Supporting information for

An Empirical Model for the Design of Batteries with High Energy Density

Yingqiang Wu,[§†] LeqiongXie,[⊥†] Hai Ming,[&†] Yingjun Guo,[£] Jang-Yeon Hwang,[ζ] Wenxi Wang,[‡] Xiangming He,[⊥] Limin Wang,[§] Husam N. Alshareef, [‡*] Yang-Kook Sun[ζ*] and Jun Ming[§*]

[§] State Key Laboratory of Rare Earth Resource Utilization, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, P. R. China.

[⊥] Institute of Nuclear and New Energy Technology, Tsinghua University, Beijing 100084, P. R. China.

[&] Research Institute of Chemical Defense, Beijing 100191, P. R. China.

[£] Huzhou Kunlun Power Battery Materials Co., LTD. Huzhou, 313000, P. R. China.

[ζ] Department of Energy Engineering, Hanyang University, Seoul 133-791, Republic of Korea.

[‡] Physical Science and Engineering Division (PSE), King Abdullah University of Science and Technology (KAUST), Thuwal, 23955-6900, Saudi Arabia.

[†] These authors contribute equally

* To whom correspondence should be addressed: husam.alshareef@kaust.edu.sa; yksun@hanyang.ac.kr; jun.ming@ciac.ac.cn.

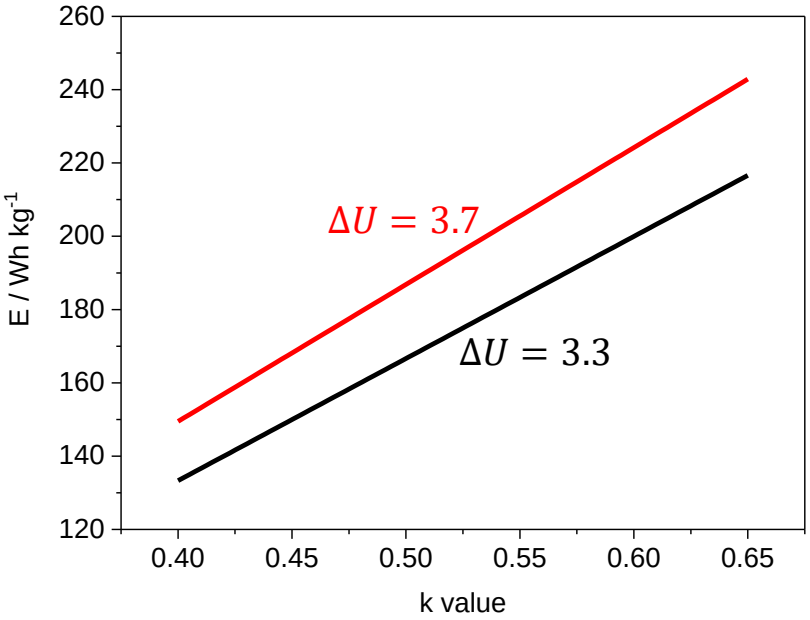

Figure S1. Dependence of energy density (E) on the k value under two different ΔU values: ΔU = 3.7 and ΔU = 3.3.

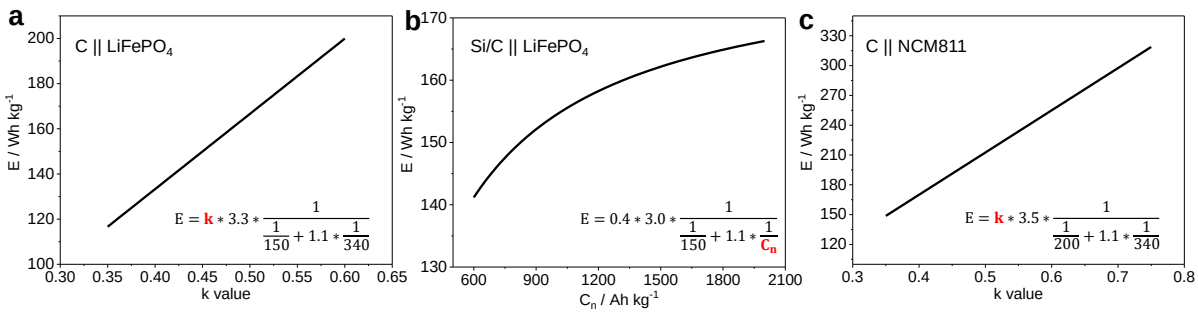

Figure S2. Dependence of E on (a) k value in C || $LiFePO_4$ battery, (b) C_n value in **Si/C || $LiFePO_4$** battery, and (c) k value in **C || NCM811** battery.

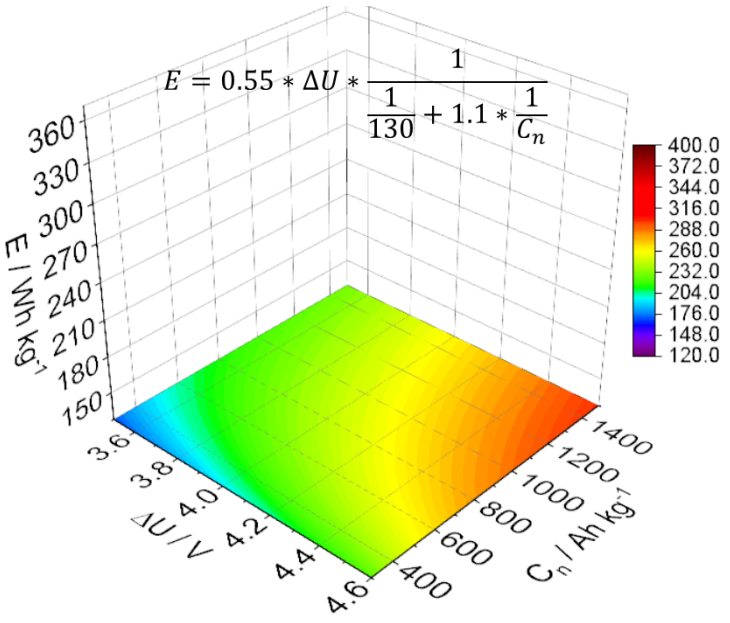

Figure S3. Variation of E value with anode capacity (C_n) and ΔU value in a hypothetical high voltage battery, where the $LiNi_{0.5}Mn_{1.5}O_4$ is used as cathode, and the k, C_p and $\chi\frac{\varepsilon_n}{\varepsilon_p}$ values are fixed at 0.55, 130 Ah kg^{-1}, and 1.1, respectively.

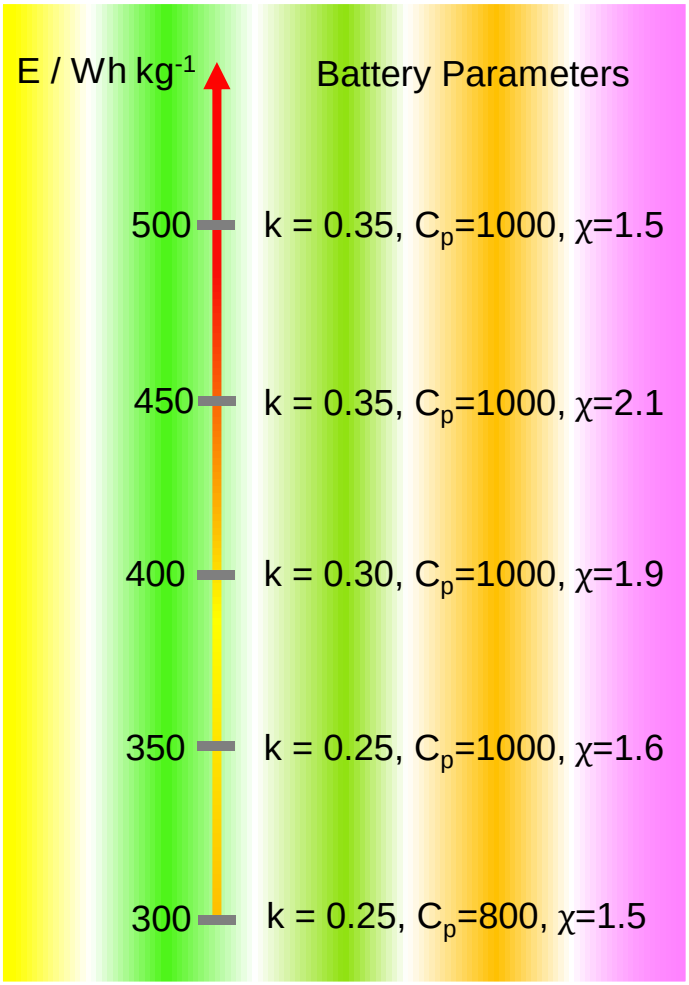

Figure S4. Strategy and parameters for designing the Li-S battery with energy densities ranging from 300 Wh kg^{-1} to 500 Wh kg^{-1} based on the proposed model.

Table S1. Estimated energy density of LIBs using the NCM811 cathode combined with various anodes. The following parameters were fix for the calculation: k = 0.55, C_p = 200 Ah kg^{-1}, $\chi\frac{\varepsilon_n}{\varepsilon_p} = 1.1$

Kind Batteries	C_n / Ah kg^{-1}	ΔU / V	E / Wh kg^{-1}
C || NCM811	340	3.6	240.4
Si/C || NCM811	800	3.3	284.7
SnO_2/C || NCM811	800	2.7	232.9
Co_3O_4/C || NCM811	800	2.0	172.5

Table S2. Electrode materials commonly used in K-ion battery[1-7]

Electrode material	Potential (vs. K/K^+) / V	Capacity / Ah kg^{-1}	Ref.
Graphite	0.01-1.5	273	[2]
Hard carbon microspheres	0.01-1.5	262	[2]
Graphene	0.6	300	[4]
Nitrogen-doped graphene	0.01-1.5	330	[2]
Sb	0.7	600	[5]
$FePO_4$	1.5-3.5	156	[7]
$KFe_4^{III}[Fe^{II}(CN)_6]$ (PB)	2.0-4.5	110	[6]
$K_{1.75}Mn[Fe(CN)_6]_{0.93}\cdot 0.16H_2O$	2.0-4.5	141	[3]
P3-type $K_{0.5}MnO_2$	1.5-4.2	140	[3]
$K_{0.7}Fe_{0.5}Mn_{0.5}O_2$	1.5-4.0	178	[3]
$KVPO_4F$	2.0-4.8	72	[1]

Table S3. Estimated energy density of KIBs calculated with k = 0.5 and $\chi \frac{\varepsilon_n}{\varepsilon_p} = 1.1$.

Battery	ΔU / V	E / Wh kg^{-1}
C || $FePO_4$	1.9	78.1
C || PB	3.45	95.8
Sb || $FePO_4$	1.5	88.2
Sb || PB	3.05	106.4
C || $K_2Mn[Fe(CN)_6]$[8]	3.5	126.4

References

1. Hosaka, T.; Kubota, K.; Hameed, A. S.; Komaba, S. Research Development on K-Ion Batteries. *Chem. Rev.* **2020**, DOI:10.1021/acs.chemrev.9b00463 10.1021/acs.chemrev.9b00463.
2. Zhang, J.; Liu, T.; Cheng, X.; Xia, M.; Zheng, R.; Peng, N.; Yu, H.; Shui, M.; Shu, J. Development Status and Future Prospect of Non-Aqueous Potassium Ion Batteries for Large Scale Energy Storage. *Nano Energy* **2019**, *60*, 340-361.
3. Sha, M.; Liu, L.; Zhao, H.; Lei, Y. Review on Recent Advances of Cathode Materials for Potassium-ion Batteries. *Energy Environ. Mater.* **2020**, *0*, 1-11.
4. Ju, Z.; Zhang, S.; Xing, Z.; Zhuang, Q.; Qiang, Y.; Qian, Y. Direct Synthesis of Few-Layer F-Doped Graphene Foam and Its Lithium/Potassium Storage Properties. *ACS Appl. Mater. Interfaces* **2016**, *8*, 20682.
5. McCulloch, W. D.; Ren, X.; Yu, M.; Huang, Z.; Wu, Y. Potassium-Ion Oxygen Battery based on a High Capacity Antimony Anode. *ACS Appl. Mater. Interfaces* **2015**, *7*, 26158.
6. Pramudita, J. C.; Sehrawat, D.; Goonetilleke, D.; Sharma, N. An Initial Review of the Status of Electrode Materials for Potassium‐Ion Batteries. *Adv. Energy Mater.* **2017**, *7*, 1602911.
7. Mathew, V.; Kim, S.; Kang, J.; Gim, J.; Song, J.; Baboo, J. P.; Park, W.; Ahn, D.; Han, J.; Gu, L. Amorphous Iron Phosphate: Potential Host for Various Charge Carrier Ions. *NPG Asia Mater.* **2014**, *6*, e138.
8. Hosaka, T.; Kubota, K.; Kojima, H.; Komaba, S. Highly Concentrated Electrolyte Solutions for 4 V Class Potassium-Ion Batteries. *Chem. Commun.* **2018**, *54*, 8387.