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Ternary $AlGe_xP$ alloy compounds for high capacity and rate capability of lithium ion battery anodes

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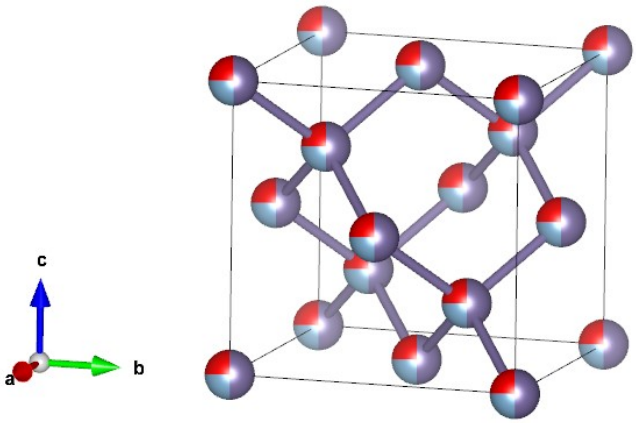

Fig. S1 Crystal structure of the as-synthesized $AlGe_2P$ compound.

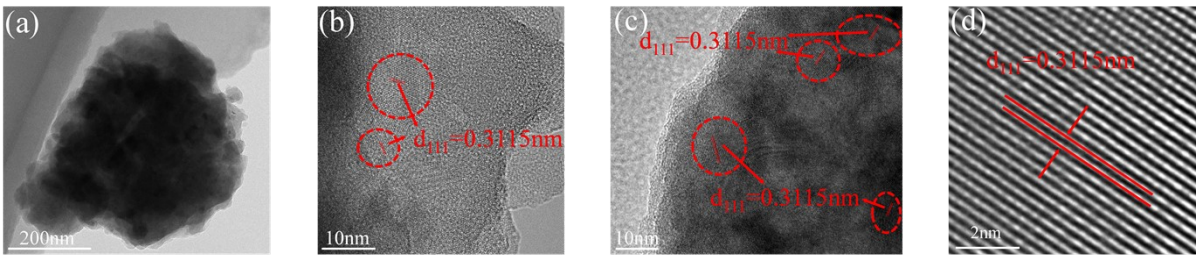

Fig. S2 (a) Low-magnitude TEM image; (b-d) HRTEM images of the as-synthesized $AlGe_2P$ compound.

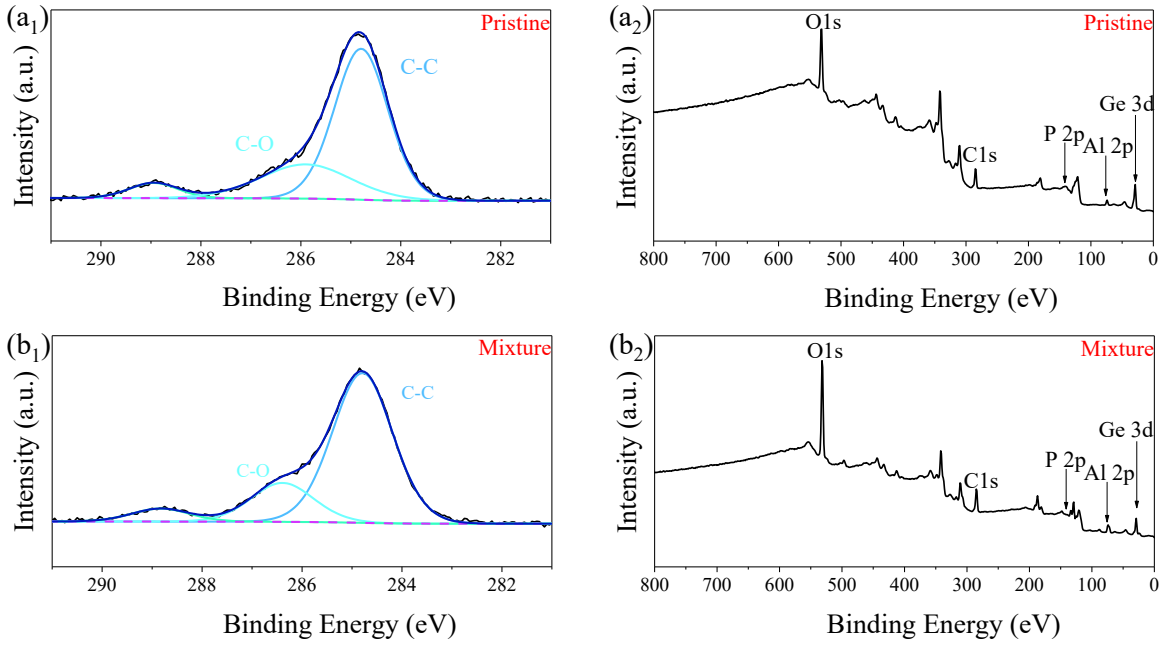

Fig. S3 High-resolution XPS spectra of C1s and full spectrum: (a) As-synthesized $AlGe_2P$ powder; (b) The Al+2Ge+P mixture.

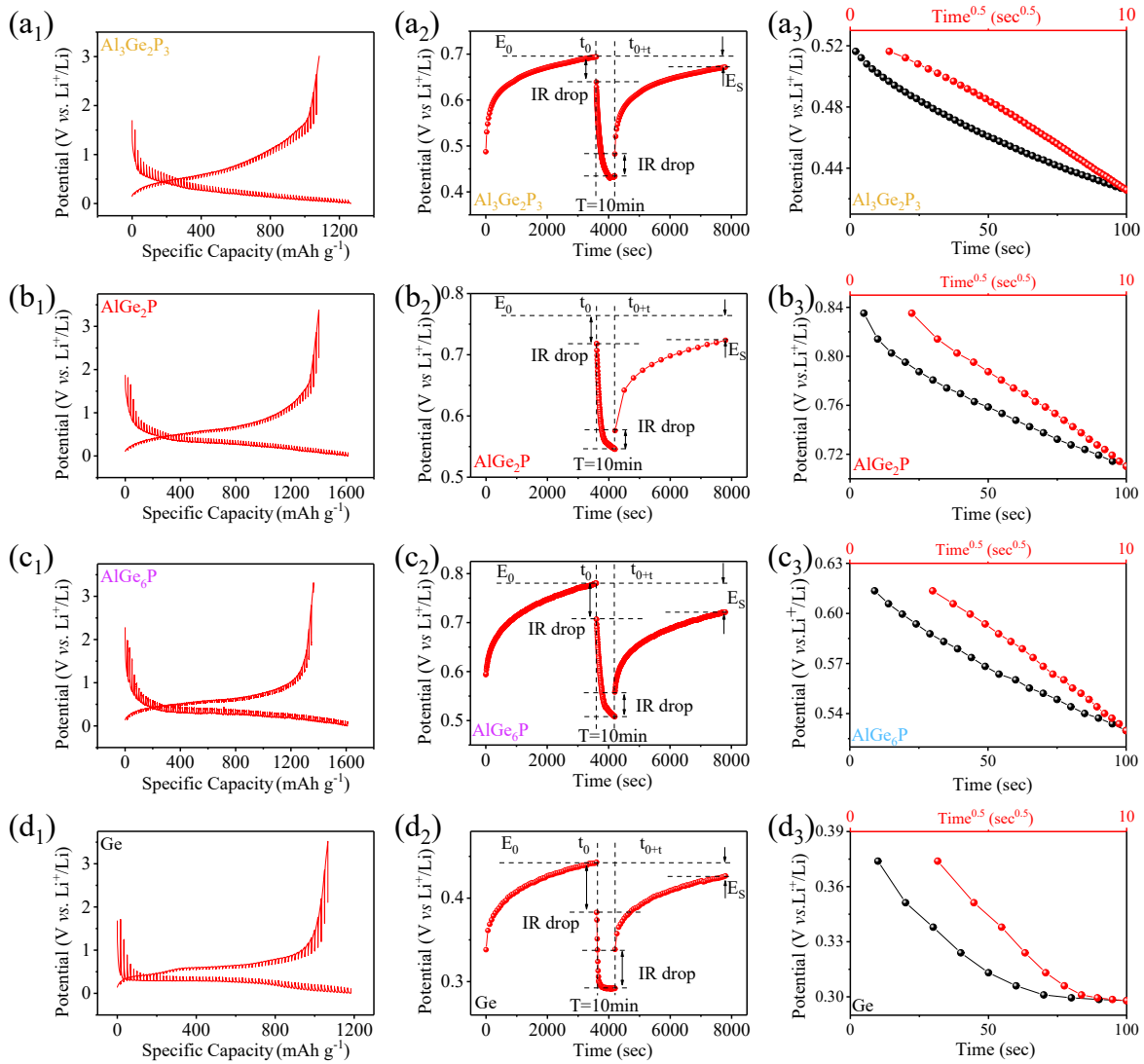

Fig. S4 GITT characterizations of the as-synthesized $Al_3Ge_2P_3$, $AlGe_2P$, $AlGe_6P$, and Ge samples: (a_1-d_1) First-cycle discharge and charge profiles; (a_2-d_2) Typical schemes of single-step GITT experiments; (a_3-d_3) $dE/dt^{(1/2)}$ curves. GITT measurement was carried out by imposing a 10 min pulse current rate at 0.1 A g^{-1}, and followed by 60 min relaxation interval for each pulse.

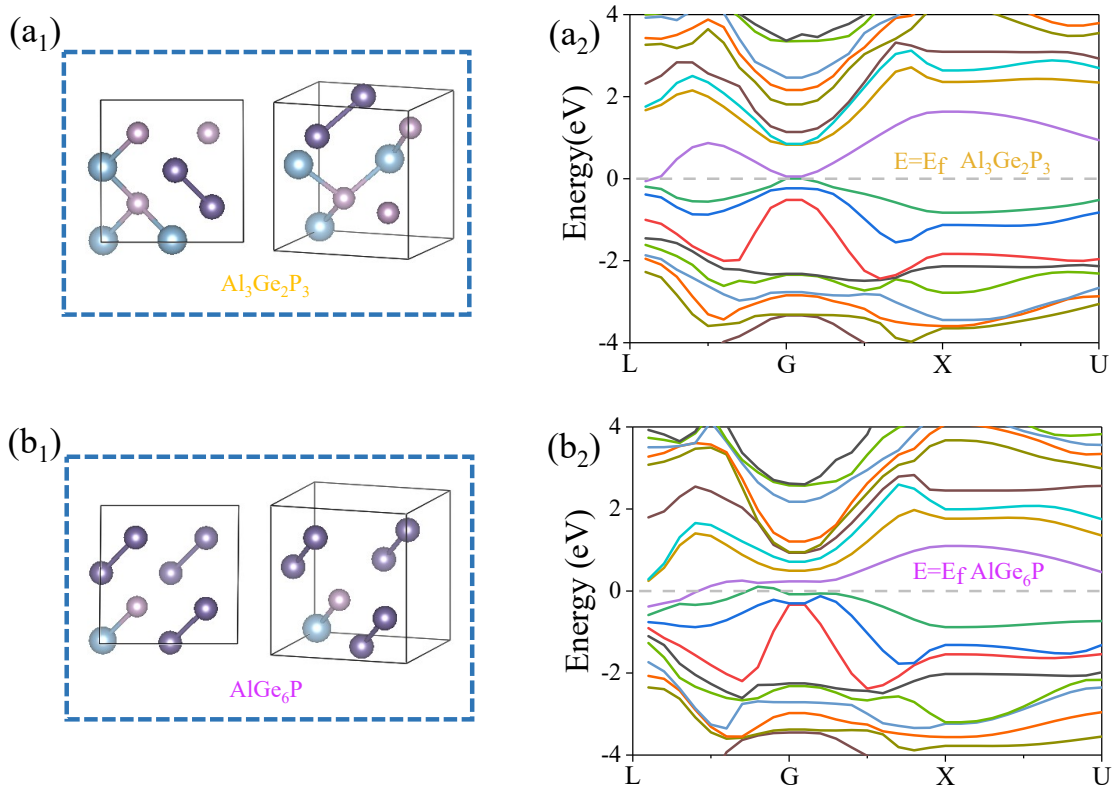

Fig. S5 (a_1-a_2): the structural model and electronic structure of the as-prepared $Al_3Ge_2P_3$ sample; (b_1-b_2) the structural model and electronic structure of the as-prepared $AlGe_6P$ sample.

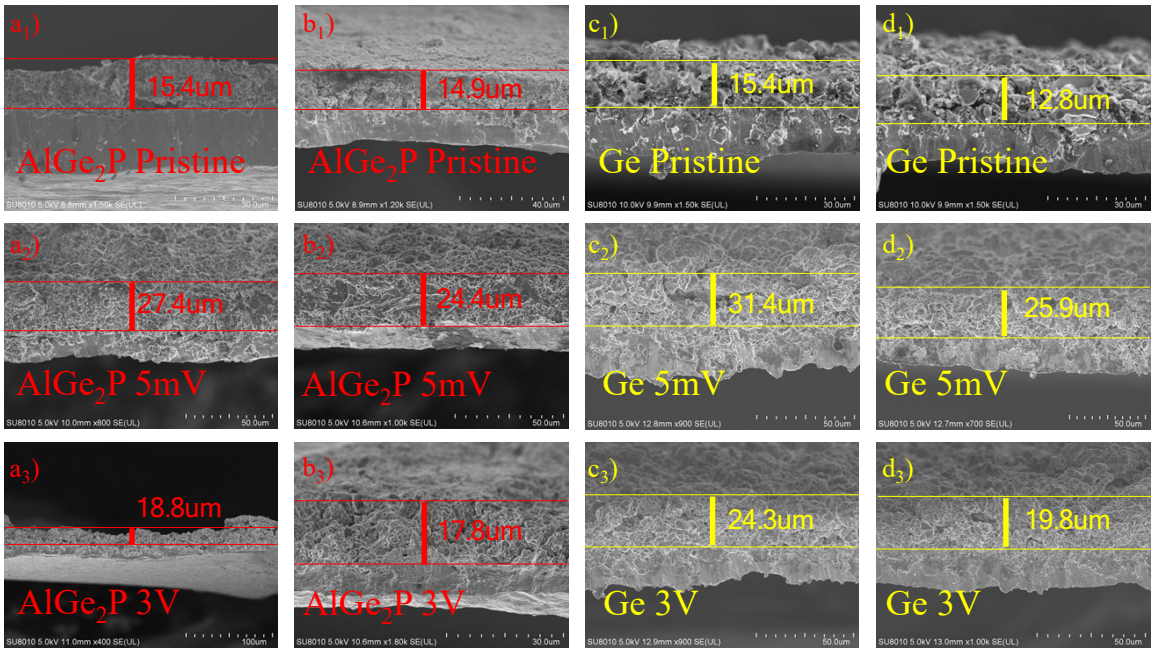

Fig. S6 Cross section images of $AlGe_2P$ with Ge electrodes at the pristine stae, discharging state of 0.005 V and charging state of 3.0 V. a, b) $AlGe_2P$ electrodes; c, d) Ge electrodes.

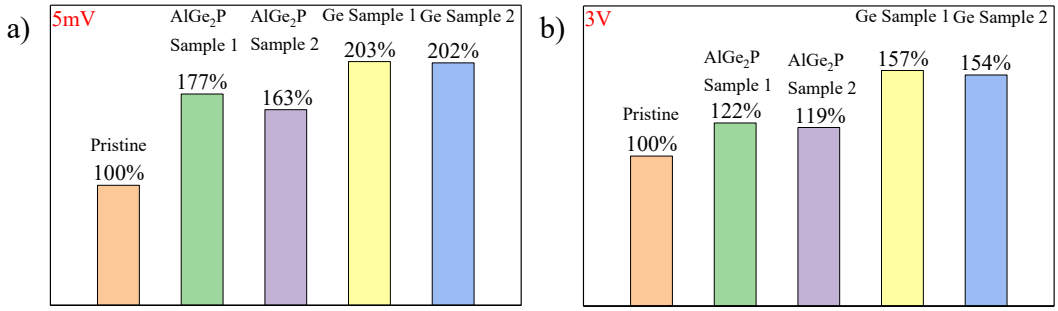

Fig. S7 Volume expansion rates of the $AlGe_2P$ and Ge electrodes calculated based on Figure S6.

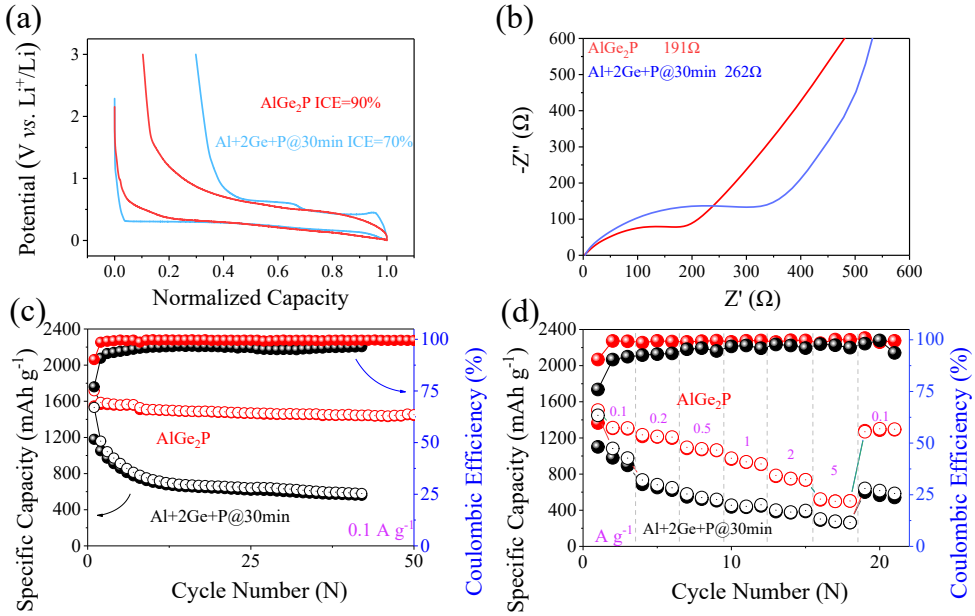

Fig. S8 Electrochemical characterizations of the $AlGe_2P$ compound and the mixture of Al+2Ge+P: (a) First-cycle discharge and charge profiles; (b) Electrochemical impedance spectra; (c) Cycling stability; (d) Rate performance.

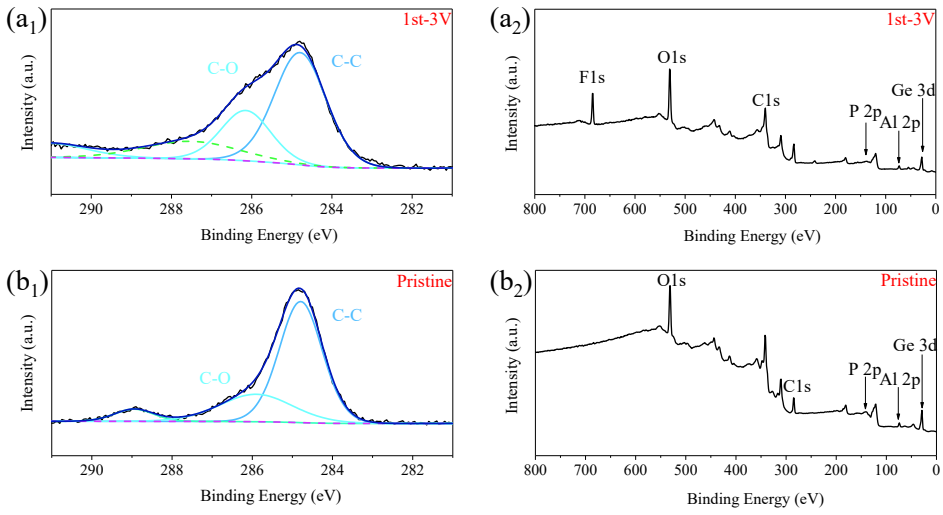

Fig. S9 XPS spectra of high-resolution C1s and full spectrum: (a) The as-prepared $AlGe_2P$ compound; (b) The as-prepared $AlGe_2P$ compound after cycling.

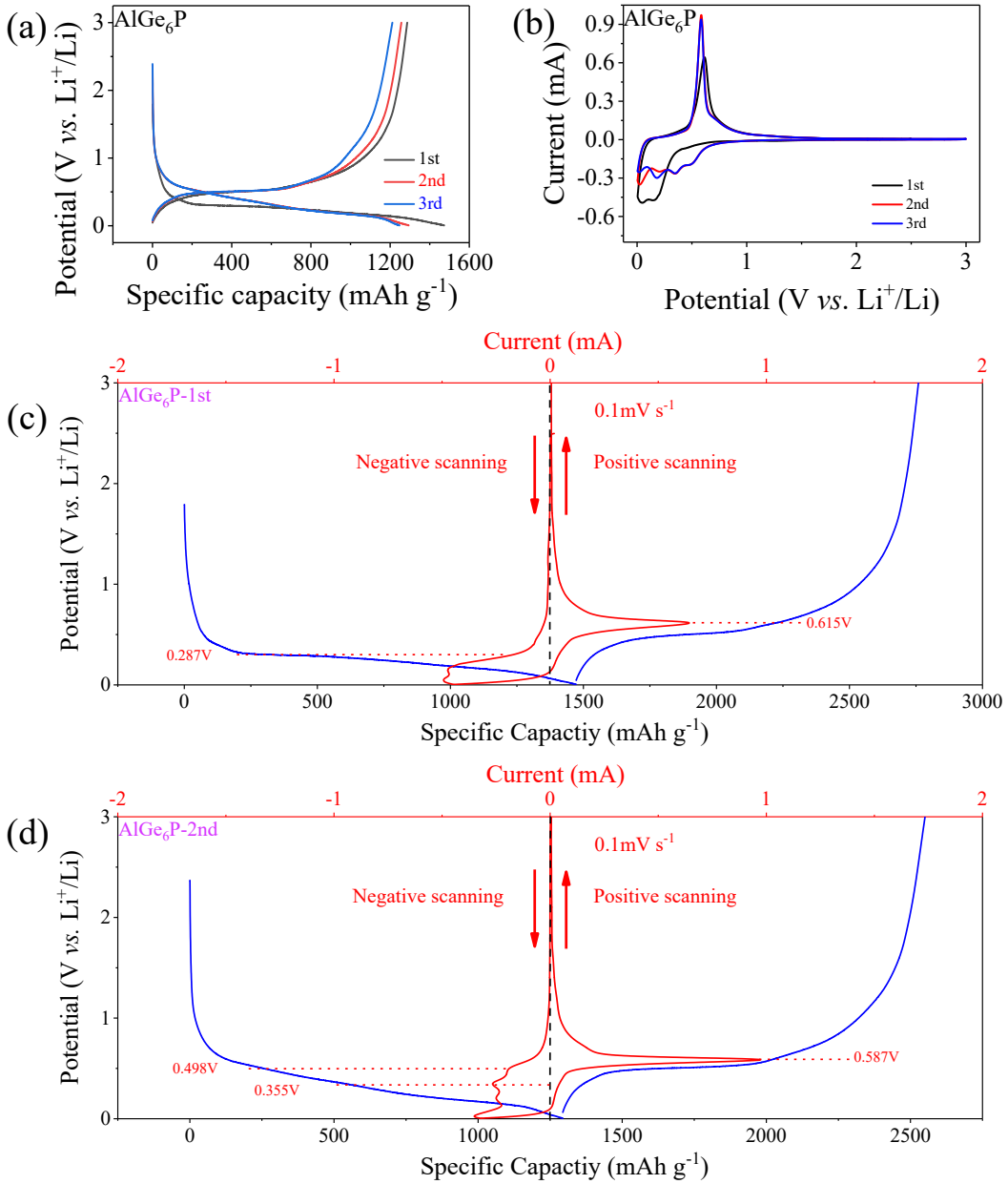

Fig. S10 Electrochemical characterizations of the as-synthesized $AlGe_6P$ sample: (a) Initial three discharge and charge profiles at 100 mA g^{-1}; (b) Cyclic voltammetry (CV) curves at 0.1 mV s^{-1}; (c) First CV curves along with the first discharge and charge profiles; (d) Second CV curves along with the second discharge and charge profiles.

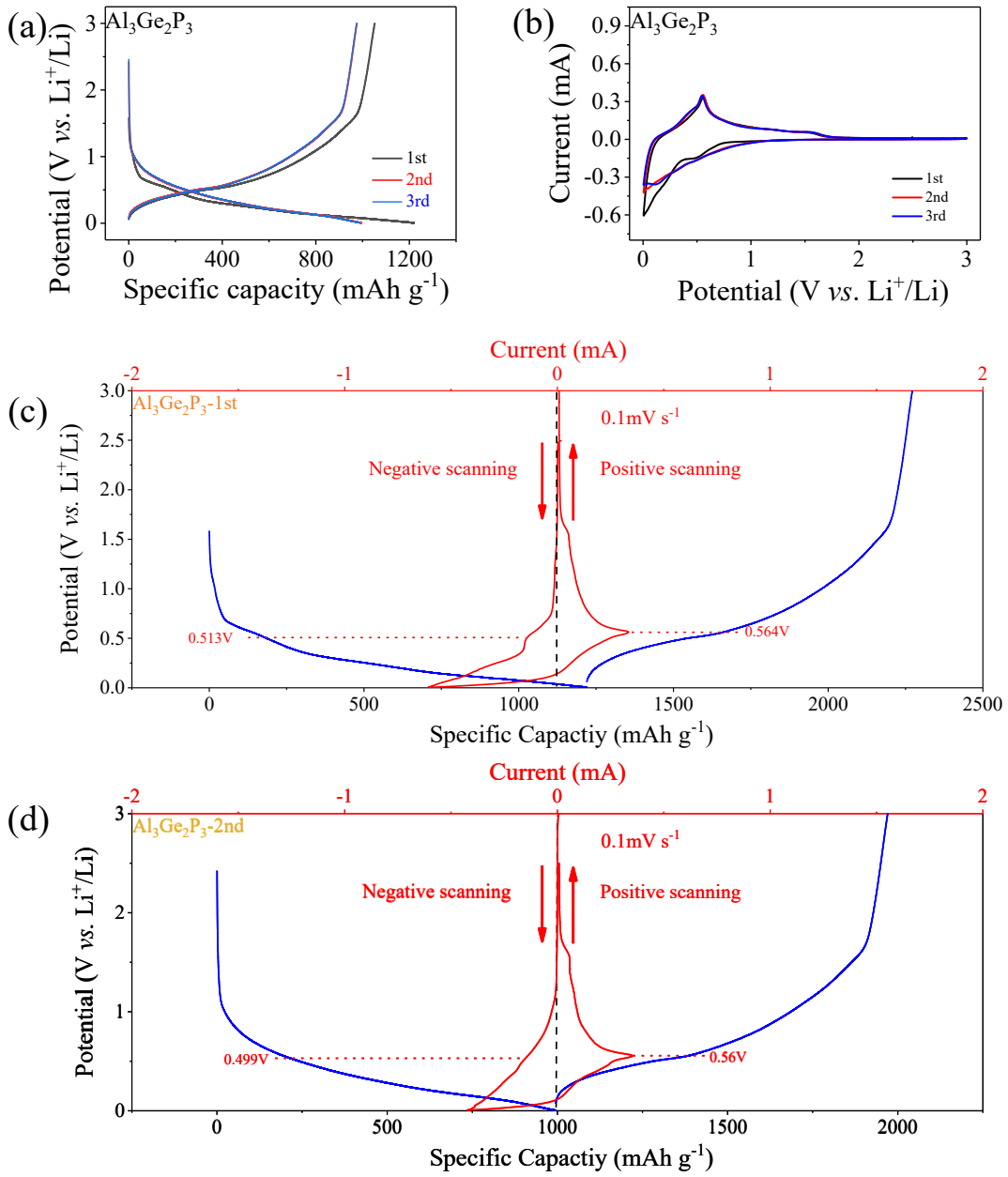

Fig. S11 Electrochemical characterizations of the as-synthesized $Al_3Ge_2P_3$ sample: (a) Initial three discharge and charge profiles at 100 mA g^{-1}; (b) Cyclic voltammetry (CV) curves at 0.1 mV s^{-1}; (c) First CV curves along with the first discharge and charge profiles; (d) Second CV curves along with the second discharge and charge profiles.

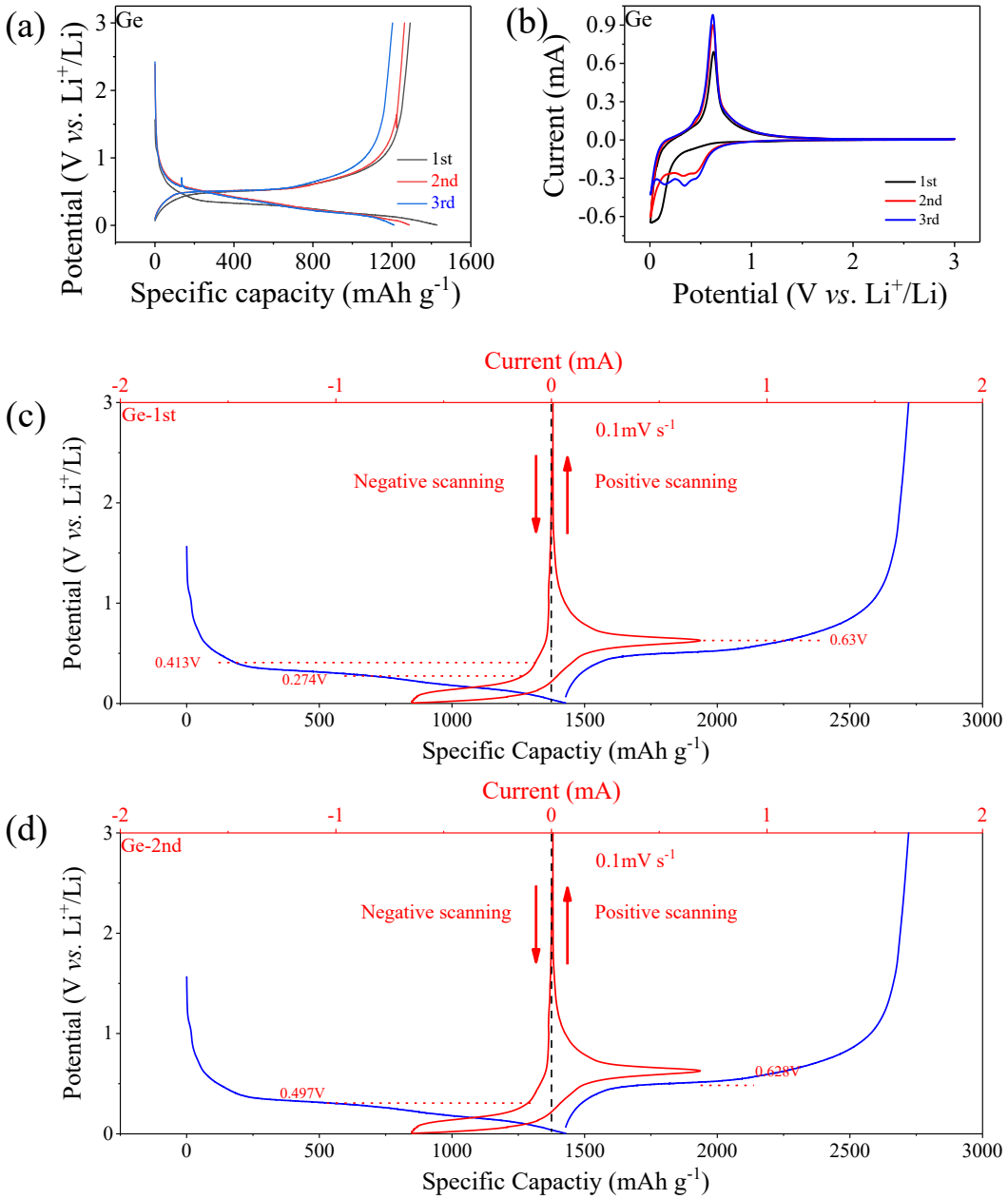

Fig. S12 Electrochemical characterizations of the single-component phase of Ge sample: (a) Initial three discharge and charge profiles at 100 mA g^{-1}; (b) Initial three cyclic voltammetry (CV) curves at 0.1 mV s^{-1}; (c) First CV curves along with the first discharge and charge profiles; (d) Second CV curves along with the second discharge and charge profiles.

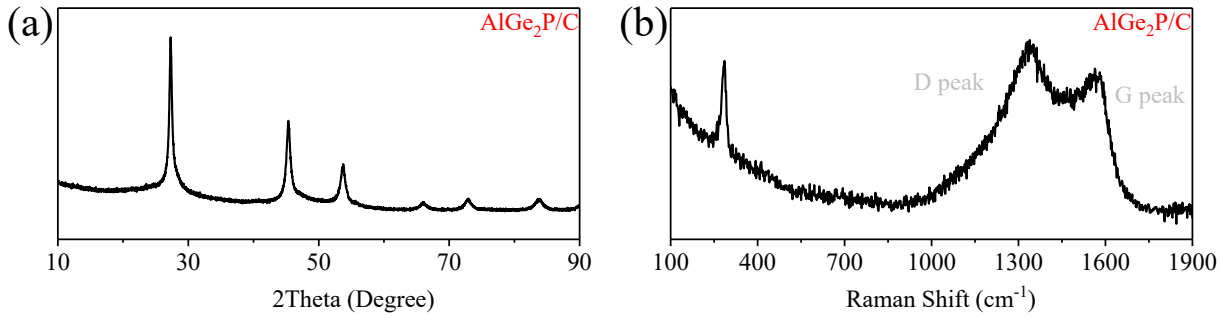

Fig. S13 (a) XRD pattern; (b) Raman spectrum of the as-synthesized $AlGe_2P/C$.

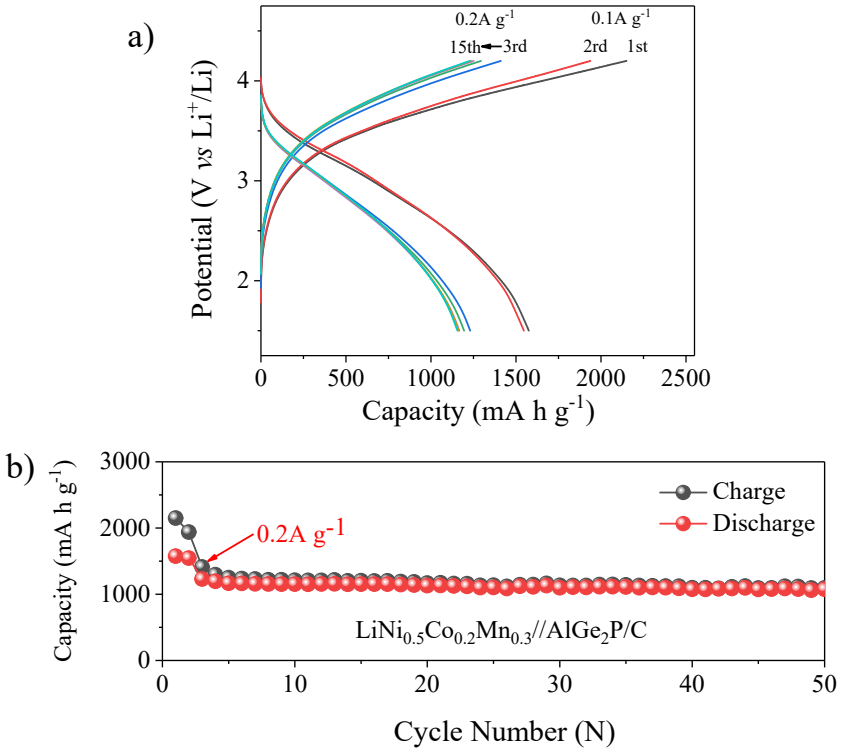

Fig. S14 a) Discharge and charge profiles, and b) Cycling stability of the $LiNi_{0.5}Co_{0.2}Mn_{0.3}O_2//AlGe_2P/C$ full cell.

Table S1. Main parameters of processing and refinement of the as-prepared $AlGe_2P$ compound.

Compound	$AlGe_2P$
Crystal System	Cubic
Space Group	Fd-3m
A, Å	5.767342
V, $Å^3$	191.1
2θ-interval, °	10–90
Z	1

Table S2. Fractional atomic coordinates and isotropic displacement parameters of the as-synthesized $AlGe_2P$ compound.

	x	Y	z	Occ
Al	0	0	0	1/4
Ge	0	0	0	1/2
P	0	0	0	1/4

Table S3. Comparison of cyclic and rate performances.

Materials	Cycle performance	Rate performance	Reference
$AlGe_2P$	2A g^{-1}, 800cycles, 867 mA h g^{-1}	20A g^{-1}, 454 mA h g^{-1}	This work
GeO_2/Ge	1A g^{-1}, 40cycles, 520.2 mA h g^{-1}	5A g^{-1}, 124.6 mA h g^{-1}	[39]
Ge/3DPG-2	0.5C, 250cycles, 931 mA h g^{-1}	5C, 494mA h g^{-1}	[40]
np-$GeSn_5$	0.2A g^{-1}, 500cycles, 520.2 mA h g^{-1}	1.5A g^{-1}, 778 mA h g^{-1}	[41]
$GeCH_3$/rGO-2	1A g^{-1}, 500cycles, 288 mA h g^{-1}	5A g^{-1}, 227 mA h g^{-1}	[42]
mGe-500	0.5C, 100cycles, 785 mA h g^{-1}	1C, 655mA h g^{-1}	[43]
Ge/3DOM-Ni	0.2C, 100cycles, 610 mA h g^{-1}	10C, 270mA h g^{-1}	[44]
GeH	1C, 100cycles, 341 mA h g^{-1}	2C, 265mA h g^{-1}	[45]
Ge/C	0.1C, 50cycles, 1095 mA h g^{-1}	2C, 972mA h g^{-1}	[46]
$CuGeO_3$@RGO	2A g^{-1}, 300cycles, 550 mA h g^{-1}	1A g^{-1}, 879 mA h g^{-1}	[47]
PC-Ge NW	0.16A g^{-1}, 50cycles, 789 mA h g^{-1}	1.6A g^{-1}, 540 mA h g^{-1}	[48]