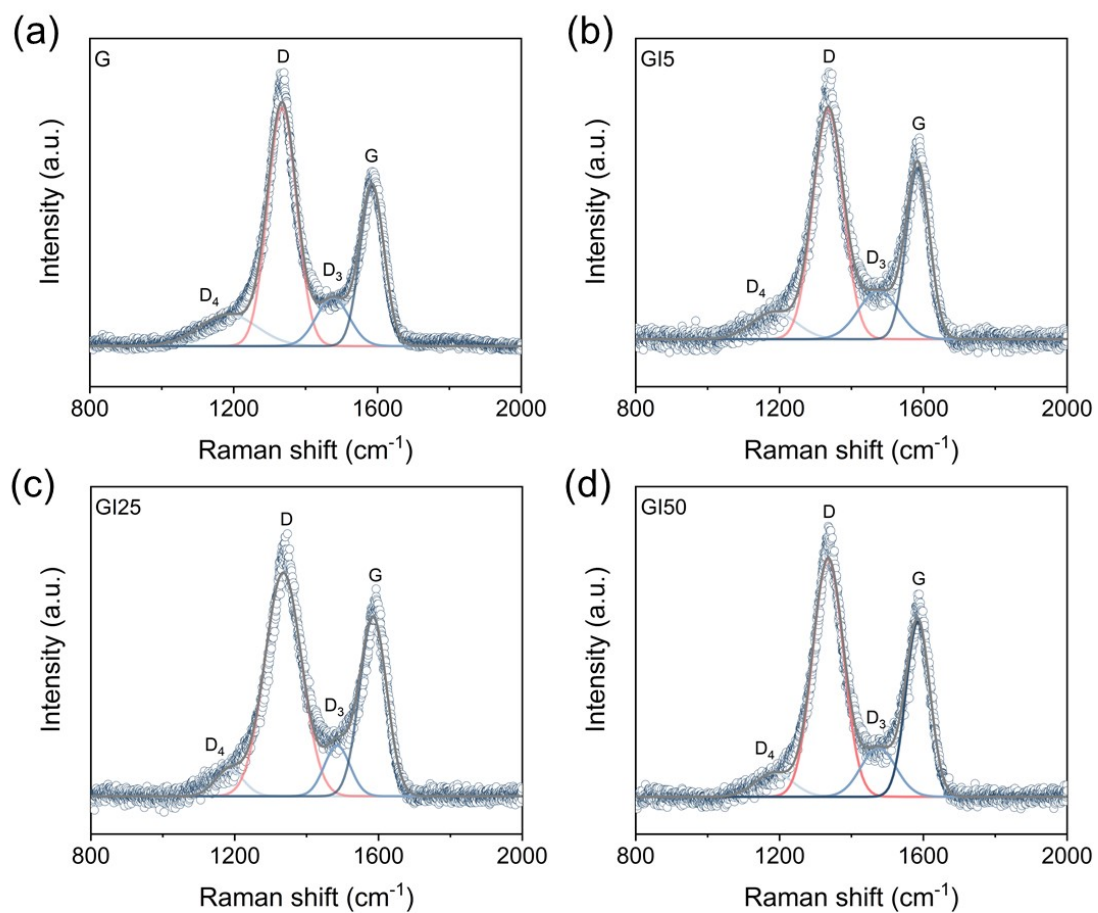


Figure S7. Fitted Raman spectra of (a) G, (b) GI5, (c) GI25 and (d) GI50.

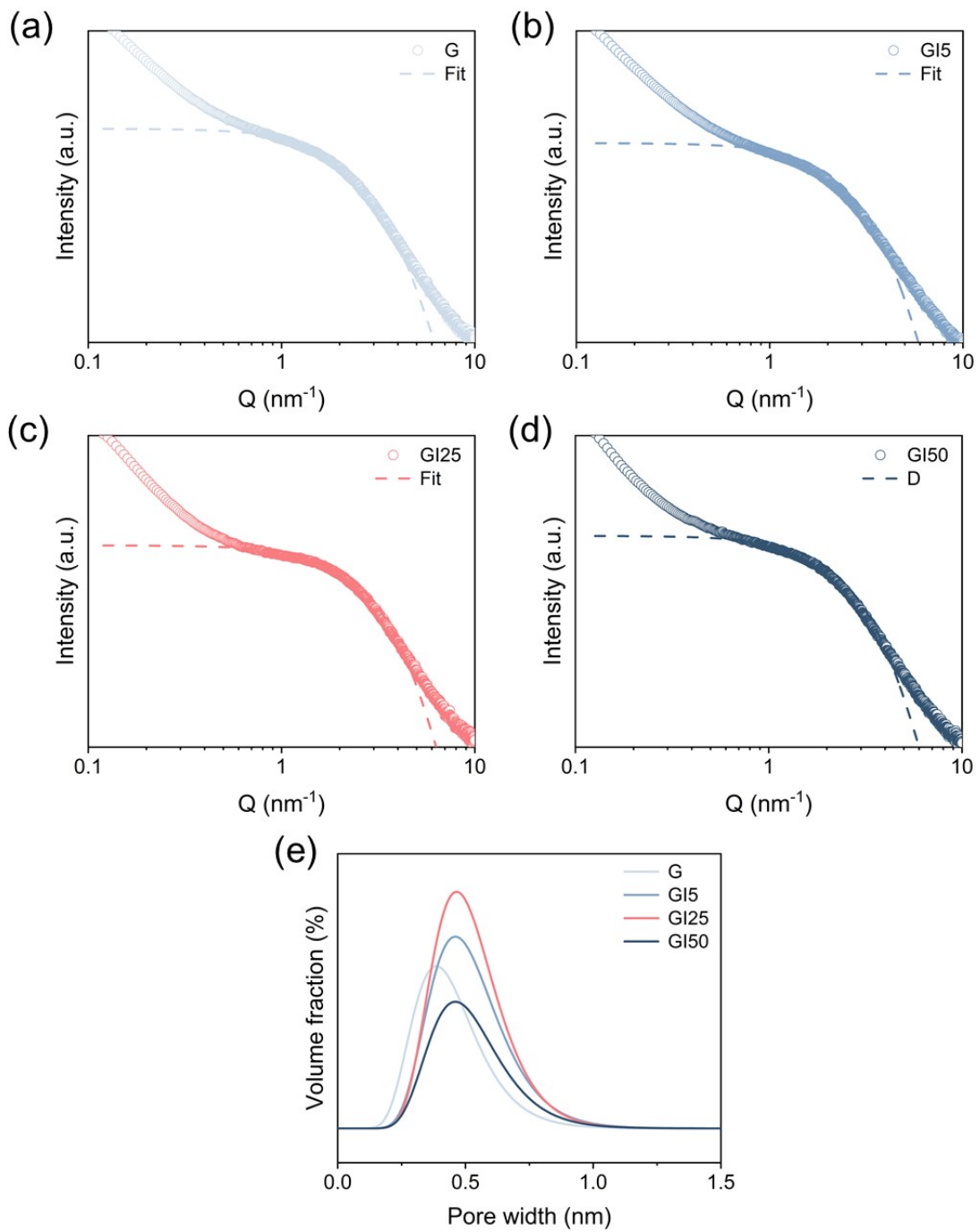


Figure S8. Fitted SAXS patterns of (a) G, (b) GI5, (c) GI25 and (d) GI50, (e) Pore distribution

curves were obtained from modeling the nanopore region of the SAXS data

Porod method:

$$I(q) = \frac{A}{q^a} + \frac{B \cdot b^4}{(1 + b^2 q^2)^2} + C \quad (\text{S-1})$$

Where:

$I(q)$ — scattering intensity;

A — the surface scattering factor at low q value is proportional to the total surface area of the open hole;

B — a factor of pore scattering, proportional to the total surface area of the pore;

b — related to the diameter of the obturator, the mean obturator diameter $R = 2 \times b \times \sqrt{10}$;

C — background constant.

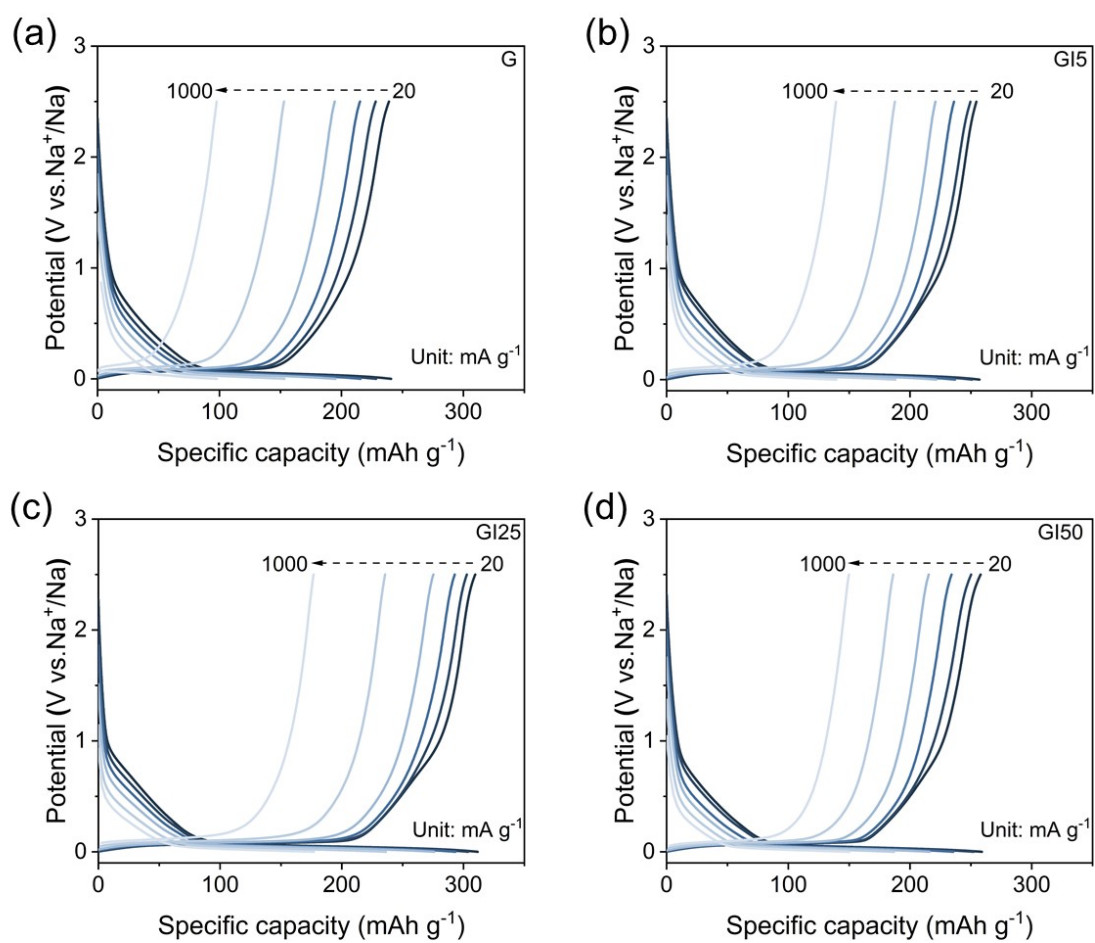


Figure S9. Discharge and charge curves at different current densities of (a) G, (b) GI5, (c) GI25 and (d) GI50).

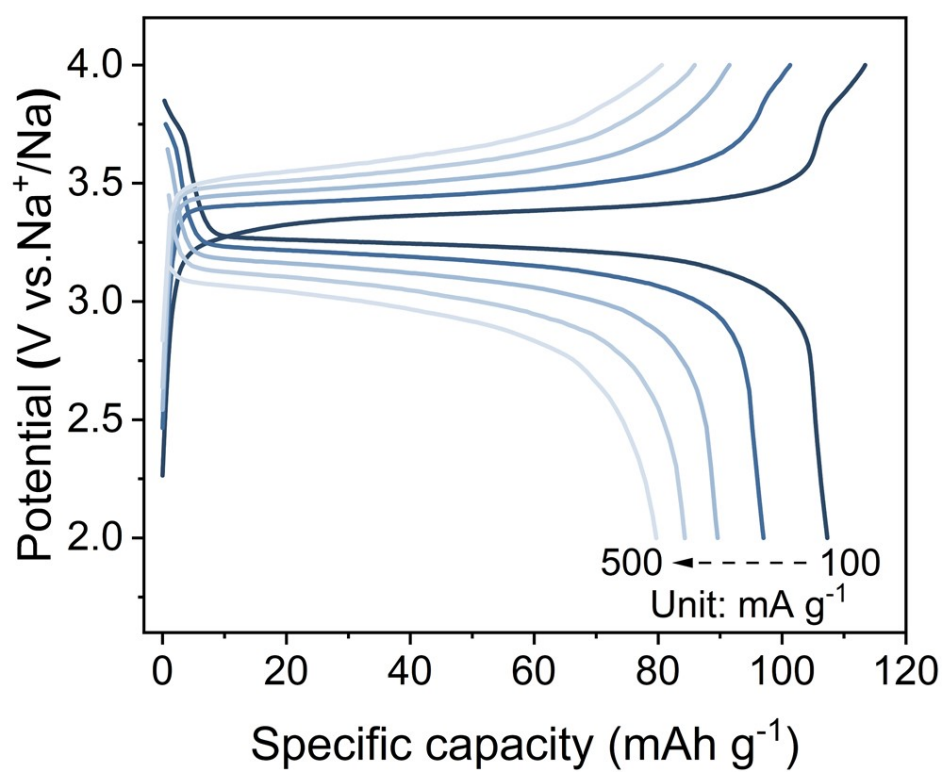


Figure S10. Discharge and charge curves at different current densities of NVP||GI25 full cell.

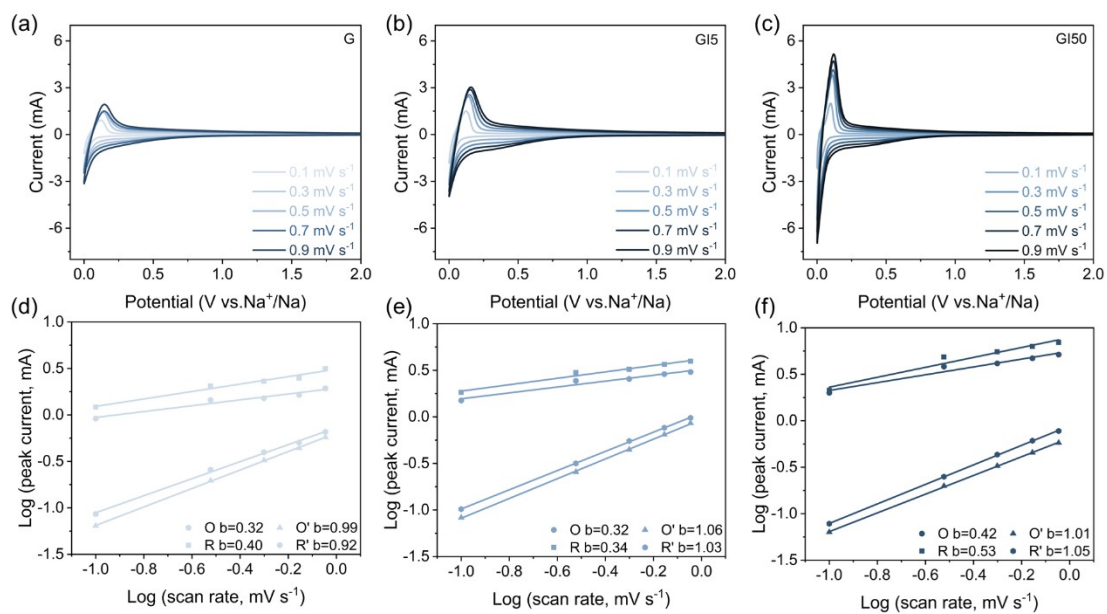


Figure S11. CV curves at different scan rates of (a) G, (b) GI5 and (c) GI50, linear relationship between scan rate and peak current of (a) G, (b) GI5 and (c) GI50.

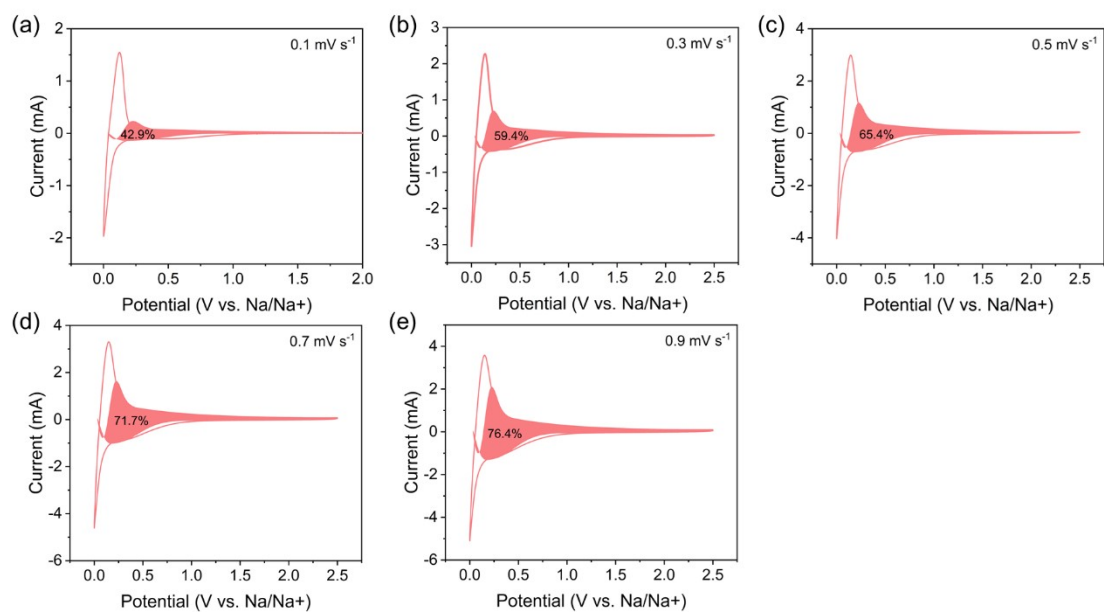


Figure S12. The contribution of capacitance and diffusion for CV curve of GI25 at (a) 0.1 mV s⁻¹, (b) 0.3 mV s⁻¹, (c) 0.5 mV s⁻¹, (d) 0.7 mV s⁻¹ and (f) 0.9 mV s⁻¹.

Table S1. Structure parameters of hard carbon materials.

Sample	d_{002} (nm)	L_a (nm)	Highly disordered (%)	Pseudo- graphitic (%)	Graphitic- like (%)	I_D/I_G	BET Surface Area ($\text{m}^2 \text{g}^{-1}$)
G	0.346	3.74	50	30	20	1.49	388.99
GI5	0.356	4.08	43	46	11	1.33	145.73
GI25	0.370	4.54	33	53	13	1.24	30.92
GI50	0.378	3.39	48	39	12	1.35	344.42

Table S2. The electrochemical properties of hard carbons.

Sample	Reversible capacity (mAh g ⁻¹)	ICE (%)
G	238.8	87.4
GI5	258.6	88.4
GI25	312.6	91.9
GI50	260.1	86.0

Table S3. Comparison of GI25 in this work with previously reported hard carbon electrodes for sodium storage.

	Reversible capacity (mAh g ⁻¹ @ A g ⁻¹)	ICE (%)	Rate performance (mAh g ⁻¹ @ A g ⁻¹)	Reference
This work	312.6 @ 0.02	91.9	293.9 @ 0.1	
CEM-G-8h	310 @ 0.02	89	263 @ 0.1	1
C-HC	310 @ 0.02	85	Not reported	2
PCS@V@C	216.7 @ 0.1	85.3	216.7 @ 0.1	3
CAC1300	308 @ 0.03	82.3	253.2 @ 0.09	4
HC	305 @ 0.02	90	Not reported	5
MoC/MCNs	289 @ 0.05	81	260 @ 0.1	6
N-CNS	304.7 @ 0.05	79.52	276.7 @ 0.1	7
PLHC1000	293 @ 0.03	75.5	241 @ 0.1	8

Table S4. Kinetic fitting parameters according to EIS test.

Sample	$R_e (\Omega)$	$R_{ct} (\Omega)$
G	2.3	564.5
GI5	2.7	223.7
GI25	3.3	166.5
GI50	6.8	274.1

References

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