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Supporting Information

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Reaction Mechanism and Performance of Innovative 2D Germanane-Silicane Alloys:
 $\text{Si}_x\text{Ge}_{1-x}\text{H}$ Electrodes in Lithium-Ion Batteries

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$\text{Si}_x\text{Ge}_{1-x}\text{H}$ Electrodes in Lithium-Ion Batteries

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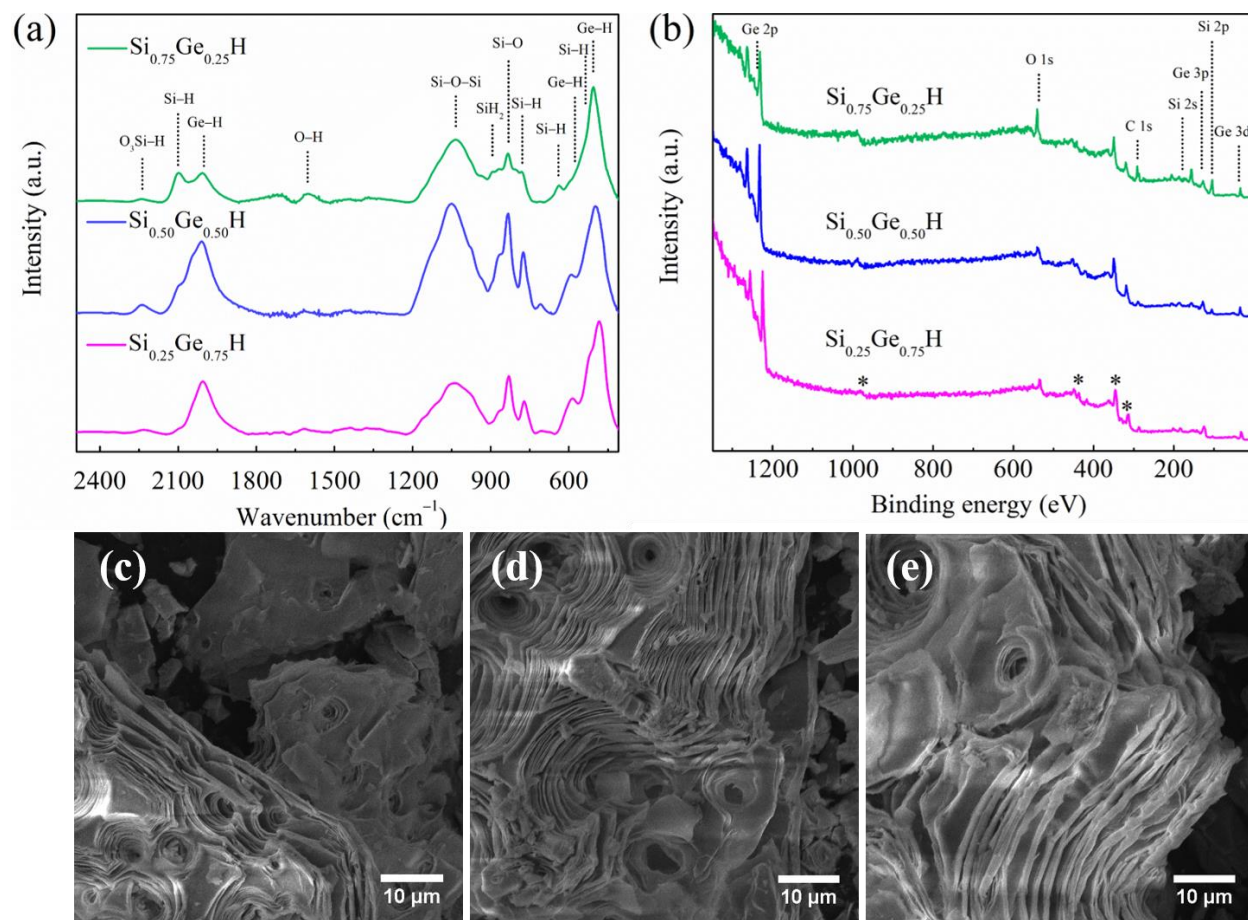


Fig. S1 FTIR spectra **a** and XPS survey spectra **b** of $\text{Si}_{0.25}\text{Ge}_{0.75}\text{H}$, $\text{Si}_{0.50}\text{Ge}_{0.50}\text{H}$ and $\text{Si}_{0.75}\text{Ge}_{0.25}\text{H}$; SEM images of $\text{Si}_{0.25}\text{Ge}_{0.75}\text{H}$ **c**, $\text{Si}_{0.50}\text{Ge}_{0.50}\text{H}$ **d** and $\text{Si}_{0.75}\text{Ge}_{0.25}\text{H}$ **e**.

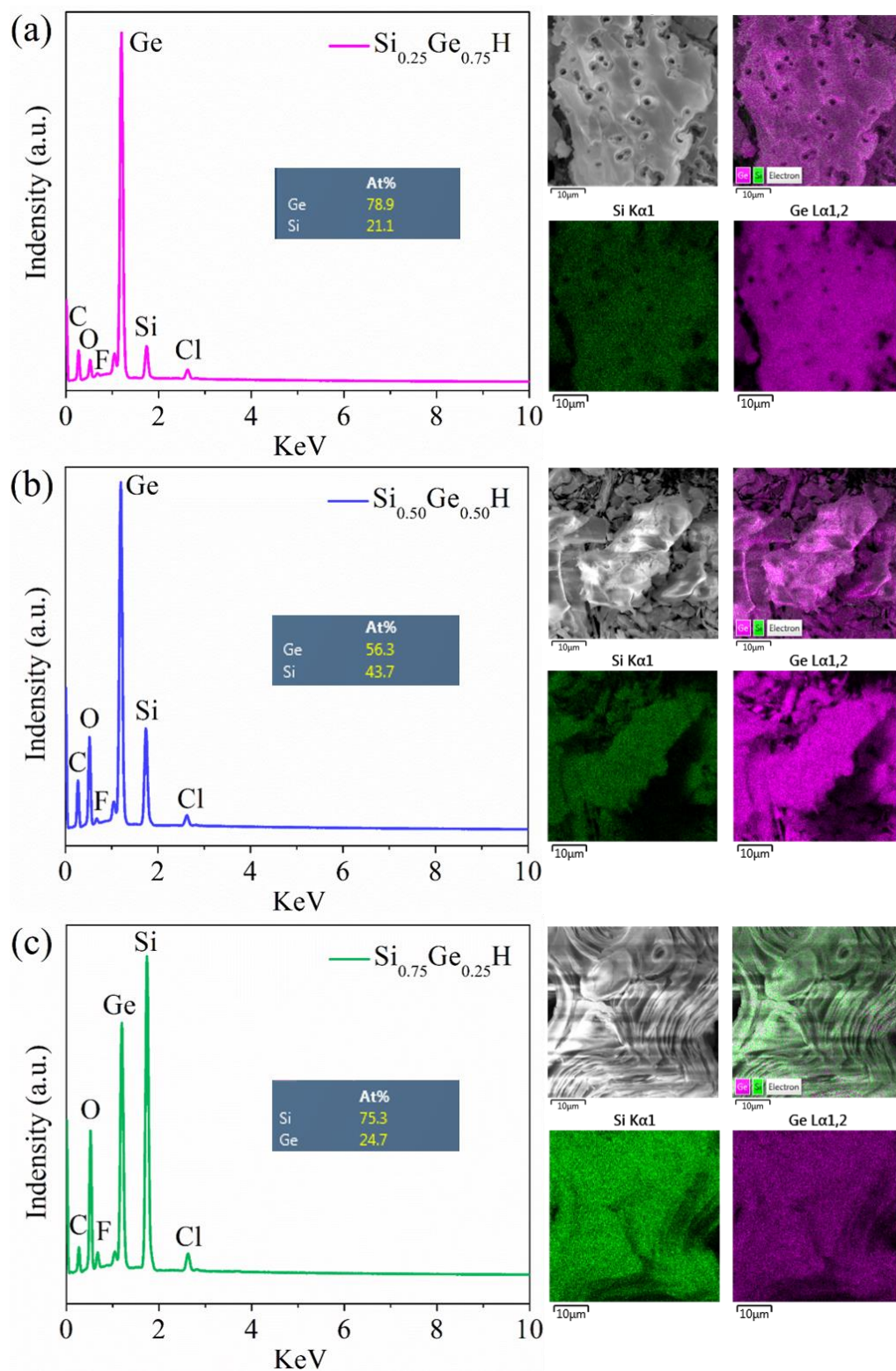


Fig. S2 Mapping of elements and respective EDX spectra of $\text{Si}_{0.25}\text{Ge}_{0.75}\text{H}$ **a**, $\text{Si}_{0.50}\text{Ge}_{0.50}\text{H}$ **b** and $\text{Si}_{0.75}\text{Ge}_{0.25}\text{H}$ **c**.

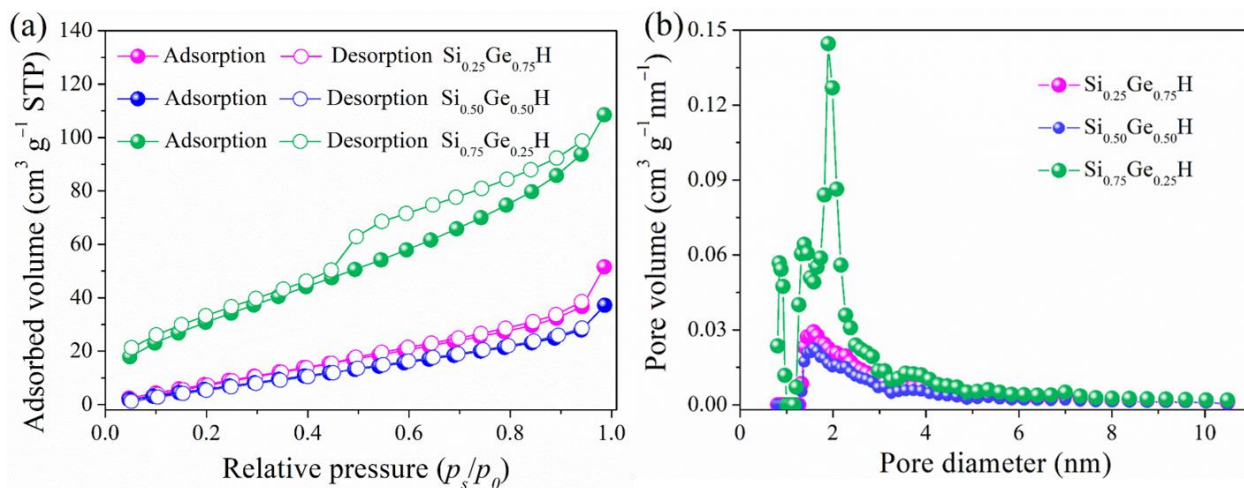


Fig. S3 Nitrogen adsorption–desorption isotherms **a** and pore diameter distributions calculated from N₂ desorption isotherms **b** for Si_{0.25}Ge_{0.75}H, Si_{0.50}Ge_{0.50}H and Si_{0.75}Ge_{0.25}H, respectively.

Table 1. Specific surface area and total pore volume of $\text{Si}_{0.25}\text{Ge}_{0.75}\text{H}$, $\text{Si}_{0.50}\text{Ge}_{0.50}\text{H}$ and $\text{Si}_{0.75}\text{Ge}_{0.25}\text{H}$.

Samples	BET surface area ($\text{m}^2 \text{g}^{-1}$)	Total pore volume ($\text{cm}^3 \text{g}^{-1}$)
$\text{Si}_{0.25}\text{Ge}_{0.75}\text{H}$	21.26	0.0562
$\text{Si}_{0.50}\text{Ge}_{0.50}\text{H}$	16.14	0.0418
$\text{Si}_{0.75}\text{Ge}_{0.25}\text{H}$	81.99	0.1434

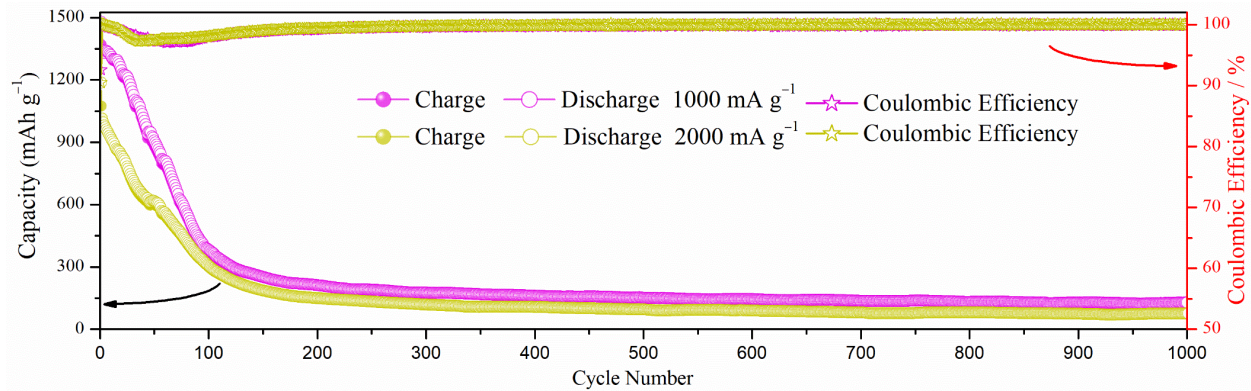


Fig. S4 Cycling stability of Si_{0.50}Ge_{0.50}H electrode at current densities of 1000 and 2000 mA g⁻¹ over 1000 cycles.

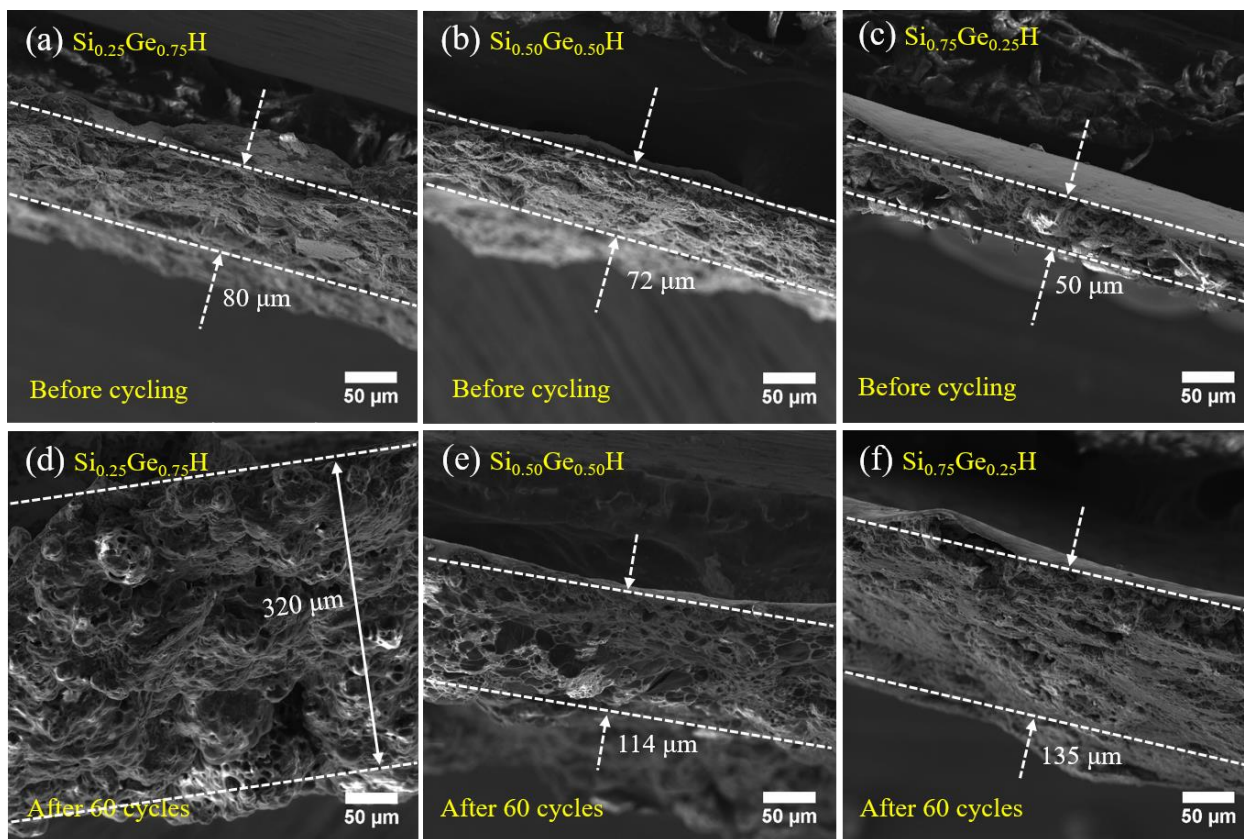


Fig. S5 Cross-section SEM images illustrating thickness deformation evolution in $\text{Si}_{0.25}\text{Ge}_{0.75}\text{H}$ (a, d), $\text{Si}_{0.50}\text{Ge}_{0.50}\text{H}$ (b, e) and $\text{Si}_{0.75}\text{Ge}_{0.25}\text{H}$ (c, f) electrodes before and after 60 cycles, respectively.

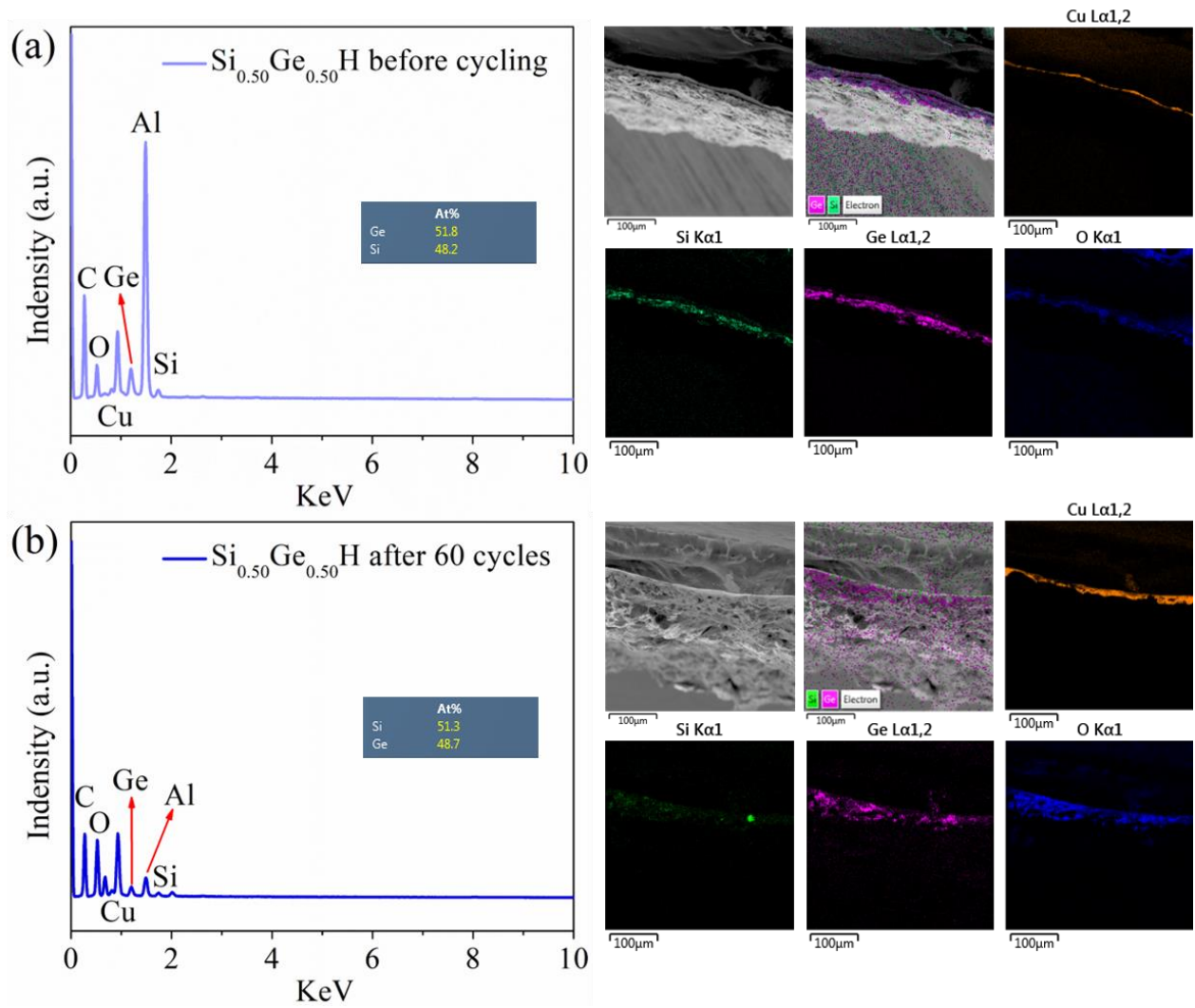


Fig. S6 Mapping of elements and corresponding EDX spectra of $\text{Si}_{0.50}\text{Ge}_{0.50}\text{H}$ electrode before and after 60 cycles (**a**, **b**), respectively.

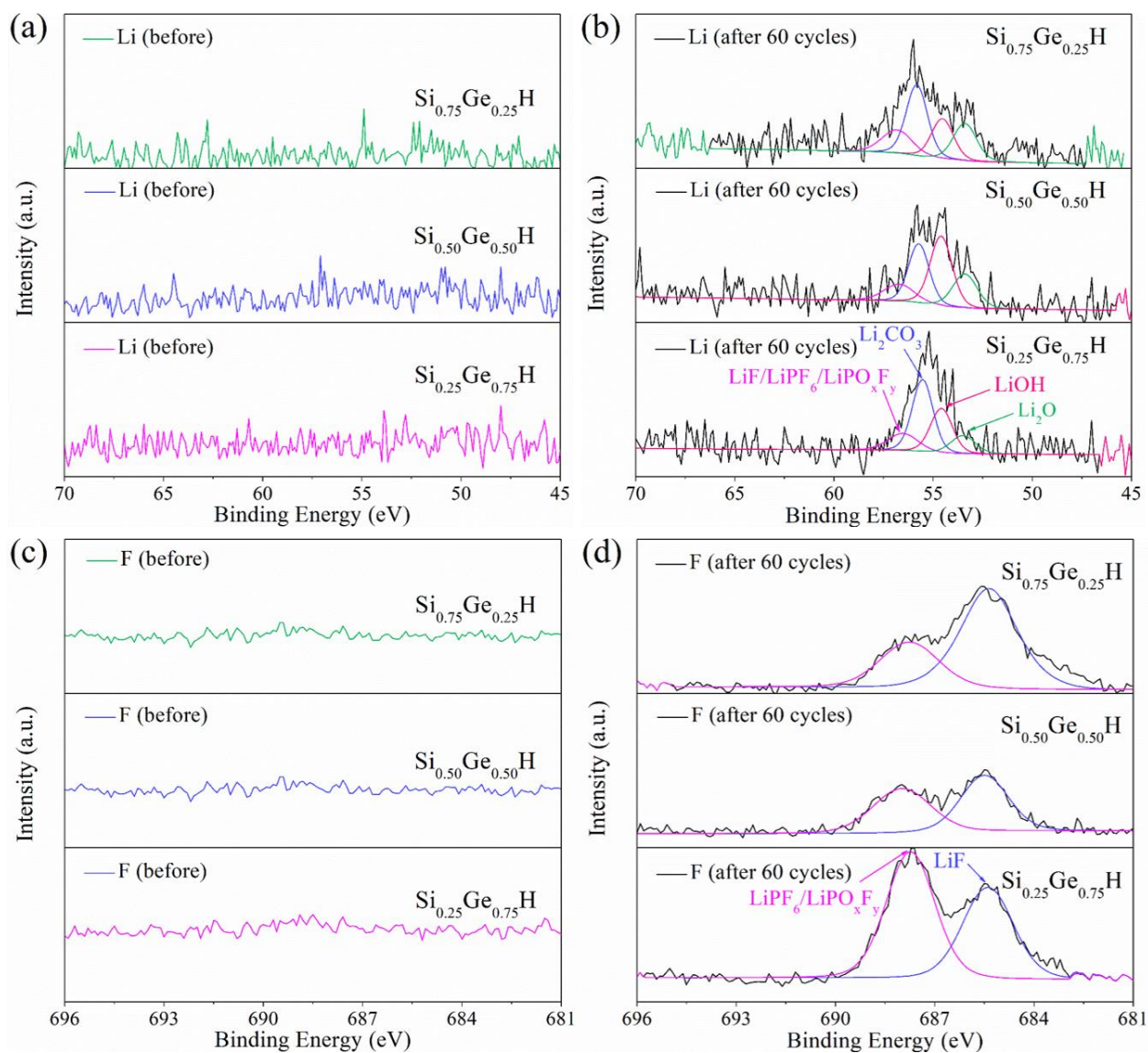


Fig. S7 XPS spectra of **a, b** Li 1s, and **c, d** F 1s core levels for $\text{Si}_{0.25}\text{Ge}_{0.75}\text{H}$, $\text{Si}_{0.50}\text{Ge}_{0.50}\text{H}$ and $\text{Si}_{0.75}\text{Ge}_{0.25}\text{H}$ before **a, c** and after 60 cycles **b, d**, respectively.

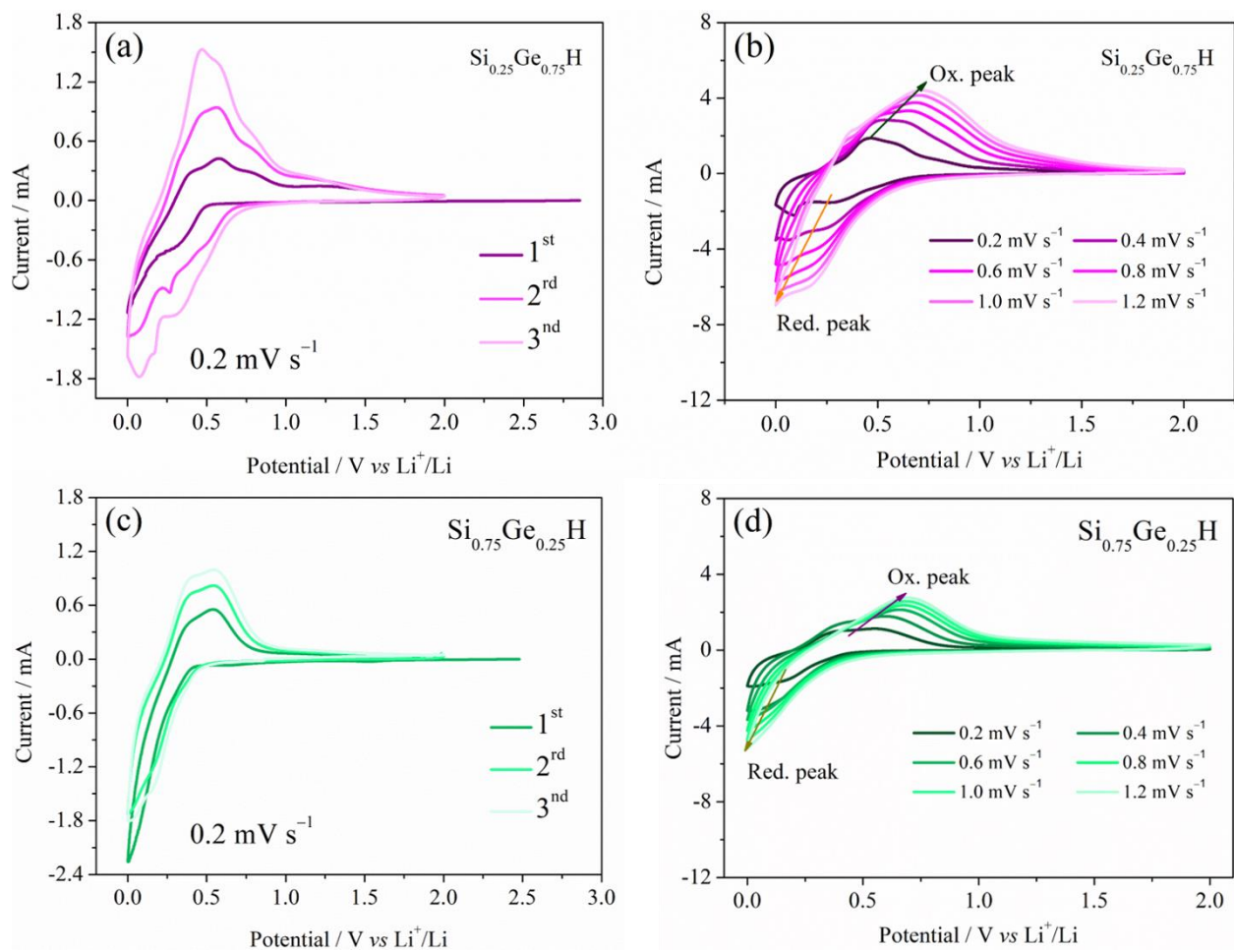


Fig. S8 **a** and **c** an initial 3-cycle CV curves of Si_{0.25}Ge_{0.75}H and Si_{0.75}Ge_{0.25}H electrodes at 0.2 mV s⁻¹; **b** and **d** CV of Si_{0.25}Ge_{0.75}H and Si_{0.75}Ge_{0.25}H electrodes at 0.2 – 1.2 mV s⁻¹.

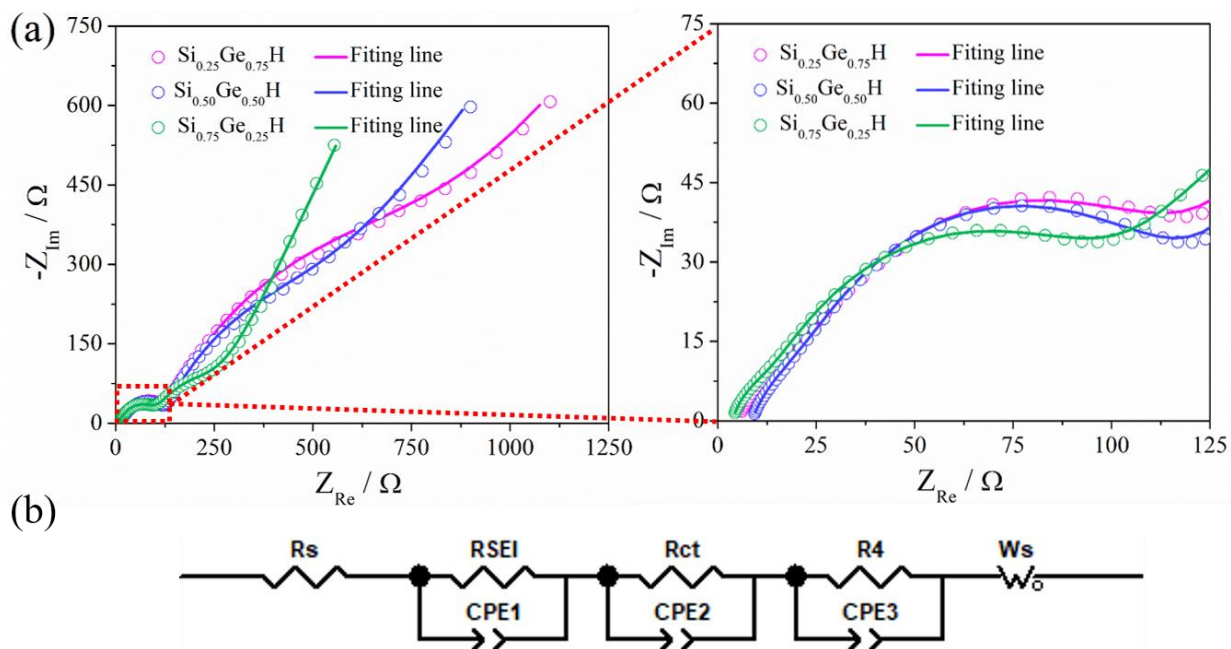


Fig. S9 Nyquist plots of $\text{Si}_{0.25}\text{Ge}_{0.75}\text{H}$, $\text{Si}_{0.50}\text{Ge}_{0.50}\text{H}$, and $\text{Si}_{0.75}\text{Ge}_{0.25}\text{H}$ electrodes after 60 cycles **a** and the corresponding equivalent circuit model **b**.

Table S2. Impedance parameters derived using equivalent circuit model (Figure S9b) for $\text{Si}_{0.25}\text{Ge}_{0.75}\text{H}$, $\text{Si}_{0.50}\text{Ge}_{0.50}\text{H}$, and $\text{Si}_{0.75}\text{Ge}_{0.25}\text{H}$ after 60 cycles under open circuit potential condition, In detail: equivalent circuit, electrode/electrolyte interface resistances (R_i , $i = s, \text{SEI}, \text{ct}, 4$) and χ^2 parameter.

Electrodes	Equivalent circuit	$R_s (\Omega)$	$R_{\text{SEI}} (\Omega)$	$R_{\text{ct}} (\Omega)$	$R_4 (\Omega)$	χ^2
$\text{Si}_{0.25}\text{Ge}_{0.75}\text{H}$	$R_s(R_{\text{SEI}}\text{CPE}_1)(R_{\text{ct}}\text{CPE}_2)$ $(R_4\text{CPE}_3)W_s$	5.190	95.07	15.07	585.5	2.0×10^{-4}
$\text{Si}_{0.50}\text{Ge}_{0.50}\text{H}$	$R_s(R_{\text{SEI}}\text{CPE}_1)(R_{\text{ct}}\text{CPE}_2)$ $(R_4\text{CPE}_3)W_s$	8.691	93.08	12.05	295.9	1.5×10^{-4}
$\text{Si}_{0.75}\text{Ge}_{0.25}\text{H}$	$R_s(R_{\text{SEI}}\text{CPE}_1)(R_{\text{ct}}\text{CPE}_2)$ $(R_4\text{CPE}_3)W_s$	3.726	90.31	7.891	135.3	1.1×10^{-4}

Table S3 Recently reported electrochemical performance of SiGe-based anode materials for LIBs.

Material structure	Specific capacity (mAh g ⁻¹)	Current density (mA g ⁻¹)	Cycling number	Battery type
Si _{0.5} Ge _{0.5}	1142	50	1	LIBs ^[1]
Ge _{0.1} Si _{0.9}	1020	C/2	100	LIBs ^[2]
Si _{0.67} Ge _{0.33}	1360	C/5	250	LIBs ^[3]
Si–Ge heterostructure nanowires	1180	C/5	400	LIBs ^[4]
This work (Si _{0.50} Ge _{0.50} H)	1059	75	60	LIBs

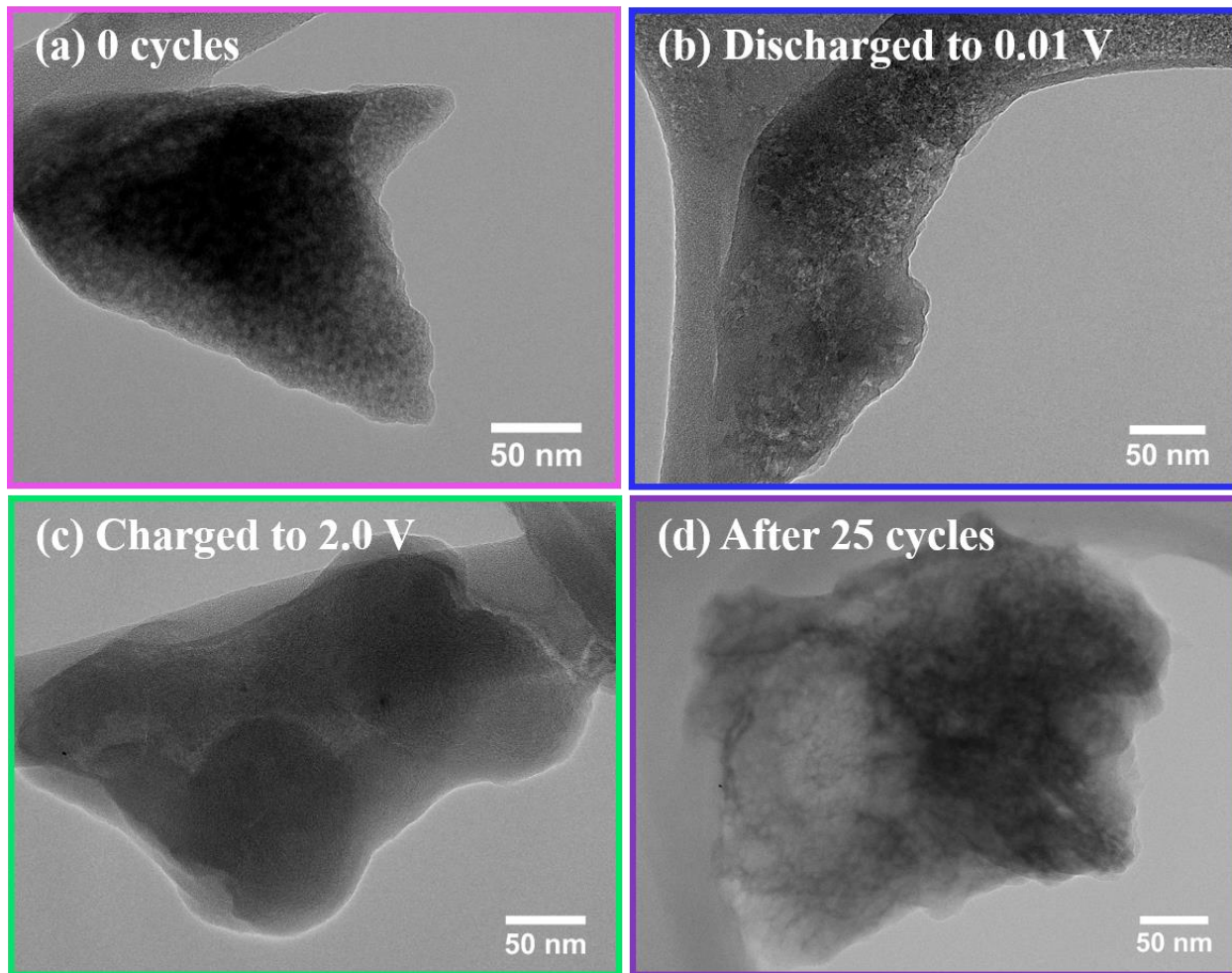


Fig. S10 TEM images depicting the evolution of morphological deformation in the $\text{Si}_{0.5}\text{Ge}_{0.5}\text{H}$ electrode during lithiation and delithiation: 0 cycles **a**, discharged to 0.01 V **b**, charged to 2.0 V **c** and after 25 cycles **d**.

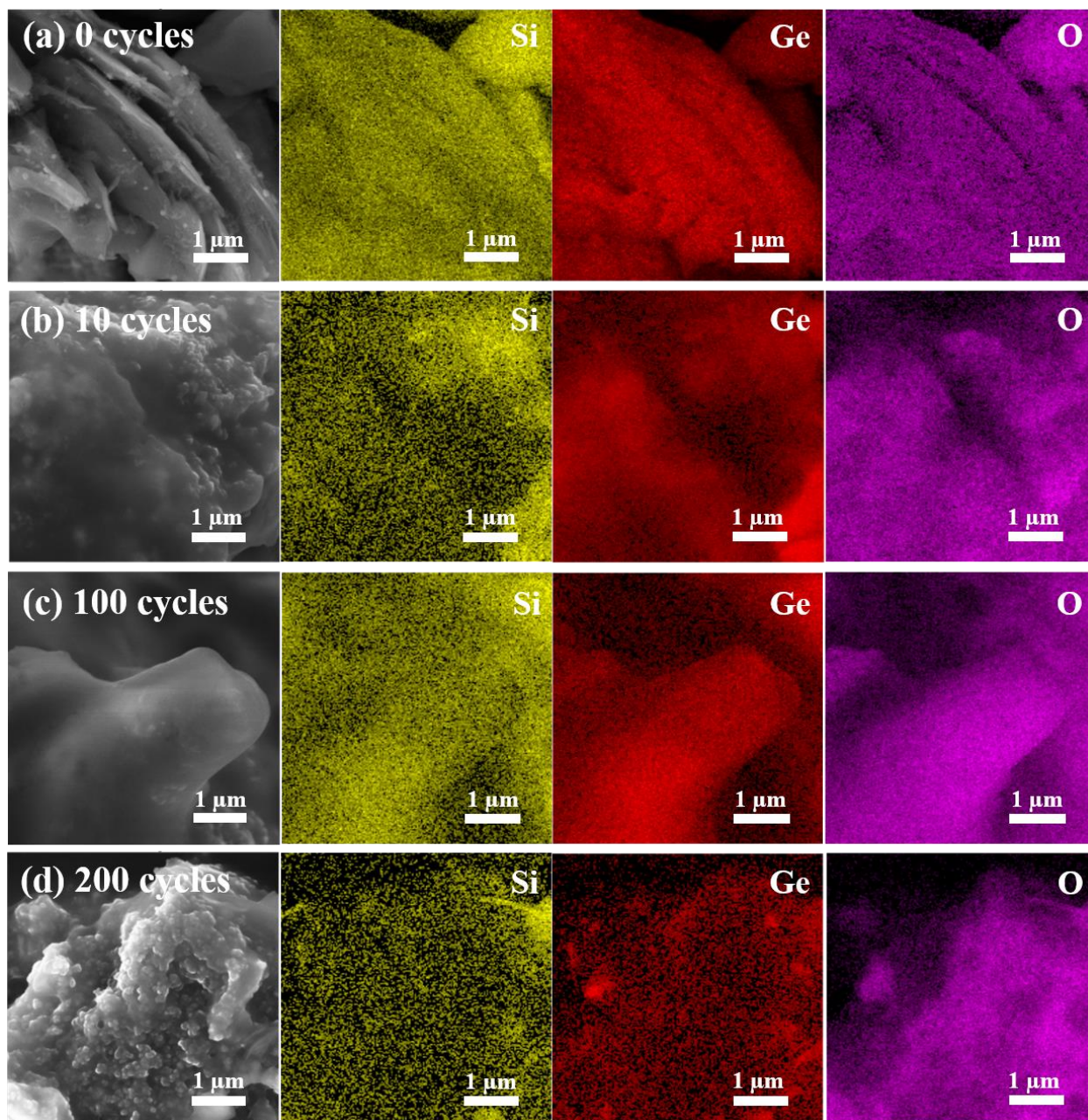


Fig. S11 SEM-EDX images illustrating morphological changes in the $\text{Si}_{0.50}\text{Ge}_{0.50}\text{H}$ electrode during lithiation and delithiation: 0 cycles **a**, after 10 cycles **b**, 100 cycles **c** and 200 cycles **d**.

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