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SnSb vs. Sn: improving the performance of Sn-based anodes for K-ion batteries by synergetic alloying with Sb

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SUPPLEMENTARY INFORMATION

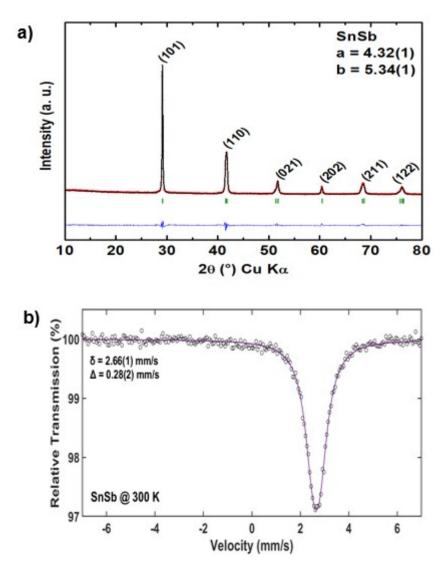


Figure S1. Characterization of SnSb powder synthesized by ball milling a) XRD pattern b) ¹¹⁹Sn Mossbauer spectrum

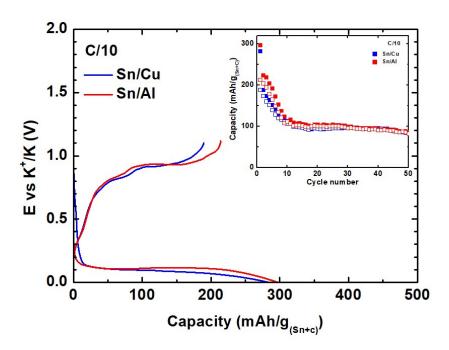


Figure S2. Voltage vs. capacity curves of the first discharge/charge in galvanostatic regime of β -Sn electrodes supported on Cu and Al current collectors and inset, the corresponding capacity retention.

Evaluation of capacity from carbon additives

In order to evaluate the electrochemical contribution of carbon additives to the capacity, galvanostatic measurements were performed on C65/VGCF/CMC electrode (wt. % 35/35/30) cycled at 20 mA/g. The carbon electrode showed a discharge/charge capacity of 310/199 mAh/g during the first cycle with an initial coulombic efficiency of 64 %. A reversible capacity of 180 mAh/g is maintained after 30 cycles corresponding to a capacity retention of 90 %. Considering that Sn and SnSb electrodes contain 18 wt. % of C65/VGCF, the contribution of carbon from the formulation to the reversible capacity of Sn and SnSb electrodes can be evaluated to 32 mAh/g.

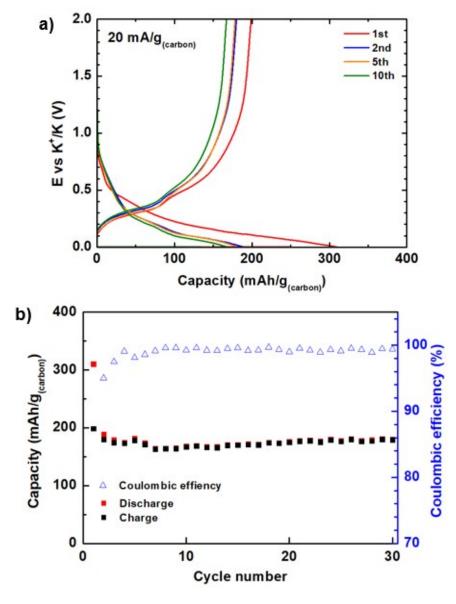


Figure S3. a) Galvanostatic discharge/charge capacity of C65/VGCF electrode at a current density of 20 mA/g and b) the corresponding capacity retention and coulombic efficiency.

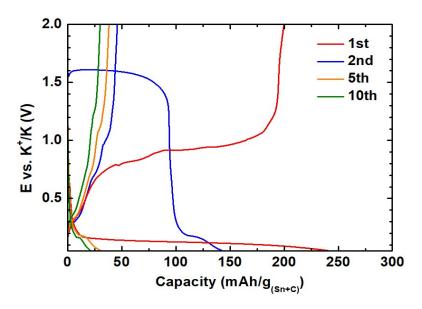


Figure S4. Galvanostatic discharge/charge profile of $\beta\textsc{-Sn}$ electrode in K half-cell at C/10 rate between 0.0 and 2.0 (V)

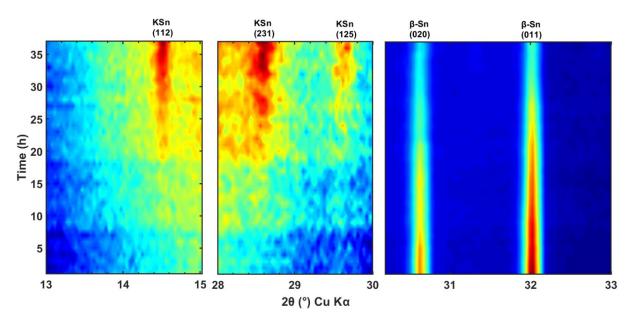


Figure S5. Contour plot of the *operando* XRD patterns of β -Sn electrode cycled at C/20.

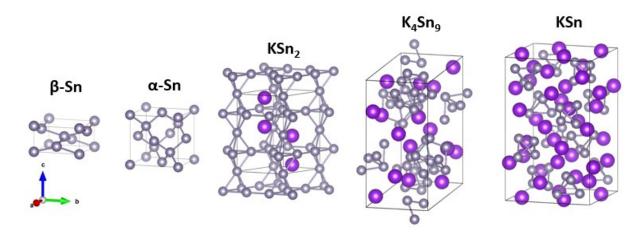


Figure S6. Crystal structures of $\beta\text{-Sn,}~\alpha\text{-Sn,}~\text{KSn}_{\text{2}},~\text{K}_{\text{4}}\text{Sn}_{\text{9}}\,\text{and}~\text{KSn}.$

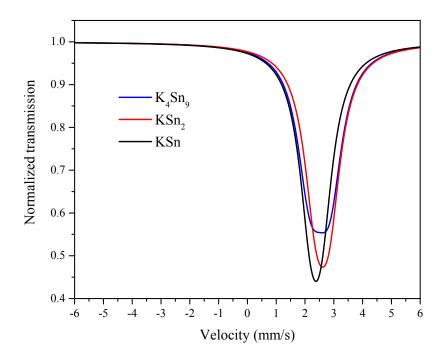


Figure S7. Theoretical ¹¹⁹Sn Mössbauer spectra of K_4Sn_9 , KSn_2 and KSn obtained from theoretical values of isomer shift and quadrupole splitting and Γ = 1 mm/s.

Phase	Space group	Lattice parameters (Å)	Z	Cell volume (ų)	Code ICSD
KSn	I4 ₁ /acd	a = 11.42 ; c = 18.57	32	2427.45	409435
KSn ₂	P6₃/mmc	a = 6.427; c = 10.43	4	373.11	190812
K ₄ Sn ₉	P2 ₁ /c	a = 14.238 ; b = 8.3554 ; c = 16.487	4	1953.1	240048
β-Sn	I4 ₁ /amd	a = 5.8310; c = 3.1820	4	108.19	040037
α-Sn	Fd-3m	a = 6.4892	8	273.28	040037

Table S1. Structural parameters of α -Sn, β -Sn, K_4 Sn $_9$, KSn $_2$ and KSn as reported in the Inorganic Crystal Structure Database (ICSD)

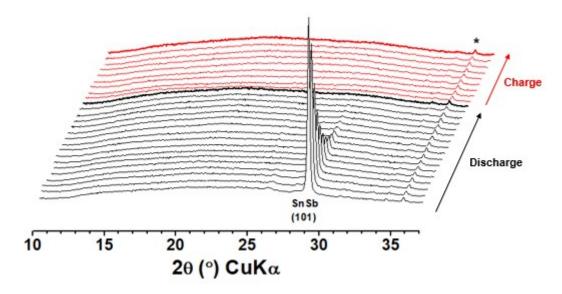


Figure S8. Operando XRD patterns of SnSb electrode cycled at C/10. The peak indicated by a star (*) is due to beryllium window.