Supplementary information

Guidelines and trends for next-generation rechargeable lithium and lithium-ion batteries

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Table S1. Operating parameters in our calculation of energy densities.

Materials	Volumetric capacity ($mAh \cdot cm^{-3}$)	Density ($g \cdot cm^{-3}$)	Average discharge voltage (V)					
			C	Fe_2O_3	NiS	TiF_3	Si	Li
$LiFePO_4$	612	3.6	3.2	2.1	2.0	1.9	3.0	3.3
LCO	714	5.1	3.6	2.5	2.4	2.3	3.4	3.7
NCA	979	4.45	3.6	2.5	2.4	2.3	3.4	3.7

NCM_{811}	930	4.65	3.6	2.5	2.4	2.3	3.4	3.7
H-LCO	944	5.1	3.75	2.6	2.5	2.4	3.55	3.85
LMP	582	3.4	3.9	2.8	2.7	2.6	3.7	4.0
LNMO	625	4.25	4.5	3.4	3.3	3.2	4.3	4.6
LCP	618	3.7	4.6	3.5	3.4	3.3	4.4	4.7
LNP	657	3.89	4.9	3.8	3.7	3.6	4.7	5.0
LVPF	471	3.1	4.1	3.0	2.9	2.8	3.9	4.2
LCPF	469	3.28	4.8	3.7	3.6	3.5	4.6	4.9
LNPF	483	3.35	5.1	4.0	3.9	3.8	4.9	5.2
LFSF	470	3.11	3.7	2.6	2.5	2.4	3.5	3.8
LNSF	500	3.36	5.1	4.0	3.9	3.8	4.9	5.2
LCSF	487	3.27	4.7	3.6	3.5	3.4	4.5	4.8
FeF_3	2196	3.649	2.44	1.54	1.44	1.34	2.24	2.6
CuF_2	2002	4.31	3.25	2.3	2.2	2.1	3.05	3.4
FeF_2	2002	4.022	2.36	1.46	1.36	1.26	2.16	2.5
NiF_2	2040	4.21	2.66	1.76	1.66	1.56	2.44	2.8
CoF_2	2038	4.21	2.5	1.6	1.5	1.4	2.3	2.6
BiF_3	1582	5.6	2.85	1.95	1.85	1.75	2.65	3.0
$CuCl_2$	1115	3.08	2.87	1.97	1.87	1.77	2.67	3.0
$FeCl_2$	1115	2.92	2.11	1.2	1.1	1.0	1.91	2.3
$NiCl_2$	1127	3.01	2.34	1.44	1.34	1.24	2.14	2.5
$FeCl_3$	1172	2.668	2.5	1.6	1.5	1.4	2.3	2.6
LiBr	1073	3.464	3.3	2.4	2.3	2.2	3.1	3.4
LiI	699	3.49	2.52	1.6	1.5	1.4	2.32	2.7
Li_2Te/Te	1277	3.379	1.6	-	-	-	1.4	1.75
Li_2Se/Se	1659	2.827	1.8	-	-	-	1.6	1.95
Li_2S/S	1937	1.66	2.0	-	-	-	1.8	2.15
$LiOH/O_2$	1634	1.46	2.6	-	-	-	2.4	2.75
Li_2O_2/O_2	2698	2.31	2.6	-	-	-	2.4	2.75

Table S2. Operating parameters in our calculation of energy densities.

Materials	Volumetric capacity ($mAh \cdot cm^{-3}$)	Density ($g \cdot cm^{-3}$)
Graphite	715	2.164
Fe_2O_3	2740	3.43
NiS	1571	3.068

TiF3	**2002**	**3.13**
Si	**2190**	**1.208**
Li	**2062**	**0.534**
Al foil	**-**	**2.70**
Cu foil	**-**	**8.96**
Separator (wet)	**-**	**1.0**

Table S3. Summary of the calculated energy densities.

Anode / Cathode	**Volumetric energy densities Wh/L**						**Gravimetric energy densities Wh/kg**					
	C	Fe_2O_3	NiS	TiF_3	Si	Li	C	Fe_2O_3	NiS	TiF_3	Si	Li
$LiFePO_4$	**673**	**651**	**544**	**580**	**888**	**964**	**268**	**225**	**195**	**205**	**345**	**403**
LCO	**819**	**877**	**726**	**780**	**1132**	**1213**	**272**	**242**	**213**	**223**	**350**	**403**
$LiMnO_2$	663	636	533	568	869	943	241	197	172	180	299	347
NCA	**934**	**1114**	**890**	**973**	**1419**	**1514**	**354**	**343**	**292**	**311**	**510**	**602**
NCM_{811}	**916**	**1073**	**862**	**940**	**1370**	**1463**	**338**	**320**	**274**	**291**	**473**	**555**
H-LCO	960	1128	906	988	1445	1537	333	317	274	290	469	546
LMP	797	833	708	753	1053	1123	325	298	261	275	422	485
LNMO	958	1073	911	972	1295	1365	351	333	296	310	449	507
LCP	**973**	**1094**	**931**	**993**	**1313**	**1383**	**383**	**372**	**328**	**345**	**501**	**568**
LNP	**1072**	**1248**	**1058**	**1132**	**1470**	**1541**	**414**	**411**	**364**	**383**	**546**	**618**
LVPF	741	749	650	685	938	998	311	283	251	263	391	445
LCPF	865	920	804	848	1102	1161	353	336	301	315	443	496
LNPF	935	1018	890	939	1200	1259	378	367	329	344	477	533
LFSF	667	646	558	589	839	900	279	244	216	225	349	400
LNSF	955	1050	915	967	1237	1297	387	378	338	354	492	551

LCSF	867	924	805	849	1112	1172	355	338	302	316	449	505
FeF_3	**774**	**1056**	**739**	**792**	**1452**	**1586**	**343**	**391**	**288**	**304**	**705**	**936**
CuF_2	**1008**	**1492**	**1088**	**1189**	**1860**	**1981**	**426**	**511**	**398**	**426**	**813**	**1027**
FeF_2	732	947	673	714	1334	1470	315	335	252	263	605	796
NiF_2	829	1155	827	891	1527	1659	353	400	305	323	678	878
CoF_2	779	1049	747	800	1431	1565	331	364	276	290	636	828
BiF_3	827	1090	825	869	1416	1533	312	320	263	268	503	616
$CuCl_2$	738	863	683	706	1137	1236	334	344	280	287	543	669
$FeCl_2$	543	525	402	399	825	930	250	215	168	166	405	520
$NiCl_2$	604	635	493	498	926	1030	275	256	204	205	448	567
$FeCl_3$	655	726	565	577	1019	1124	310	309	245	250	527	669
LiBr	836	1022	821	855	1279	1373	363	384	320	329	569	685
LiI	527	488	401	399	699	776	223	182	154	152	294	353
Li_2Te	432	-	-	-	630	748	191	-	-	-	291	396
Li_2Se	530	-	-	-	849	982	246	-	-	-	443	613
SeS_2	576	-	-	-	959	1098	266	-	-	-	498	689
Li_2S	**614**	**-**	**-**	**-**	**1044**	**1184**	**315**	**-**	**-**	**-**	**691**	**1004**
LiOH	719	-	-	-	1126	1239	386	-	-	-	765	1029
Li_2O_2	**829**	**-**	**-**	**-**	**1508**	**1639**	**407**	**-**	**-**	**-**	**935**	**1285**