Supporting information

Voltage Plateau Variation in a Bismuth-Potassium Battery

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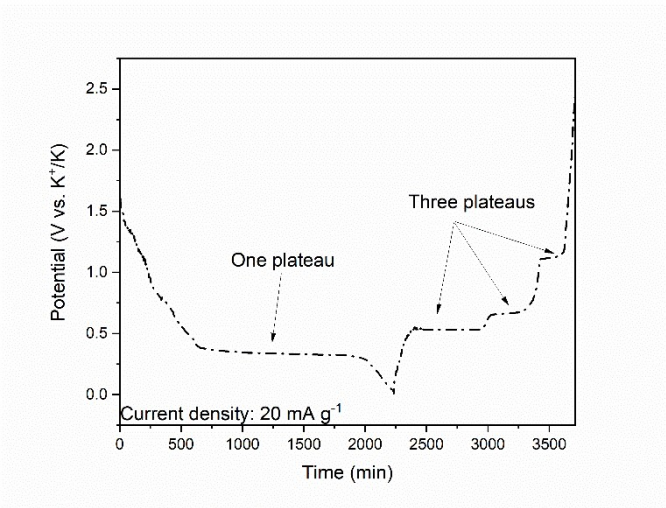

Fig. S1 Discharge-Charge curves of the bismuth-potassium cell (current density: 20 mA g^{-1}).

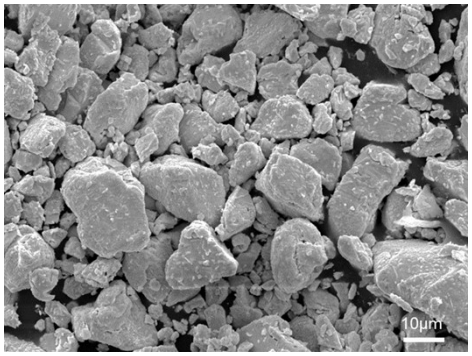

Fig. S2 Scanning electron microscope image of pristine bismuth material.

Tab. S3 Material details, space group and lattice parameters of each K_xBi phase.

	KBi_2	K_3Bi_2	K_3Bi
ICDD card number	00-003-0698	/	01-074-1165
Space group	Fd-3m	C2/c	$P6_3/mmc$
Space group number	227	15	194
a (Å)	9.52	6.86	6.178
b (Å)	9.52	6.86	6.178
c (Å)	9.52	9.55	10.933
α (°)	90	78.881	90
β (°)	90	78.881	90
γ (°)	90	92.095	120

Tab. S4 DFT simulated formation energy (E_{mix}), voltage (V), and Bader charges (q) for Bi and K in K_xBi.

Composition	E_{mix} (eV)	V (V vs. K^+/K)	q_{Bi} (e)	q_K (e)
Bi			0	
Bi_2K	-0.32	0.95	-0.37	0.66
Bi_2K_3	-0.35	0.67	-1.06	0.71
BiK_3	-0.39	0.52	-1.97	0.75

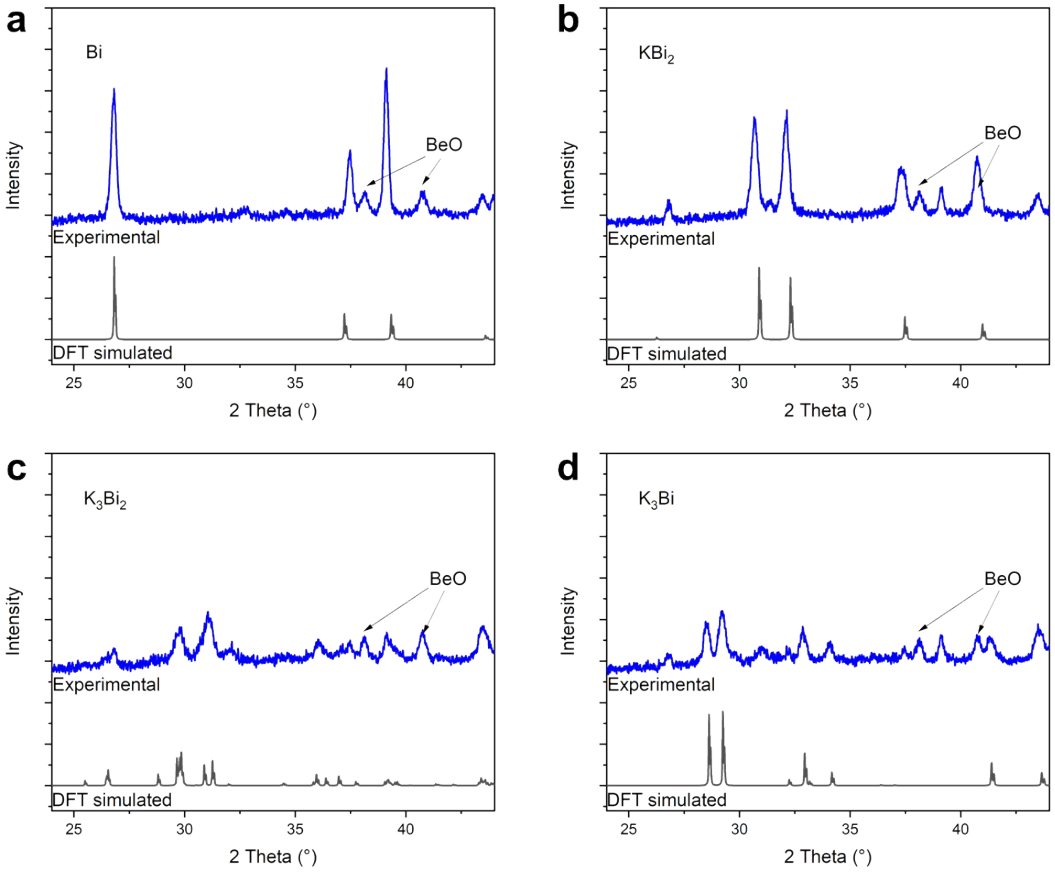

Fig. S5 Comparison of DFT simulated (in black) and experimental XRD (in blue) for a) Bi, b) KBi_2, c) K_3Bi_2, and d) K_3Bi.

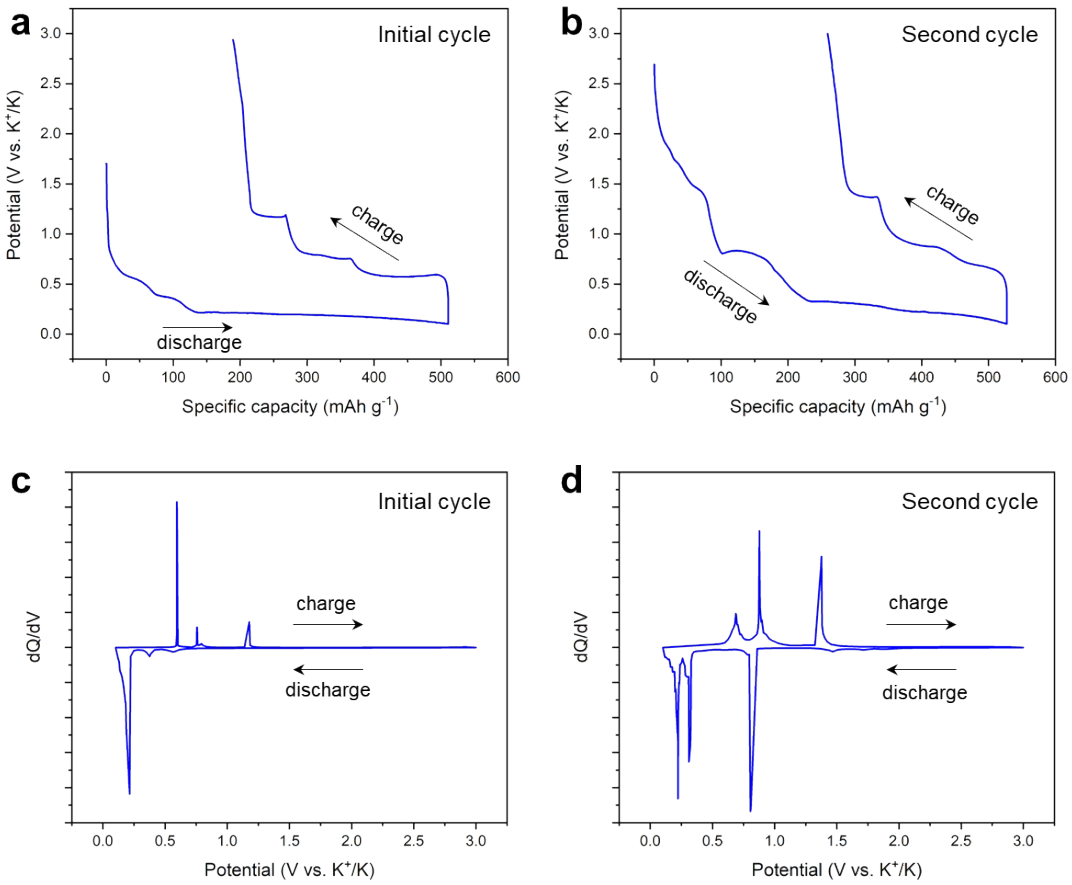

Fig. S6 The voltage profile of bismuth-potassium cell in the (a) initial cycle and (b) second cycle. The corresponding dQ/dV curve of the (c) initial cycle and (d) second cycle, showing one reduction peak for the initial discharge and three reduction peaks for the second discharge.

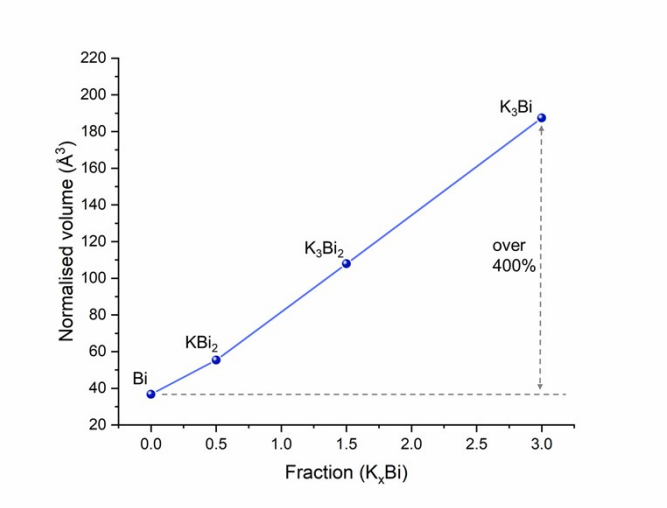

Fig. S7 Volume change of the identified K-Bi alloys.

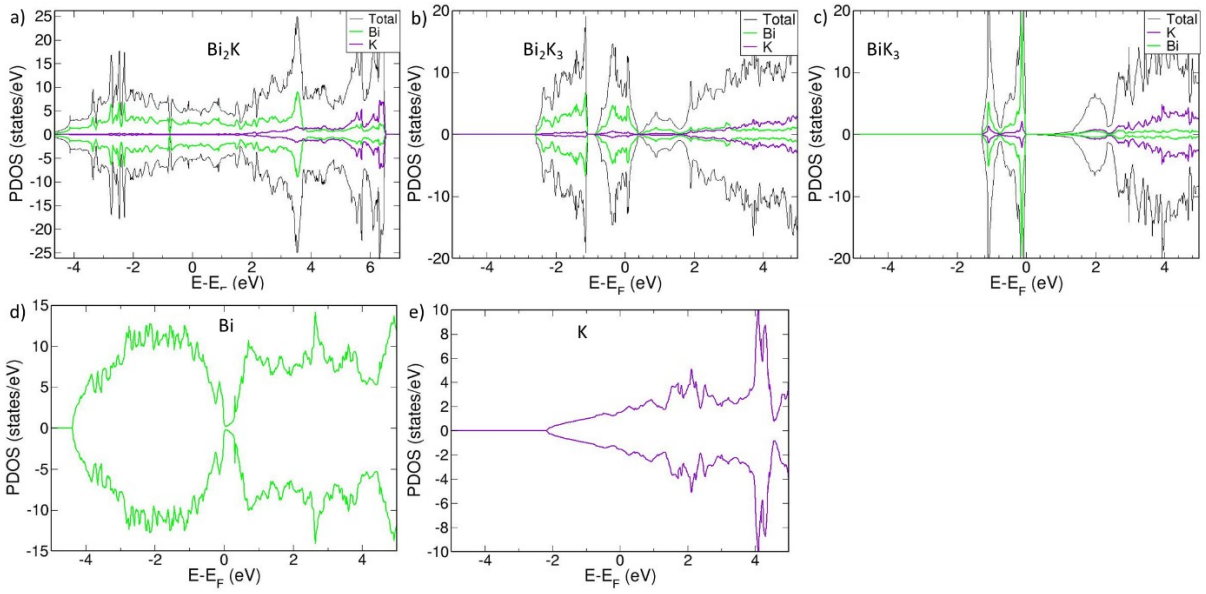

Fig. S8 Projected density of states (PDOS) for (a) Bi_2K, (b) Bi_2K_3, (c) BiK_3, (d) Bi, and (e) K.

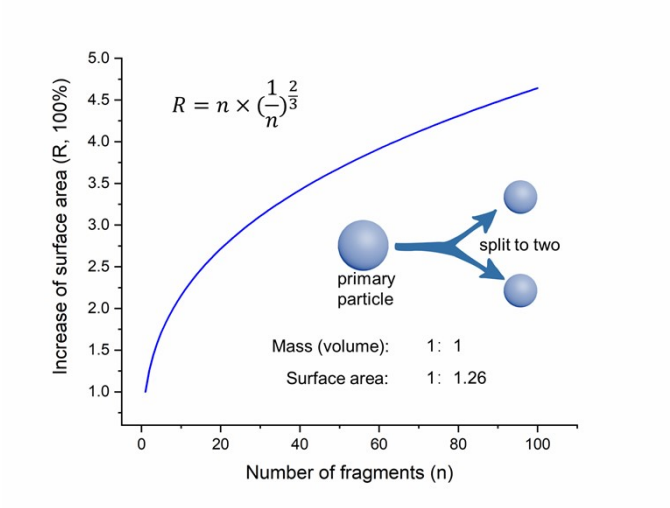

Fig. S9 The geometric relationship in ideal condition, showing the increase of surface area as the function of increased fragments. Inset: the illustration of the relationship that the surface area increases to 1.26 when the pristine particle is split into two spheres.