ARTICLE

Supporting Information

Reactive Boride as Multifunctional Interface Stabilizer for Garnet-Type Solid Electrolyte in All-Solid-State Lithium Batteries

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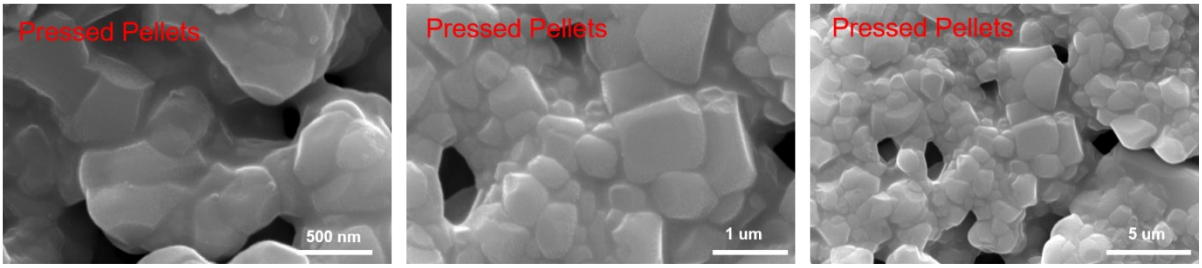

Fig.S1 SEM images of the surface of as-prepared LLZTO pellets.

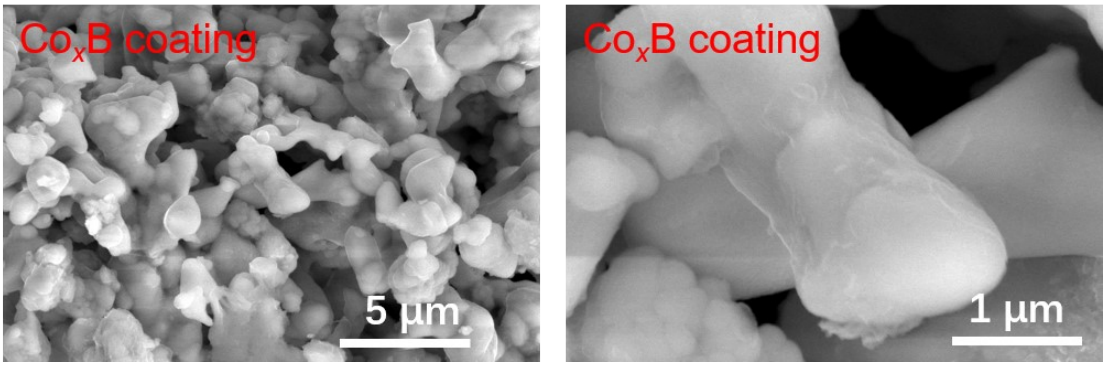

Fig.S2 SEM images of the surface of the Co_xB coated LLZTO particles with enlarged magnifications.

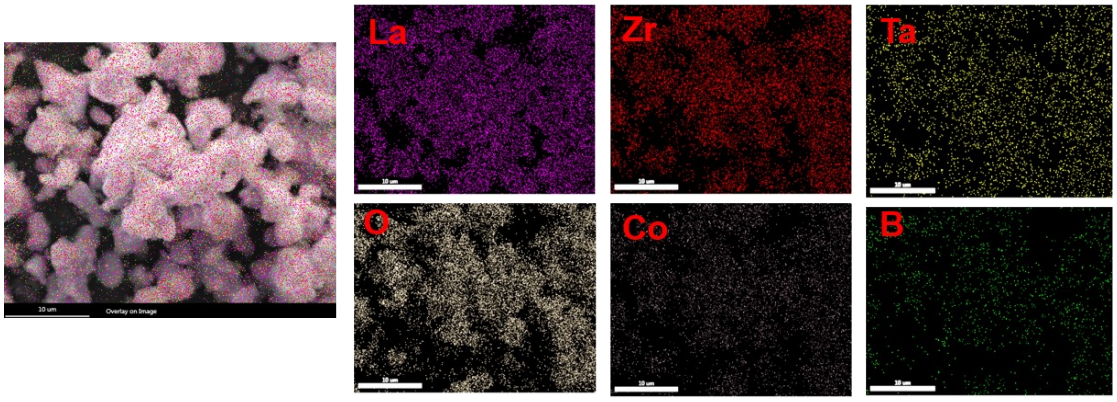

Fig. S3 SEM-EDS mapping results of Co_xB coated LLZTO particle.

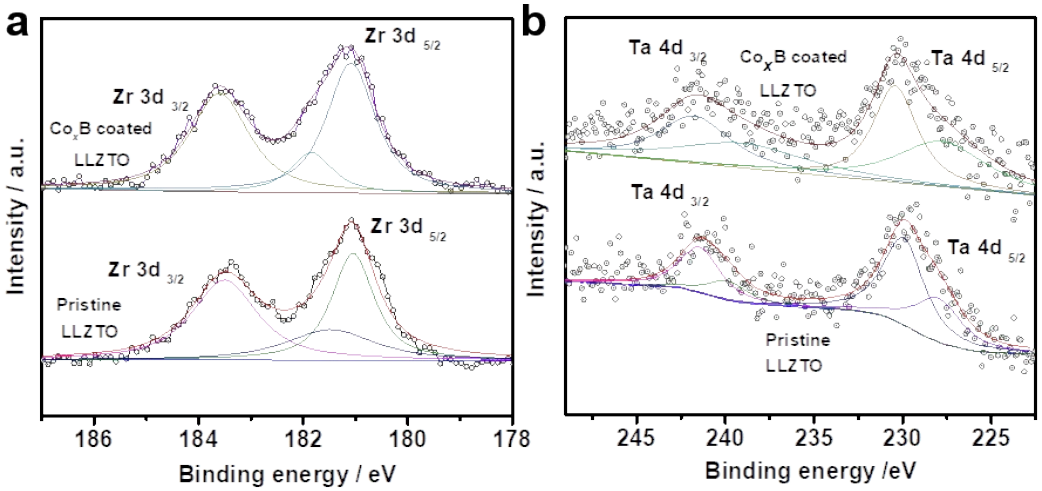

Fig. S4 The XPS spectra of (a) Zr 3*d* and (b) Ta 4*d* of both pristine LLZTO and Co_xB coated LLZTO.

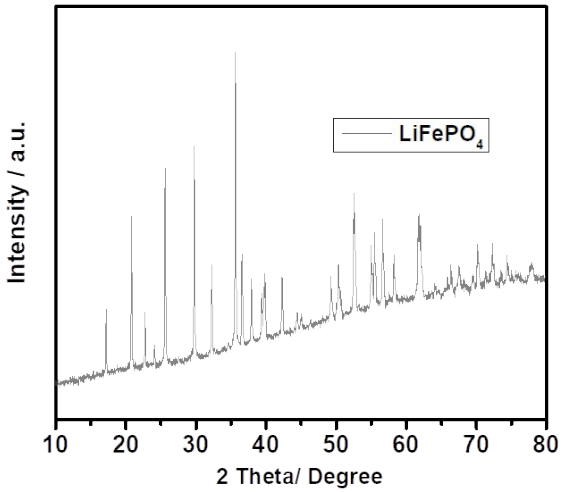

Fig. S5 The XRD patterns of the purchased carbon-coated $LiFePO_4$ cathode material.

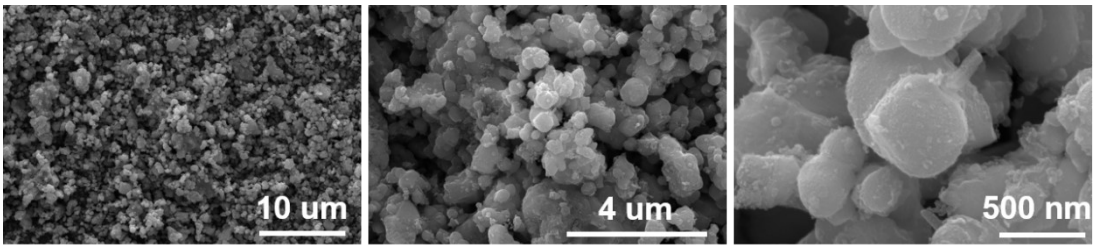

Fig. S6 The SEM images of purchased $LiFePO_4$.

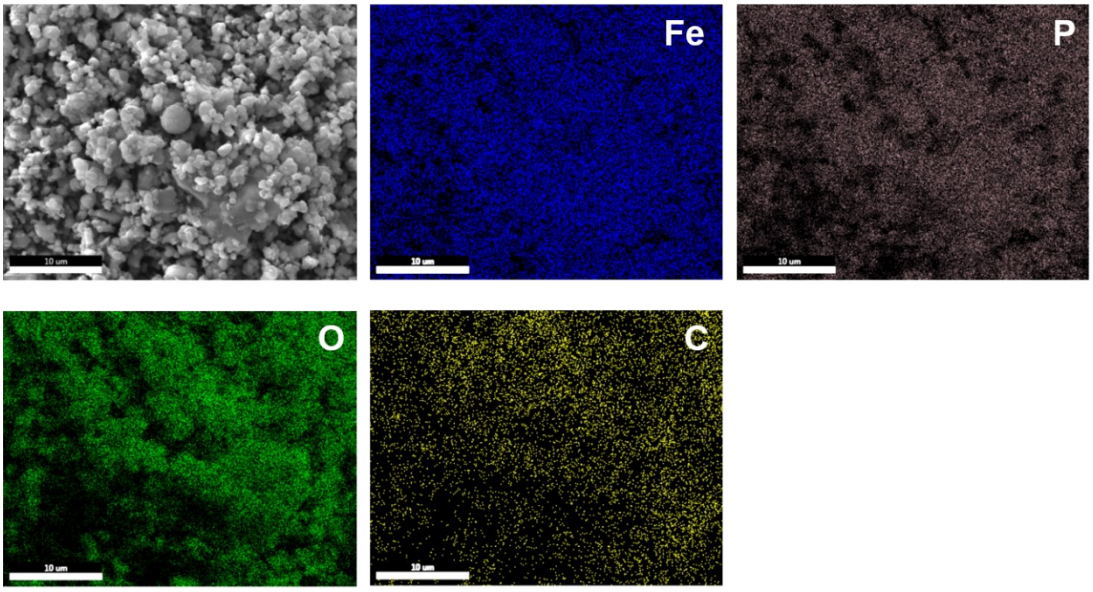

Fig. S7 The SEM-EDS mapping results of Fe, P, O and C in the purchased $LiFePO_4$ cathode material.

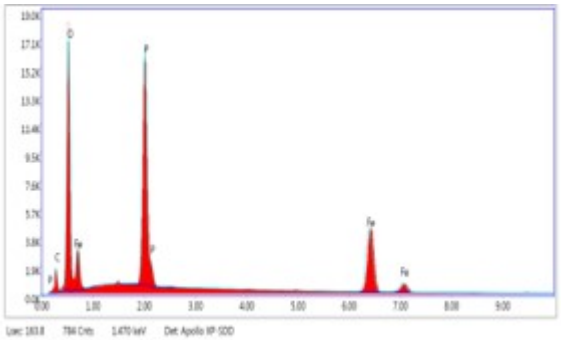

Fig. S8 The point EDS result of the purchased $LiFePO_4$ cathode material.

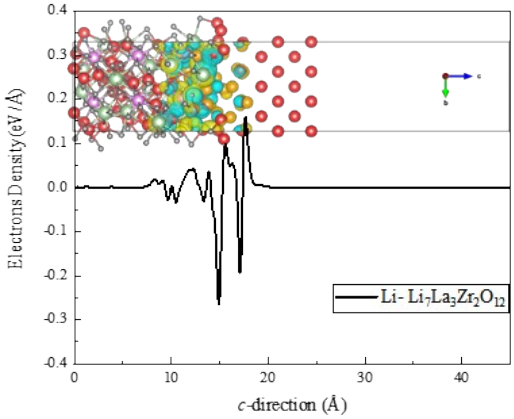

Fig. S9 The charge density difference plot of isosurface of Li|LLZTO interface.

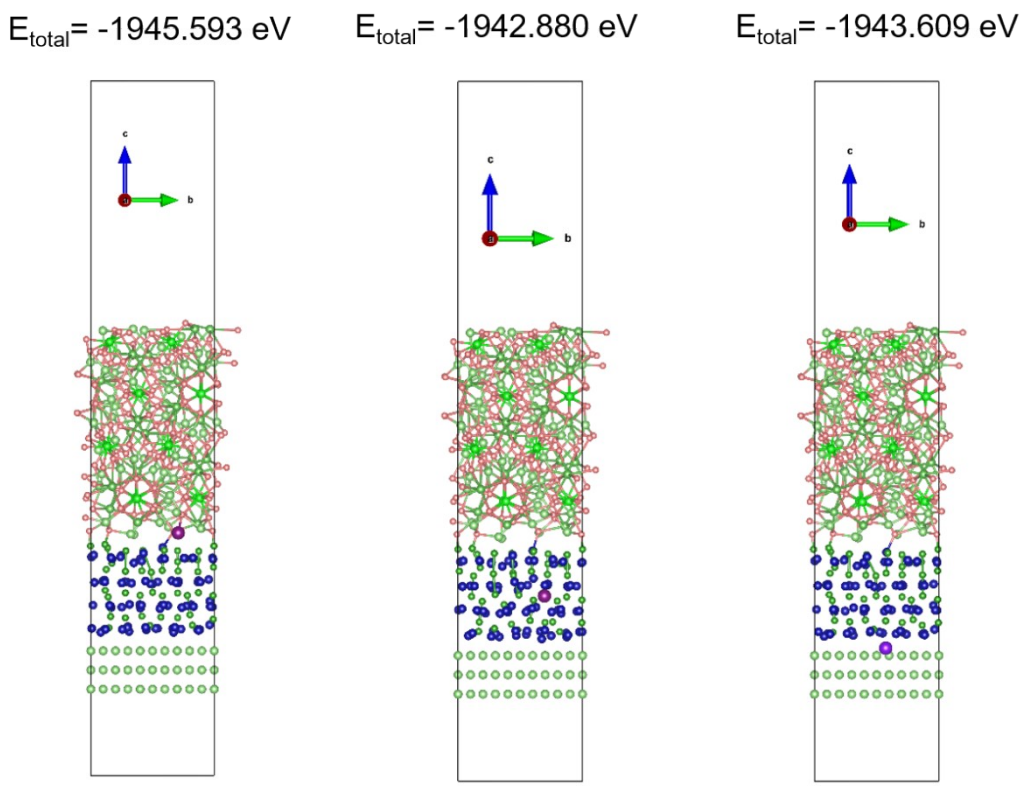

Fig. S10 The total energies of different status of Li ion in the Li|Co_2B|LLZTO interfaces.

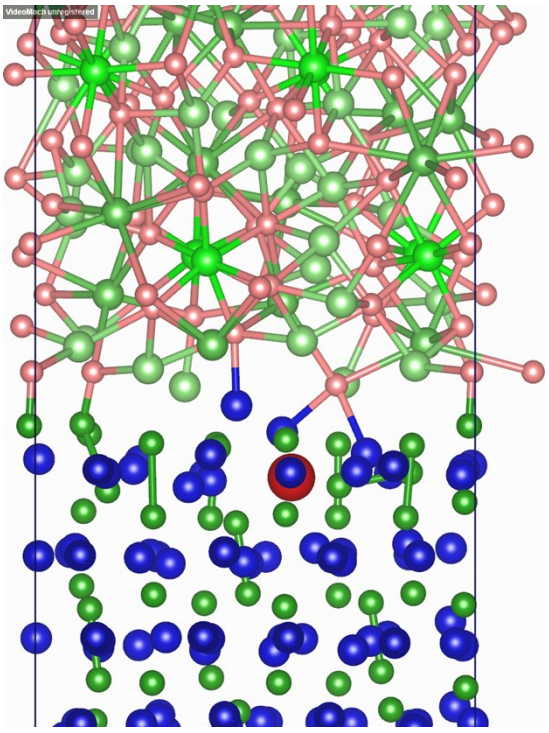

Fig. S11 The animation of the overall Li ion transportation through the Li|Co_xB|LLZTO interfaces.

Table S1 The detailed refined results of $Li_{6.4}La_3Zr_{1.4}Ta_{0.6}O_{12}$ powder sample using GSAS-II software.

	x	y	z	fraction	multi	Uiso
Li1	0.6500(0)	0.1790(0)	0.3773(9)	0.2930	96	0.02459
Li2	0.2500(0)	0.3750(0)	0.0000(0)	0.9600	24	0.01562
La	0.2500(0)	0.1250(0)	0.0000(0)	1.0000	24	0.02835
Zr	0.0000(0)	0.0000(0)	0.0000(0)	0.7000	16	0.02478
Ta	0.0000(0)	0.0000(0)	0.0000(0)	0.3000	16	0.03074
O	0.0538(0)	0.1483(0)	-0.0048(4)	1.0000	96	0.07340

Table S2 The pellet density and chemical composition of pristine LLZTO and Co_xB coated LLZTO by ICP-OES.

	Relative density	ICP-OES results			
		Li	La	Zr	Ta
Pristine LLZTO	92.44 %	6.36	3.01	1.39	0.59
Co_xB-coated LLZTO	93.15 %	6.35	3.02	1.39	0.59

Table S3 The heterogenous junction energy of each component in Co_2B/LLZTO, Li/Co_2B and Li/LLZTO.

Co_2B/LLZTO-B	Co_2B	LLZTO	Formation (eV)	Area (Å^2)	Specific Formation energy (eV Å^{-2})
-1872.766 eV	-552.227 eV	-1309.896 eV	-10.64332	119.076	-0.08938
Co_2B/LLZTO-Co	Co_2B	LLZTO	Formation (eV)	Area (Å^2)	Specific Formation energy (eV Å^{-2})
-1865.461 eV	-546.888 eV	-1309.896 eV	-8.67724	119.076	-0.07287
Li-Co_2B-B	Co_2B	Li	Formation (eV)	Area (Å^2)	Specific Formation energy (eV Å^{-2})
-135.862 eV	-112.475 eV	-21.620 eV	-1.7672	23.4589	-0.07533
Li-Co_2B-Co	Co_2B	Li	Formation (eV)	Area (Å^2)	Specific Formation energy (eV Å^{-2})
-136.315 eV	-111.384 eV	-21.624 eV	-3.3078	23.4589	-0.14100
Li-LLZTO	LLZTO	Li	Formation (eV)	Area (Å^2)	Specific Formation energy (eV Å^{-2})
-1156.360 eV	-1020.790 eV	-127.575 eV	-7.99525	122.238	-0.06540

Note: Co_2B/LLZTO-B means the interface main contacting atom in Co_2B is B atom, Co_2B/LLZTO-Co means the interface main contacting atom in Co_2B is Co atom.