

Theoretical Specific Capacity

$Q_{\text{theoretical}} = nF / (3600 \cdot MW)$ in mAh/g

Atomic Mass	g/mole
Li	6.94
Fe	55.845
P	30.974
O	15.999
Ni	58.693
Co	58.933
Mn	54.938
Al	26.982

Faraday Constant (A-s/mol) 96485.33

											EX. 4		EX. 3		Uemura	
	A.M.U.	NCM111	NCM523	NCM811	LiCoO2	LiNiO2	LiMn2O4	LiFePO4	Li0.83Mn0.5Co0.5O1.5	Li0.967Mn0.5Co0.5O1.5	Li0.83Mn0.75Ni0.25O1.75	Fe0.125O1.875	LiMnO2			
Li	7	1	1	1	1	1	1	1	0.83	0.967	0.83	0.75	1			
Ni	58.693	0.333	0.5	0.8		1						0.25				
Co	58.933	0.333	0.2	0.1	1				0.5	0.5						
Mn	54.938	0.333	0.3	0.1			2		0.5	0.5		0.75	0.875	1		
O	15.999	2	2	2	2	2	4	4	1.5	1.5		1.75	1.875	2		
Al	26.982															
Fe	55.845							1					0.125			
P	30.974							1								
Molecular Weight	g/mol	96.46	96.61	97.34	97.93	97.69	180.87	157.82	86.74	87.70	89.69	90.30	93.94			
Li ions	n	1	1	1	1	1	1	1	0.83	0.967	0.83	0.75	1			
Theoretical Specific Capacity (Q)	mAh/g	277.8	277.4	275.3	273.7	274.3	148.2	169.8	256.4	295.5	248.0	222.6	285.3			
									3.08	3.55	2.98	2.67	3.42			
									2.24	2.60	2.24	2.00	2.70			
									1.37	1.36	1.33	1.34	1.27			

Calculating the N/P Ratio for the Lithium Metal Battery

For the ease of calculating N/P ratio for Li metal batteries, often areal capacities in unit of mAh cm⁻² for Li metal anode and cathode material are used. It is worth noting that the often theoretical capacity of Li and the practical capacity of the cathode are used for calculating N/P ratio. It is because Li metal is often industrially processed as a thin film (ranging from 500 μm to 20 μm in the thickness), and the initial capacity of Li is not dramatically affected by cycling conditions. However, the major reason for using practical capacity, equivalently measured capacity, for the cathode is that the actual cathode capacity is sensitive to operating conditions such as operating voltage window, C rate, temperature, and etc. Therefore, it is common in the field to consider measured cathode capacity from the defined operating conditions to calculate N/P ratio. Since the battery electrodes are relatively thin, the capacity values are normalized by the electrode size to derive the areal capacity of the anode and cathode. Gravimetric capacities are reported as well, but it became common in the field to use areal capacities to find N/P ratio. Since Li metal anode comes as a thin film, a useful equation to calculate N/P ratio with Li metal foil is relating Li thickness to areal capacity. The below equation relates to how the thickness of Li metal foil is related to its theoretical areal capacity.

Li Areal Capacity	Li thickness
1 mAh cm ⁻²	4.85 μm
4 mAh cm ⁻²	19.40 μm
7 mAh cm ⁻²	33.95 μm

Table 3: Areal capacity of Li with respect to its thickness. Note that these are theoretical values. The thickness is calculated by assuming perfectly flat and smooth film of Li.

Benefits of Using Li Metal Anodes

Lithium metal is an ideal anode material for Li batteries due to the following properties. [1]

- Low density: 0.534 g cm⁻³
- Low reduction potential: -3.04 V vs SHE
- High theoretical specific capacity: 3861 mAh g⁻¹ and 2061 mAh cm⁻³

The low density of Li helps to reduce overall cell mass and volume, which helps to improve both gravimetric and volumetric capacities and energy densities of Li battery. Also, the low reduction potential of Li enables the cell to operate at relatively high cell voltage that also increases the energy density of the Li battery.

The theoretical gravimetric and volumetric capacities of Li metal anode are

$Q_g = nF M_w = 3861.328 \text{ mAh g}^{-1}$
 $Q_v = Q_g \cdot \rho = 2061.949 \text{ mAh cm}^{-3}$

where

Q_g = Gravimetric capacity of Li [mAh g⁻¹]
 n = Number of electrons transferred = 1
 F = Faraday's constant = 26.8014814 [Ah mol⁻¹]
 M_w = Molecular weight of Li = 6.941 [g mol⁻¹]
 Q_v = Volumetric capacity of Li [mAh cm⁻³]
 ρ = Density of Li = 0.534 [g cm⁻³]

The capacity values calculated above are the upper limit of the all the possible anode materials that could be utilized as the anode for Li batteries, meaning that Li is intrinsically the highest energy-dense anode material for Li batteries. [1-3] However, these theoretical values are difficult to achieve in reality as the high chemical and electrochemical reactivities of Li induce side reactions during the battery cycling. [4]

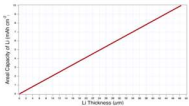


Fig. 1: Li metal anode areal capacity Q_A vs Li thickness T_{Li} computed using Eq. (1). (Source: M. S. Kim)