



PURE LITHIUM

BATTERY METRICS AND MISCONCEPTIONS

Addressing the nebulous language on lithium battery performance metrics

Desislava R. Dikova and Professor Donald R. Sadoway

Pure Lithium Corporation
56 Roland Street Suite 309
Boston, Massachusetts 02129
Inquiries: info@purelithium.io

I. Introduction.

Since the Nobel-winning discovery of lithium-ion batteries, researchers have kept demonstrating higher performance, lower costs, better chemistries, faster charging. Driven by the clean energy transition, an unprecedented amount of investment has triggered a surge in the battery market [1]. Unfortunately, the technology has far outpaced the precision of language we use to describe it. Definitions of key battery performance metrics have become increasingly ambiguous, inconsistent, and nebulous. Left unchecked, this well-documented phenomenon [2, 3, 4, 5] will irreparably erode the integrity of the battery industry. To maintain investor confidence and public trust, the battery industry must uphold the highest level of rigorous, ethical communication. The first step is speaking the same language.

This paper suggests more precise language for reporting properties, performance, and components of lithium-based battery systems. Sections II, III, and IV discuss methodologies for responsibly measuring and disclosing performance metrics. Section V defines the language used to describe lithium-specific electrochemistry and charge-discharge mechanisms. Section VI addresses safety considerations and misconceptions. Conclusions, figures, and references can be found in sections VII-X.

II. Theoretical vs. Functional Metrics.

Theoretical properties are metrics intrinsic to materials and governed by natural law; they represent upper limits and are meaningful for justifying design choices. However, they are not only insufficient but unsuitable for demonstrating real-world performance. Comparison between theoretical metrics and experimental or dated systems is highly misleading [2, 3]. Responsible reporting must identify all reported values as theoretical or functional.

Key theoretical limits of battery materials include energy density, power density, capacity [4], and electrochemical potential. These values are widely reported and derived from standardized methodology. “Functional metrics” are values calculated from experimental data under standardized methods and conditions [4, 6, 7]. Some functional metrics can be reported as mean, initial, or best values over battery lifetime. The absence of these qualifiers, assumptions, and raw values renders performance reports incomparable and possibly misrepresentative [2, 5].

As noted in Figure 1, certain values are presented on a “per volume” or “per mass” basis. The adjective “gravimetric” and “specific” both mean “per mass.” The adjective “volumetric” means “per volume.” Gravimetric

and volumetric values are also distinguishable by the denominator of the units of the reported value – kg or cm³, respectively. Using the mass or volume of just the active materials is an example of a theoretical value. This value neglects the mass and volume of the indivisible cell [2, 3, 8]. Consider for example, a system that relies on excess lithium. All lithium-ion batteries face some lithium depletion upon their first charge. To avoid capacity and energy density losses, researchers introduce excess lithium to the cell [9]. The excess mass must be included in gravimetric mass calculations to enable comparison between different systems [5]. The use of excess lithium also poses safety implications, as discussed in Section VI.

Figure 2 is an example of responsible reporting of theoretical upper of the internal combustion engine (ICE), lithium-ion batteries (LIB), and lithium metal batteries (LMB). The values in Figure 2 are derived from the graphite negative electrode in LIB and ICE fuels gasoline and natural gas to represent commerciality [10, 11, 12, 13, 14, 15].

III. The Scourge of Unspecified “Energy Density.”

“Energy density” is one of the most deafeningly reported battery metric. The lack of standardization leads to non-trivial misrepresentations that spiral into further inconsistencies, rendering it impossible to compare battery systems meaningfully – especially across the academic and industrial gap [3].

First, let’s define “energy” - the ability of a force to displace an object. The International Standard (SI) units for energy are Joules (J), though for electrochemical systems, energy is reported as watt-hours or kilowatt-hours (Wh, kWh).

Next, “power” - energy transferred per unit of time, expressed in Joules per second (J/s) or watts (W) [Equation 1]. Power in an electric system is calculated as the product of the current in amperes (A) and potential or voltage in Volts (V) [Equation 2]. Current and voltage are related by Ohm’s Law [Equation 3] so power is experimentally measured by setting one as the independent variable and recording the other as the dependent variable.

1) Definition of power and energy

$$\text{Power (W)} = \frac{\text{Energy(Wh)}}{\text{Time (h)}}$$

2) Definition of electrical power

$$\text{Power (W)} = \text{Current(A)} * \text{Voltage(V)}$$

3) Ohm's Law

$$\text{Voltage (V)} = \text{Current (A)} * \text{Resistance(Ohm)}$$

Now that we have a power value, we can back-calculate energy, the product of power and time [Equation 1]. By definition, "energy density" is theoretical volumetric energy density or the energy generated per volume of material [Figure 1]. However, "energy density" can be reported per mass or volume, as a theoretical limit, or as an observable, functional metric. Thus, reporting "energy density" lacking adjectives is insufficient.

"Gravimetric energy density" or "specific energy" is the theoretical upper limit of energy that can be generated per mass of material. The theoretical upper limit metrics are kilowatt-hours per kilogram (kWh / kg) or megajoules per kilogram (MJ / kg). We will refer to experimental values as "functional specific energy." Gravimetric energy density refers to this value for just the *active material* of an electrode – the interactions, mass, and volume of the rest of the battery system are not included. Experimental systems always face non-zero thermal losses due to inevitable interaction between layers of materials. Thus, reporting gravimetric energy density as

"energy density" misrepresents real-world performance. Furthermore, it is unfair to contrast the theoretical value - gravimetric energy density - with the experimental value - functional specific energy [5]. Experimental values must be measured in identical conditions and calculated using the same subset of system mass. In the absence of experimental values, comparisons may be reported against other theoretical values or must be labeled as optimistic [2].

IV. Capacity, Depth of Discharge, and Trade-offs.

An equivalent definition of electrical power is the product of capacity (ampere-hours, Ah) and discharge potential (V) per certain length of time (hours, h) [Equation 4].

4) Equivalent definition of electrical power

$$\text{Power (W)} = \frac{\text{Capacity (Ah)} * \text{Potential (V)}}{\text{Time (h)}}$$

"Nameplate" or "nominal" capacity is the theoretical maximum capacity of a system in its fully charged state [Equation 5]. Another theoretical metric closer to reality is the "usable capacity," also called "initial discharge capacity." We can equivalently define usable capacity as the product of nameplate capacity and depth of discharge (DOD) [Equation 6].

DOD is the ratio of output capacity to available capacity, calculated as the ratio of initial discharge capacity to initial charge capacity, expressed as a percentage [Equation 7]. Experimentally, DOD is pre-defined by setting threshold values for charge potential and discharge potential. At the threshold value, the system reverses polarity until it reaches the next potential threshold. One cycle of hitting both thresholds represents one charge-discharge cycle, defined by the variable n . The nameplate capacity, usable capacity, and DOD are theoretical limits measured during the first cycle, $n=1$.

5) Definitions of nameplate capacity

$$\begin{aligned} \text{Nameplate capacity(Ah)} &= \frac{\text{Charge power(W)} * \text{Time(h)}}{\text{Charge potential(V)}} \\ &= \text{Charge capacity(Ah, } n = 1) \end{aligned}$$

6) Definitions of usable capacity

$$\begin{aligned} \text{Usable capacity(Ah)} &= \frac{\text{Discharge power(W)} * \text{Time(h)}}{\text{Discharge potential(V)}} \\ &= \text{Discharge capacity(Ah, } n = 1) \\ &= \text{Nameplate capacity(Ah)} * \text{DOD(\%)} \end{aligned}$$

7) Definition of the depth of discharge (DOD)

$$\text{DOD(\%)} = \frac{\text{initial discharge capacity(Ah)}}{\text{initial charge capacity(Ah)}} * 100\%$$

Functional power has a linear relationship with functional discharge capacity and an inverse relationship with time [Equation 4]. Careful selection of DOD can be used to achieve fast charging at the expense of power and vice versa. Too high of a DOD can lead to degradation and shorter lifetimes, while too low of a DOD leads to a prohibitively slow charging system. Figure 3 summarizes the trade-offs. Since DOD can affect lifetime, DOD must be reported in tandem with Coulombic efficiency (CE) [16] and C-rate over time.

CE is equal to the ratio of discharge capacity for one charge-discharge cycle (n) to the usable capacity ($n=1$) [Equation 8]. The number of stable charge-discharge cycles, N , that demonstrate CE above some threshold value can be used as an estimation of battery lifetime.

8) Definition of Coulombic efficiency

$$\begin{aligned} \text{CE (\%)} &= \frac{\text{discharge capacity for cycle } n}{\text{discharge capacity for cycle } n = 1} * 100\% \\ &= \frac{\text{discharge capacity for cycle } n}{\text{usable capacity}} * 100\% \end{aligned}$$

C-rate is the observed rate at which the battery discharges. First, the theoretical current is the current needed to deliver nameplate capacity for one hour [Equation 9]. Then, the C-rate is the ratio of current drawn during one charge-discharge cycle (n) to theoretical current, per time [Equation 10].

9) Theoretical current for C-rate calculation

$$\text{Theoretical Current (A)} = \frac{\text{Nameplate capacity (Ah)}}{1 \text{ hour}}$$

10) Definition of C-rate

$$\text{C - rate (h}^{-1}\text{)} = \frac{\text{Measured current (A)}}{\text{Theoretical current (A)} * \text{Time(h)}}$$

Side reactions, mechanical stress, and thermal losses are observed as decreases in CE and C-rate [16, 17]. The rate of decrease in CE past N cycles is equally significant – systems that experience an accelerated, sudden drop pose substantial safety concerns [16].

The selection of DOD affects electrochemical performance, charge speed, safety, and lifetime. Specifically, the variables usable capacity, functional power, CE, C-rate, and N: summarized in Figure 1 and contrasted in Figure 3. It is incomplete to report less than all these metrics and inconsistent to cherry-pick from different experimental conditions [5]. DOD optimization is an understudied but growing area of research [6, 17].

V. Lithium Electrochemistry and the Negative Electrode.

Note that the title of this section uses the term “negative electrode” rather than “anode” or “cathode.” By definition, a cathode is an electrode where a reduction half-reaction occurs, and an anode is an electrode where an oxidation half-reaction occurs. The sum of the two half-reactions is called a “redox reaction.” A redox reaction is an electrochemical process where charge carriers are transferred between materials. Charge carriers are any electrically charged species that can flow in a specific medium: electrons flow through conductors, ions flow through solutions. In other words, electrons can’t swim, ions can’t walk.

In a secondary battery, the redox reaction occurs reversibly. A “Galvanic cell” is a forward or discharge reaction which outputs energy. The reverse is an “electrolytic cell.” Upon charge, one electrode experiences an oxidation half-reaction, but on discharge, it undergoes a reduction half-reaction [Figure 4]. Assessing the chemistry at this electrode requires identifying it by an unchangeable property between charge and discharge – or the polarity. The negative electrode will always be the negative electrode, regardless of the type of half-reaction, and the same for the positive electrode. Therefore, it is most appropriate to identify electrodes as “negative” or “positive” rather than “anode” or “cathode.”

Lithiation is the migration of lithium ions towards the negative electrode, also known as the forward reaction and discharge reaction [Figure 5]. The most common negative electrode for Li-ion batteries is a graphite scaffold, represented formulaically as C_6 . When researchers study the graphite electrode, they mean to study the negative electrode, not the “anode, when charging” or “cathode, when discharging.”

Of course, graphite is not the only negative electrode used or researched for Li-ion batteries. Lithiation functions by two different mechanisms, dependent on the negative electrode material, summarized in Figure 5. Graphite lithiation occurs by the intercalation mechanism, where lithium ions occupy the pores of a scaffolding material [12, 14]. The alternative is “conversion,” where lithium ions burrow into metallic vacancies in the negative electrode. The two types of conversion mechanisms are diffusion (Type A) or alloying (Type B) [12]. The negative electrode experiences volumetric expansion proportional to the volume of transferred ions. Extreme volumetric expansion, due to overcharging, results in physical strain that can cause degradation and shorts. As a result, volumetric expansion is a critical metric for indirectly assessing batteries' lifetime, durability, and safety. Reported volumetric expansion coefficients of commercially available Li-ion negative electrodes are shown

in Figure 6. Lithiation occurs at a fixed electrochemical potential. This potential, the discharge potential, is used to calculate the upper limit of power output [Equation 2]. Lowering the DOD to prevent overcharging can extend battery lifetime, at the expense of functional power output. The reverse process, de-lithiation, suggests the power input needed to recharge a battery. Figure 7 shows the lithiation and de-lithiation potentials for commercially used Li-ion negative electrodes. These are immutable limits that cannot be engineered away, nor do they represent real-world performance.

All electrochemical systems need an electrolyte and two electrodes which participate in two half-reactions. No system can generate power without these components. Therefore, no system can be “anode-free.” So-called “anode-free” systems signify that the “anodic” reaction occurs within the electrolyte rather than on or in a substrate. For example, in a wet-state “anode-free” lithium metal battery system, the negative electrode is metallic lithium, and the positive electrode is some reaction within the electrolyte. The potential of the positive electrode reaction is collected by an electrochemically inactive metal current collector. The positive electrode or “anode” still exists in this system, just not as a traditional solid [18]. Instead, the electrolyte serves as both the electrolyte and the site of the positive

electrode reaction. The exciting novelty of these systems is that the electrolyte and positive electrode are “phase-unified,” or “mutually solvated.” These phase-unified electrode-electrolyte systems are truly revolutionary. They don’t need imprecise buzzwords to sell.

VI. Safety: Misconceptions on Solid-State and High-Temperature Batteries.

Any battery that contains flammable materials and/or is vulnerable to thermal runaway is dangerous. Most research focuses on preventing thermal runaway that ignites flammable materials [7, 17, 19], and less so on excluding flammables [20, 21]. These notable flammables are organic electrolytes and excess lithium [9].

All batteries warm up as they are used. Thermal runaway is an extreme, accelerated version of this, triggered when a cell shorts or rapidly discharges [19]. A short occurs when the separator between the negative and positive electrode is compromised due to mechanical abuse. Possible sources of this abuse are volumetric expansion from lithiation or dendrite formation. Both mechanisms are affected by the choice of DOD. A rapid decrease in CE also suggests the possibility of thermal runaway in the case of cell failure.

A proposed solution has been solid-state batteries, though the term has been liberally overused to the point of losing meaning. Many so-called “solid-state” batteries contain a separator and/or positive electrode wetted with flammable electrolyte [5]. Firstly, marketing a battery as “solid-state” when it includes a wetted separator is just incorrect. Second, marketing “solid-state” as inherently safe without disclosing the flammability of the constituent materials or thermal management is misleading. Case in point: safety is not a guarantee in solid-state or wet systems unless the battery can prevent thermal runaway.

The inherent issue is *runaway*, not elevated temperatures. A battery operated at higher than ambient temperatures [22, 23] is not inherently unsafe if it can prevent thermal runaway. Of course, device temperature depends on the application: a hand-held mobile device with a hot battery would be uncomfortable, if not dangerous, to handle.

There is little standardization on reporting thermal performance, though methods for determining cooling coefficient have been proposed [7, 24]. Safe operating conditions become much more flexible if flammable materials are excluded AND thermal management is insured. To date, no such battery exists in the market.

VII. Conclusions.

- The integrity of the battery industry is at stake if we do not adopt standardized, consistent definitions for metrics of battery performance.
- Most notably, the ambiguous term “energy density” lacking adjectives must be eliminated from the vocabulary of the battery industry.
- Any reported performance values must be explicitly identified as theoretical upper limits or experimentally observed; average or best; initial or throughout the lifetime.
- The choice for depth of discharge (DOD) reveals unavoidable trade-offs, and therefore, metrics must be reported together from consistent experimental conditions. Affected properties include functional discharge capacity, functional power, coulombic efficiency, C-rate, lifetime, and volumetric expansion. Research into DOD optimization is overlooked but crucial.
- The terms “positive electrode” and “negative electrode” are properties that remain unchanged regardless of charge-discharge direction. The terms “anode” and “cathode” are reversible and inappropriate for describing secondary batteries.
- The term “anode-free” must be replaced with a term that more accurately reflects

that the electrolyte and positive electrode are the same material – “phase-unified” or “mutually solvated.”

- Removing flammable materials and the possibility of thermal runaway is the only guarantee of battery safety. Substitutes for flammable electrolytes, removal of excess lithium, and thermal management metrics are critically under-researched.
- No battery that relies on wetted components should be branded a “solid-state” system. Furthermore, solid-state does not inherently guarantee safety unless the previously outlined conditions are met.

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IX. Figures.

	THEORETICAL PROPERTY	FUNCTIONAL METRIC	UNITS	UNIT CONVERSIONS	Want to be:
Relative to Mass	Gravimetric Energy Density (<i>syn.</i> Specific Energy)	Functional Specific Energy	kWh / kg MJ / kg	1 kWh \rightleftharpoons 3.6 MJ	High
	Gravimetric Power Density (<i>syn.</i> Specific Power)	Power-to-weight ratio	kW / kg	1 kWh \rightleftharpoons 3.6 MJ	High
	Gravimetric Capacity (<i>syn.</i> Specific Capacity)	Functional Specific Capacity	Ah / kg mAh / g	1 Ah / kg \rightleftharpoons 1 mAh / g	High
Relative to Volume	Volumetric Energy Density (<i>syn.</i> Energy Density, unspecified)	Functional Energy Density	kWh / cm ³ kWh / m ³	1 cm ³ \rightleftharpoons 1x10 ⁶ m ³	High
		Volumetric Expansion	%		Low
Electrochemical	Lithiation Potential	Discharge potential	V		High
	De-lithiation Potential	Charge potential	V		Low
	Nameplate capacity (<i>syn.</i> Nominal rated capacity, initial charge capacity)	Functional Charge Capacity	Ah C	1 Ah \rightleftharpoons 3600 C	High
	Usable Capacity (<i>syn.</i> Initial discharge capacity)	Functional Discharge Capacity	Ah C	1 Ah \rightleftharpoons 3600 C	High
	Depth of Discharge (DOD)		%		Varies*
		Coulombic efficiency	%		High
		C-rate	Per hours, h ⁻¹		High
	Lifetime	Hours, h Cycles, N		High	

Figure 1. Precise language distinguishing metrics of battery performance as theoretical or functional. Synonyms are listed in parentheses and labeled "syn." Functional values over time must also be identified as "mean" or "initial." The units used to report these values can also be a source of misinterpretation, so the commonly used units and conversions between them are listed. *Pros and cons of high DOD are identified in Figure 3.

		ICE [10, 11]		LITHIUM-ION [12, 13]	LITHIUM METAL [13, 14, 15]	
		Gasoline	Natural Gas	Graphite	Substrate agonistic	
ELECTROCHEMICAL	Gravimetric Energy Density (mAh / g active material)	/	/	372	3862	
	Volumetric Energy Density (mAh / cm ³)			756	2046-2062	
	Discharge potential (V vs. SHE)			-3.040	-3.040	
MATERIAL	Mass density (g / cm ³)	715-780	0.7-0.9	2.27	0.53	
	Functional Specific Capacity	(kWh / kg)	12.8	15.3	0.25-0.30	0.35-0.56
		(MJ / kg)	45.8-47.5	53-55	0.3-1.1	2.0

Figure 2. Some theoretical limits of fuels for internal combustion engine (ICE), Li-ion batteries (LIB), and lithium metal batteries (LMB). While other chemistries exist, gasoline and natural gas for ICE and graphite-based Li-ion batteries are assessed for the sake of representing commerciality. These values represent theoretical properties based on active material. This data is useful for designing new systems and assessing what metrics must be demonstrated to outperform existing technology. It is critical to include and compare theoretical and functional metrics throughout the design, development, and deployment processes for a holistic assessment. Data sources: [10, 11, 12, 13, 14, 15]

Pros of high DOD	Cons of high DOD
More usable capacity	Low C-rate
Higher functional power	Possibly shorter lifetime
Higher CE	Possibly hazardous system failure

Figure 3. The selection of a high depth of discharge (DOD) reveals non-trivial performance trade-offs. The efficient, high-power battery would result in slower charging, faster degradation, and possibly hazardous failure. Optimization of DOD is needed to achieve a balance of these metrics.

PROPERTY		FORWARD REACTION	BACKWARD REACTION
Generalizable to all Electrochemical Cells	Energy Pathway	Discharging, or energy output	Charging, or energy input
	Type of Cell	Galvanic Cell	Electrolytic cell
	Half-Reaction at Negative Electrode	Reduction (So, this is the Cathode)	Oxidation (So, this is the Anode)
Specific to Lithium Batteries	Example Half-Reaction at Negative Electrode	$C_6 + Li^+ + e^- \rightarrow LiC_6$	$LiC_6 \rightarrow C_6 + Li^+ + e^-$
	Mechanism at Negative Electrode	Lithiation	De-lithiation

Figure 4. Language for generalizable and lithium-based properties of electrochemical cells at the negative electrode. These terms switch depending on the direction of the reversible reaction – charging and discharging. The negative electrode is the same – the C_6 carbon scaffold in a Li-ion system – regardless of directionality. Conversely, the “anode” and “cathode” designations switch depending on directionality, making them inappropriate terms for describing electrodes in secondary batteries.

	LITHIATION MECHANISM		
	Intercalation	Conversion	
		Type A	Type B
Examples [12]	Graphite, LTO, MOF	Li_2O , MnO , MgH_2	Si, Sn, Ge, Zn, Cd, Pb, P, Sb
Lithiation Mechanism	Intercalation	Diffusion	Alloying
Storage sites	Pores	Metallic vacancies	
Reason for expansion	Overfilling porous sites Strain on electrode	Lack of vacancies Electroplating	

Figure 5. Language for distinguishing mechanisms of lithiation at negative electrodes in lithium-based batteries.

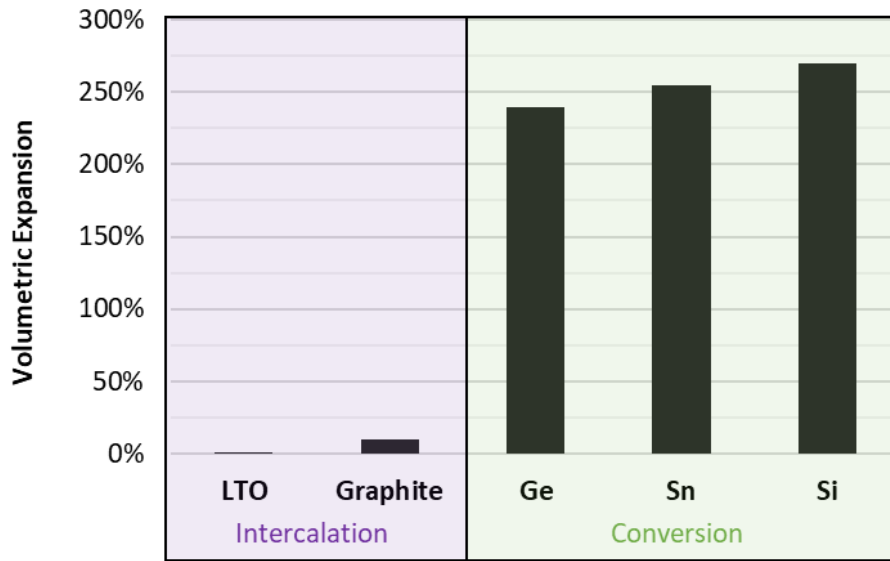


Figure 6. The reported volumetric expansion of commercially available Li-ion negative electrodes, distinguished by lithiation mechanism, as described in Figure 5. Data source: [12]

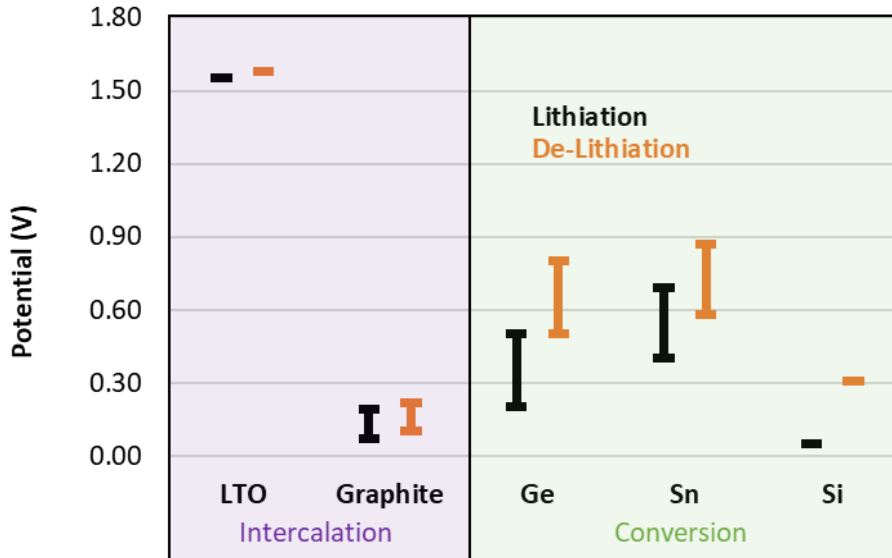


Figure 7. The lithiation and de-lithiation potentials of commercially available negative electrodes for lithium-ion batteries. Negative electrodes are grouped by lithiation mechanism described in Figure 5. Data source: [12]

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