Cost and performance analysis as a valuable tool for battery material research

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Cost and performance analysis is a powerful tool to support material research for battery energy storage, but it is rarely applied in the field and often misinterpreted. Widespread use of such an analysis at the stage of material discovery would help to focus battery research on practical solutions. When correctly used and well detailed, it can effectively direct efforts towards selecting appropriate materials for commercial applications. Using sodium-ion batteries as an example, we simulate the energy density and the cost of battery packs with several sodium-ion cathode materials taken from the literature in three case studies that illustrate how to identify the most promising solutions from the results of the model. Using publicly available information on material properties and open-source software, we demonstrate how a battery cost and performance analysis could be implemented using typical data from laboratory-scale studies on new energy storage materials.

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Introduction

The analysis of cost and performance is a crucial aspect of battery research, as it provides insights and guidance for researchers and industry professionals on the current state and possible future of electrochemical energy storage[1–5]. Typically, cost and performance analysis has been used with a high-level approach that addresses the directions that battery technology should take to achieve specific targets of energy density and price without focusing on specific materials or using actual experimental data, but by making assumptions on the properties that batteries have (or should have)[6].

By contrast, an accurate low-level approach that focuses on the implementation of cost and performance analysis in the material discovery phase is seldom seen[7–10]. Even when cost and energy density estimations for new materials are given, very simplistic calculations and assumptions are often done. For example, estimating the energy density of a new cathode material by multiplying the maximum obtainable specific capacity by the average voltage value gives only a partial, optimistic picture of the true energy density that can be achieved by a battery cell with such a cathode in realistic conditions. Similarly, it is an oversimplification to assume that a cathode material with low-price precursors translates automatically into an inexpensive battery pack, without considering the share of the cathode cost in the whole system, or how the conditions for scale-up to a commercial solution influence the final cost[11]. But if properly applied, cost and performance analysis can effectively support the research of new energy storage materials, such as those being explored as complementary solutions or substitutes to lithium-ion batteries.

Lithium-ion batteries represent the state-of-the-art battery technology for energy storage, currently enabling the shift to a sustainable society through the widespread use of electric vehicles and renewable energy[12,13]. However, predictions about the necessary capacity to achieve a full mobility electrification and support photovoltaic and wind power plants point to tenths of terawatt hours in the next 30 years[5,14]. The strains on battery supply chains owing to this continuously growing demand are already evident, with the prices of many raw materials having increased consistently over the past few years[15]. Therefore, much effort is being dedicated to researching new battery chemistries that can rely on cheaper and more homogeneously distributed raw materials while still offering comparable performance[16,17].

Sodium-ion batteries[18,19], lithium–sulfur batteries[20,21], multivalent cation batteries[22,23], dual-ion batteries[24], halogen batteries[25] and organic batteries[26–28] are among these alternative solutions. Each battery chemistry has its own advantages and disadvantages, but sodium-ion batteries are at present the only new chemistry near the commercialization stage, with both startups and established companies producing practical cells on the amp hour scale[29,30]. In the quest to find viable solutions, and with the plethora of new materials proposed as cathodes and anodes, exaggerated claims about electrochemical performance and projected costs often occur[31–34]. This leads to baseless assertions and sensational headlines, in a moment when battery energy storage is in the spotlight thanks to the exponential growth of its market. If reiterated, this could undermine the credibility not only of the research area but also of the entire industry.

The use of cost and performance analysis in research could be a way to put the results obtained in a laboratory setting in the right perspective. But to obtain sound outcomes, such an analysis requires a comprehensive understanding of battery manufacturing processes: setting a cell format (pouch, cylindrical, prismatic) and designing the full battery pack accordingly, considering the electrical cables and the thermal management system, modelling the investment and operating cost of a production plant, and so on. Nowadays, peer-reviewed open-source tools such as BatPaC and CellEst that enable this level of analysis are available, allowing a detailed simulation of the price and size of commercial-scale battery packs (applicable to closed systems only, not open like lithium–air or analogous solutions) that starts from the definition of the electrochemical and physical properties of the cathode and anode materials[35,36]. Such software can empower every researcher in the field to assess the performance of their newly synthesized materials in an upscaled system using the experimental data as input and to compare them with commercial chemistries or with other innovative solutions. Moreover, these tools can support the planning and design of experiments by preliminarily assessing the potential impact of modifications to the anode, cathode or electrolyte that are carried out to improve battery capacity and voltage. This process helps researchers to critically evaluate whether it is worth undertaking potentially complex and/or expensive treatments.

To illustrate how a low-level approach to cost and performance analysis can be a valuable tool for battery material research, this Perspective explores three case studies on sodium-ion battery packs using comprehensive software for cost and energy density modelling (BatPaC 5.0)[36,37]. The objective is to illustrate how to select the most promising active materials, or to identify treatments to improve their performance, for further experiments and investigation. We do this by quantitatively analysing the results of these simulations, assessing as examples the effects of lower cut-off voltage and pre-sodiation strategies on the cost and energy density of sodium-ion batteries.

Case studies

Our analysis draws from published works on sodium-ion batteries, using experimental data retrieved from the literature (Supplementary Table 1). Each case study considers three cathode materials, while the anode material used in all cases is hard carbon. Among all the metrics provided by the simulations, the focus is placed on the pack gravimetric and volumetric energy densities (in Wh kg^{-1} and Wh l^{-1}), and pack cost per kWh (in US\$ kWh^{-1}), which are used to assess the size and cost of the resulting battery packs. For more details about the necessary data for the simulation, refer to Box 1 and the Supplementary Information. In Table 1, results of the simulations for the three case studies are reported. The energy density and cost of all the modelled battery packs and commercial lithium-ion batteries are compared in Supplementary Figs. 3–5.

Variation of lower cut-off voltage

The key to achieving (sodium-ion) batteries with good energy density and low cost is to develop cathode materials that can combine a high average working voltage with a high specific capacity. Equally important, the voltage should not excessively decrease while discharging the battery, as a battery pack must be designed to provide the required power performance even at a low state of charge. If the voltage sinks too much on discharge, the current must increase accordingly to keep the electric power (the voltage by current product) constant while in the low state of charge. All the cables and busbars connected to the current collectors must be bigger and heavier to withstand the increasing current without excessive heating and voltage drop, contributing to the energy density decrease of the battery pack. Moreover, there are limits related to the power electronics: the United States Advanced Battery

Box 1

Required data for cost and performance analysis

Simulation of the cost and energy density of battery packs requires a minimum set of data on the active materials to gain a preliminary understanding of their performance in a realistic configuration. This set includes specific capacity, voltage profile, density and material cost of the anode/cathode couple that will be simulated (see the figure).

Voltage profile and specific capacity. The voltage profile and specific capacity are typical data obtained from laboratory tests on coin cells or small pouch cells. It is advisable to use values obtained with low-current experiments, as the model will then calculate the losses owing to a C/3 current when simulating the battery operation (where the C-rate is a measure of charge or discharge rate relative to battery capacity). Therefore, it is recommended to conduct tests at a current of C/10 or lower and use these as input. Another option for the voltage curve is to perform measurements using the galvanostatic intermittent titration technique to obtain equilibrium voltage points for input into the program. Considering typical half-cell data, the discharge curve is the one required for the cathode and the charge curve is the one for the anode. The voltage behaviour of the full cell can be obtained by properly subtracting the latter from the former.

Density. The required density for the model is the true particle density of the active material, which excludes the volume of open pores inside the polycrystalline (secondary) powder particles and the open space between them. This property can be measured using, for instance, helium pycnometry. If measuring density directly is not possible owing to equipment limitations or material properties (such as sensitivity to the atmosphere or measuring gas), one can calculate the crystallographic density by using X-ray diffraction data on single crystals and fitting the diffractogram. This allows evaluation of the unit cell, its volume and the atoms it contains, enabling calculation of the material's density. Alternatively, if none of these methods is feasible, a reasonable density value can be assumed based on the material class being investigated and the related literature. For example, a particle density of 4.6–$5.0\,\mathrm{g\,cm^{-3}}$ is a good approximation for lithium-based layered oxide cathode materials. It is important not to use the 'tap density' of the material (the density obtained after mechanically tapping a container of the powder sample), which includes the void volume between packed particles as well as the porosity inside the particle.

Material cost. There are various methods available for cost estimation. For commercial materials, one can consult sources that track current prices of common precursors and materials used in the battery industr . If the material is not commercial, one can calculate the cost by modelling the synthesis process and considering the cost of reactants, along with a rough estimation of processing costs[15,67]. In such cases, it is crucial to use bulk quantities for reactant prices, rather than relying on speciality chemistry catalogues, as the latter will result in unrealistically high battery costs. This type of cost modelling becomes particularly valuable when analysing the impact of raw material prices on the studied materials or assessing the effects of variations in precursor prices on the final battery cost. Estimating the production costs can be challenging because of the diversity of reactions and production methods for battery materials, especially those in the early research stage. However, several publications suggest a plausible range of US$6–10 kg^{-1} for an initial estimate[4,35,67]. This estimate can be further refined with in-depth analyses of the production process. In cases where modelling the synthesis process is also unfeasible, owing for instance to a lack of bulk prices for the chemicals used, the final active material price may be (optimistically) assumed based on values typical of commercial materials, such as US$10–30 kg^{-1}. Subsequently, the effect of material price variations on the final battery cost can be assessed.

Battery pack design. The last fundamental component for modelling is the definition of a battery pack that needs to be simulated using the chosen materials. This involves selecting its rated capacity or energy, rated power and pack architecture (that is, the number of cells in series and parallel per module, the number of modules in series and parallel in the pack, and the number of packs in parallel). The ratio between the nominal power and the nominal energy of the battery determines the 'power-to-energy' ratio (P/E), which indicates whether the battery is designed for power or energy applications. The minimum dataset described above can be comfortably used to simulate high-energy battery packs (indicatively, $P/E < 1.5$). However, when simulating high-power battery packs, additional data are required, for instance the area-specific impedance of the battery at different states of charge and pulse durations, the conductivity of the electrolyte, or the kinetics of the electrochemical reactions at the electrodes. Therefore, for a preliminary assessment of the energy density and cost of a battery pack made with new materials, simulating high-energy battery packs requires fewer measurements and is more straightforward.
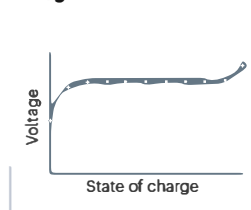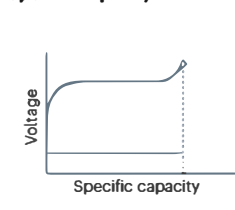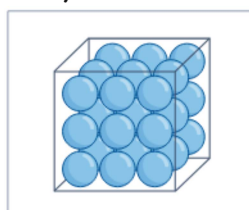
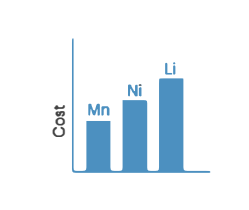Consortium (USABC) recommends that the minimum battery voltage should not be lower than 50–55% of its maximum voltage to stay within the working range of the power converters[38,39].

Nevertheless, the sodium-ion battery literature (and that of many other innovative post-lithium-ion chemistries) is full of examples of cathode materials with relatively high specific capacity that are cycled in large voltage windows, from about 4 V to well below 2.5 V. This feature is usually the result of voltage profiles with several plateaux and strong gradients. Commercial lithium-ion battery cathodes, instead, have a lower cut-off voltage between 2.5 V and 3.5 V, depending on the type of material. Also, they are characterized by high and gently sloping voltages, as in the nickel–manganese–cobalt or nickel–cobalt–aluminium families, or by single or double high-voltage plateaux, as in lithium iron phosphate and lithium manganese oxide[40]. These properties help to keep the power provided by the battery stable even at a low state of charge.

Moreover, the anode materials of choice for sodium-ion batteries are hard carbons – that is, disordered carbonaceous materials where sodium ions can be reversibly stored in their closed nanoporous and graphitic domains[41]. Hard carbon anodes are characterized by a voltage profile that combines a plateau region around 0.1 V (versus Na^+/Na) and a sloping region where the voltage rises gradually to about 1.5 V (versus Na^+/Na)[42]. When a sodium-ion cathode and anode are combined in a full cell, the anode's sloping voltage region causes a progressive drop of the battery voltage from the mid to low state of charge of the battery, regardless of the voltage profile of the cathode. This effect is not present in commercial lithium-ion full cells, where the graphite anode voltage rises steeply only for extremely low states of charge[43]. Hence, sodium-ion batteries are even more affected than lithium-ion batteries by a drop in the voltage towards the end of discharge. A strongly sloping voltage can be found also in other classes of negative electrodes still in the research phase, such as conversion-alloying materials[44] and organic anodes[45].

The voltage window in which a sodium-ion battery is cycled is, then, a fundamental parameter not only for the stability of the electrodes and the capacity retention[46], but also for the design of the battery pack. By increasing the lower cut-off voltage of the battery, its average voltage is increased and there are benefits related to the battery pack architecture, but this comes at the expense of the available capacity.

A material with a large specific capacity fraction delivered at low voltages could then have the same or even worse overall performance in battery packs compared with a lower-capacity material that lies entirely at higher and more stable voltage values.

To study the effect of this variable, we varied the lower cut-off voltage of each battery (comprising a cathode material and a hard carbon anode) and simulated the cost and energy density. The cut-off voltage targets used are either 55% of the maximum cell voltage (as in USABC specifications) or 1.5 V, which was reported as a typical minimum cell voltage in recent publications and datasheets on commercial sodium-ion batteries[47]. The material subjects of this analysis are the maricite-phase $NaFe(PO_4)$ (NFP)[48]; $Na[Ni_{0.3}Fe_{0.4}Mn_{0.3}]O_2$ (NFMO), an O3-phase layered oxide[49]; and $Na_3V_2(PO_4)_2F_3$ (NVPF), a vanadium-based polyanionic compound[50].

Looking at Fig. 1 and the results in Table 1, we can observe how the three materials are affected in very different ways by the minimum cut-off voltages, depending on their cathode voltage profile. The higher the slope, the larger is the lost capacity associated with the targeted cut-off voltage, which is detrimental for the performance of the pack. The removal of this capacity comes, however, with an increase of the average operative voltage, which is beneficial for the energy density. The relative impact of these two effects depends on the shape of the voltage curve. For instance, the average voltage of the NFP battery increases from 2.17 V to 2.58 V (+19%) or 2.88 V (+33%) when setting the cut-off to 1.5 V or to 55% of the maximum voltage (later referred to as USABC cut-off voltage or USABC target), respectively. However, the stronger effect of the two is the capacity drop: in fact, there is a 10% decrease in pack gravimetric energy density (and a 9.2% pack cost increase) for the 1.5-V cut-off, respectively rising to a 26.6% decrease (and 31.1% cost increase) for the USABC cut-off voltage. The NFMO-based battery already has an initial cut-off voltage of 1.3 V, so raising it to 1.5 V does not cause a relevant drop of the pack metrics (approximately 2% capacity loss). With the USABC cut-off voltage of 2.09 V, the capacity decreases more than 17%. However, the average cell voltage increases only 7%, resulting in a 9.1% decrease of pack energy density and a cost increase of 8.6%. Finally, the NVPF battery shows an initial lower cut-off voltage very near to the USABC target (2.30 versus 2.37 V), and its increase to this value causes virtually no detrimental effect on the battery pack performance.

Table 1 | Results of simulations for case study on variation of lower cut-off voltage

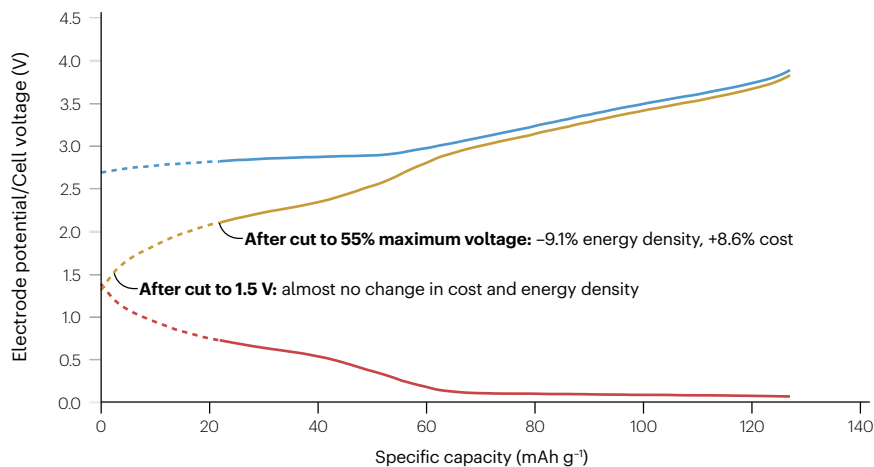| Material	Lower cut-off voltage target	Lower cut-off voltage (V)	Pack volumetric energy density (Wh l⁻¹)	Pack gravimetric energy density (Wh kg⁻¹)	Pack cost per kWh (US$)	Capacity loss after cut (%)	Battery average voltage (V)
$NaFe(PO_4)$	Initial value	0.30	157.0	84.2	156.9	0.84[a]	2.17
	1.5 V	1.50	141.4	75.7	171.4	26.95	2.58
	USABC target	2.28	116.3	61.8	205.7	48.53	2.88
$Na[Ni_{0.3}Fe_{0.4}Mn_{0.3}]O_2$	Initial value	1.30	208.4	108.0	136.9	0.26[a]	2.77
	1.5 V	1.50	207.0	107.2	137.7	2.02	2.80
	USABC target	2.09	190.4	98.1	148.6	17.46	2.97
$Na_3V_2(PO_4)_2F_3$	Initial value	2.30	199.9	106.0	158.9	0.36[a]	3.61
	1.5 V	–	–	–	–	–	–
	USABC target	2.37	199.3	105.7	159.3	0.99%	3.62

USABC, United States Advanced Battery Consortium. [a]The capacity loss at the initial value of cut-off voltage is greater than 0 because this initial cut-off voltage was slightly adjusted to obtain a round number.
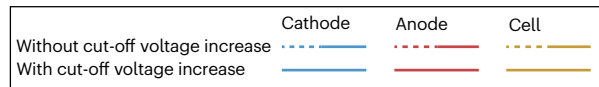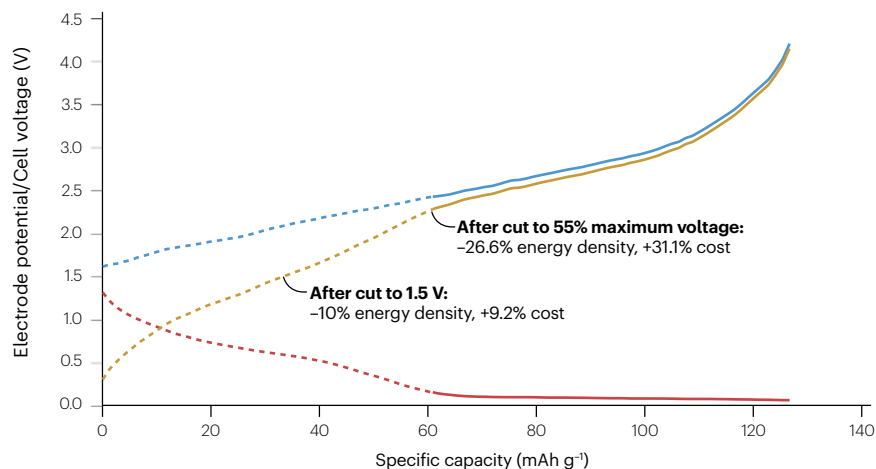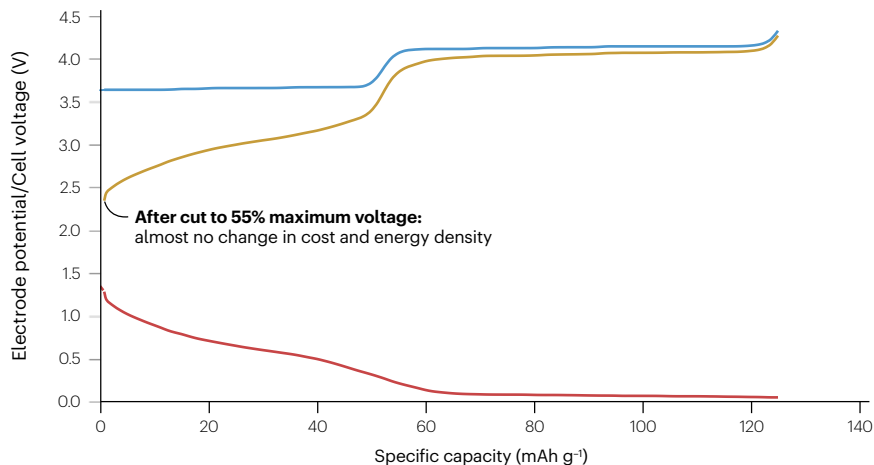
Fig. 1 | Electrode potentials of cathode and anode and resulting cell voltages of the materials analysed in the lower cut-off voltage study. The materials analysed are NaFe(PO$_4$) (panel **a**), Na[Ni$_{0.3}$Fe$_{0.4}$Mn$_{0.3}$]O$_2$ (panel **b**) and Na$_3$V$_2$(PO$_4$)$_2$F$_3$ (panel **c**). The dashed line represents the part of battery voltage and capacity removed after the increase of the lower-cut-off voltage to the USABC target of 55% of the maximum voltage.

From the above, it is clear that there are limitations in terms of available capacity when considering practical cut-off voltage restrictions to limit the voltage drop during discharge. However, in many reports, (sodium-ion) battery cathode materials are cycled within a very wide voltage range. Considering this, it is recommended to calculate the actual battery voltage curve after coupling with a suitable anode material. Then, when reporting the capacity and energy density achievable with a specific cathode material, it is crucial to consider the cut-off voltage limitations. This approach ensures that the evaluated performance of the materials aligns more closely with realistic applications, helping the selection of new materials for use in cells and, ultimately, battery packs. A decrease in performance owing to higher cut-off voltages, if reasonably limited, may be acceptable if it yields strong benefits in the pack architecture, as in the 1.5-V cut-off case for NFP and the 2.09-V cut-off case for NFMO, where the relevant metrics suffer a change lower than 10%.

Pre-sodiation to increase capacity of cathode materials

Some sodium-ion cathode materials are synthesized with less than the maximum sodium content – for instance, materials in the P2-phase layered oxide class[51], and certain polyanionic compounds[50]. Consequently, their complete capacity cannot be harvested without the addition of sodium to their structure. However, in a metal-ion battery, the source of metal cations is the cathode, with the anode being in its discharged form when the battery is manufactured. Pre-sodiation is a treatment applied to the anode or cathode material that provides additional sodium ions to enable the cathode's full capacity to be used[52].

Electrochemical pre-sodiation of anodes and cathodes with sodium metal is possible at the laboratory scale, but it is not regarded as a scalable and industrially viable pathway. Solutions that can be easily used in the roll-to-roll production process, such as chemical treatments in baths (so far reported only for lithium-based systems), are interesting for the anode side[53–55]. The pre-sodiation of cathodes with sacrificial salts may be another viable approach: during the first charge of the battery, the electrochemical decomposition of the sacrificial salt, assumed here to be sodium oxalate, results in sodium ions and gases as products, hence providing cations that can be used for full sodiation of the cathode structure[56–59]. This comes at the expense of porosity of the positive electrode, which increases owing to the void space left behind by the decomposition of the sacrificial salt. Salts that

are compatible with the solvents used during the electrode processing can be used, and the gases generated by the reaction are then evacuated from the cell after the formation cycles.
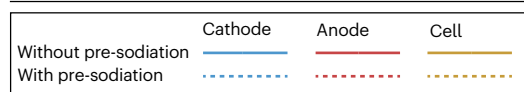
However, the capacity unlocked by pre-sodiation in these partially sodiated cathode materials resides primarily at low potentials, typically below 2.5 V. Therefore, the energy that can be extracted from this additional capacity is lower than that already present in the as-synthesized cathode material, in particular considering the additional drop caused by the sloping region of the hard carbon anode. An assessment of the energy density and cost of the battery, both with and without the pre-sodiation treatment, is essential to determine the utility of this strategy for increasing the cathode capacity.

Here, we simulate two scenarios: a sacrificial salt addition in the cathode, which increases its porosity; and an 'ideal' pre-sodiation of the anode. The latter method does not induce a detrimental porosity increase and is assumed to be an inexpensive strategy implemented in the roll-to-roll processing of the anode. These represent the worst- and best-case scenarios, respectively, for assessing the impact of this treatment on the energy density and cost of battery packs. The cathode materials chosen for the study, all requiring additional sodium to fully exploit their capacity, are $Na_3V_2(PO_4)_2FO_2$ (NVPFO), an oxygen-substituted NVPF[50]; and $Na_{0.6}[Ni_{0.22}Al_{0.11}Mn_{0.66}]O_2$ (NNAMO)[60] and $Na_{0.6}[Ni_{0.22}Fe_{0.11}Mn_{0.66}]O_2$ (NNFMO)[61], both P2-phase layered oxides. The calculations regarding the pre-sodiation with sacrificial salt are described in the Supplementary Information.
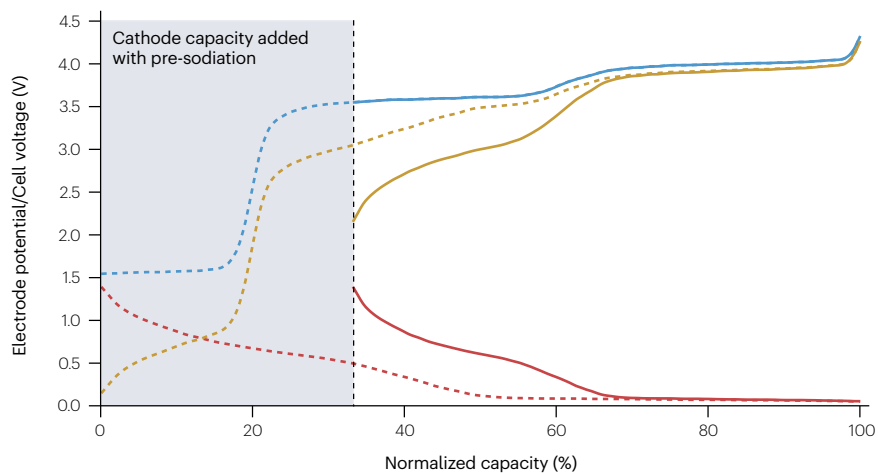
The results of the simulations (Table 2) demonstrate that the battery performance is improved in the best-case scenario, with an increase in volumetric and gravimetric energy density of at least 3.5% and 9%, respectively, and a cost decrease per kilowatt hour of the battery pack of at least 11%. This improvement holds true for pre-sodiation of the anode across all three batteries tested, under the most optimistic hypothesis. However, with the use of sacrificial salt in the cathode, the energy densities decrease below the non-pre-sodiated case. The increase in capacity, which is almost 50% for NVPFO and more than 60% for the two layered oxides, is not sufficient to counteract the increase in porosity caused by the presence of sacrificial salt. An increase of porosity results in more void space in the battery that has to be filled with electrolyte, decreasing the compactness of the battery and increasing the weight (and cost) due to inactive components (current collectors, separator, electrolyte, hardware)[15]. Nevertheless, the cost of the pack

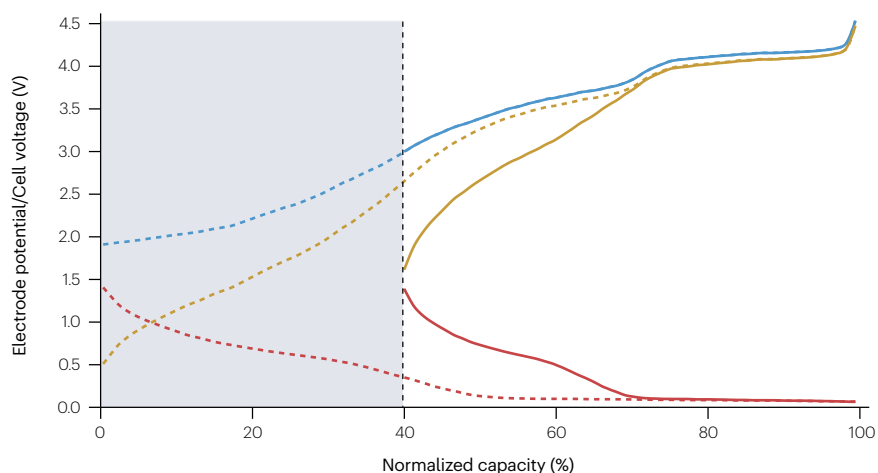**Table 2 | Results of simulations for case study on pre-sodiation for increasing capacity of cathode materials**

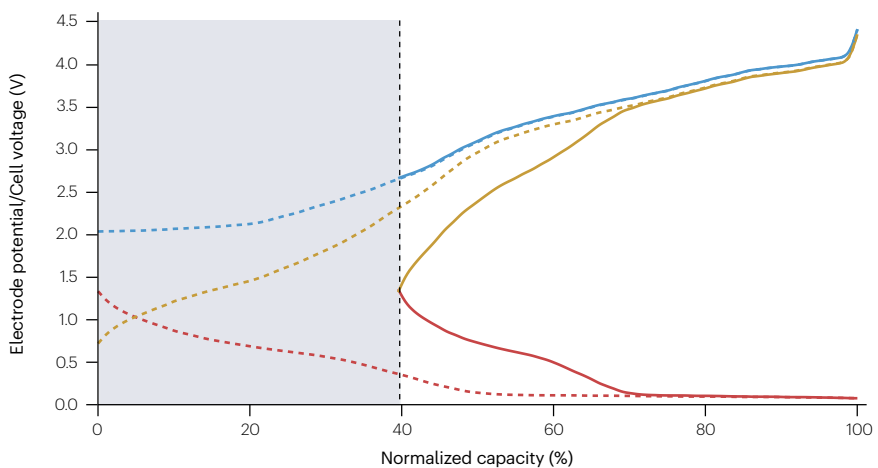| Material	Pre-sodiation	Lower cut-off voltage (V)	Pack volumetric energy density (Wh l⁻¹)	Pack gravimetric energy density (Wh kg⁻¹)	Pack cost per kWh (US$ kWh⁻¹)	Capacity gain with pre-sodiation (%)	Battery average voltage (V)
$Na_3V_2(PO_4)_2FO_2$	No	2.15	203.4	108.4	161.7	–	3.47
	Yes (anode)	0.15	214.3	118.1	142.3	49.6	2.98
	Yes (cathode)	0.15	196.8	110.3	148.0	49.6	2.98
$Na_{0.6}[Ni_{0.22}Al_{0.11}Mn_{0.66}]O_2$	No	1.60	230.6	119.2	126.0	–	3.43
	Yes (anode)	0.50	238.8	129.9	111.9	66.9	2.83
	Yes (cathode)	0.50	209.5	117.3	119.7	66.9	2.83
$Na_{0.6}[Ni_{0.22}Fe_{0.11}Mn_{0.66}]O_2$	No	1.30	211.8	108.5	138.0	–	3.17
	Yes (anode)	0.70	221.7	119.7	120.8	66.4	2.65
	Yes (cathode)	0.70	194.7	108.3	129.1	66.4	2.65

Fig. 2 | Electrode potentials of cathode and anode and resulting cell voltages of the materials analysed in the study of pre-sodiation for capacity increase of cathode materials. The materials analysed are $Na_3V_2(PO_4)_2FO_2$ (panel **a**), $Na_{0.6}[Ni_{0.22}Al_{0.11}Mn_{0.66}]O_2$ (panel **b**) and $Na_{0.6}[Ni_{0.22}Fe_{0.11}Mn_{0.66}]O_2$ (panel **c**). The light grey region represents the part of cathode capacity that is added by the pre-sodiation. The capacity is normalized by dividing by the specific capacity with pre-sodiation of the cathode material.

a $Na_3V_2(PO_4)_2FO_2$

b $Na_{0.6}[Ni_{0.22}Al_{0.11}Mn_{0.66}]O_2$

c $Na_{0.6}[Ni_{0.22}Fe_{0.11}Mn_{0.66}]O_2$

is still lower than the base case, because the quantity of (expensive) active materials required to achieve the target pack energy reduces thanks to the higher capacity.

Moreover, it is observed that for all materials, the average battery voltage substantially decreases after both types of pre-sodiation. For instance, in the case of NVPFO, it drops from 3.47 V to 2.98 V, a 14% decrease. This is also evident in Fig. 2, where the capacity added by the pre-sodiation of the cathode is highlighted in light grey. For NVPFO, the added capacity consists mostly of a plateau at around 1.5 V, which, after subtraction of the anode voltage, falls well below 1 V. In the case of the two layered oxides, the capacity unlocked by pre-sodiation lies between 2.5 and 2 V, resulting in a sharply sloping profile of the battery voltage that ends with a cut-off below 1 V. As a result, after integrating the area below the curve and dividing by the capacity of the battery, the average voltage decreases considerably, which is detrimental to the energy and cost of the battery. Lastly, note that the cut-off voltage after pre-sodiation is much lower than both the 1.5-V and USABC targets discussed in the case study on varying the lower cut-off voltage. Therefore, when considering cut-off voltage limits, it becomes questionable whether all or part of this additional capacity can be used.

In summary, based on the results of this case study, we recommend a critical discussion of the voltage at which the capacity obtained from pre-sodiation (or, more broadly, from the addition of cations to enhance the capacity of active materials) is situated. Modelling the impact of the cathode capacity increase with a cost and performance model can provide valuable support for studies aimed at quantitatively assessing the improvements resulting from such treatments.

Pre-sodiation to compensate for first-cycle sodium loss

Pre-sodiation strategies can also be used to overcome the loss of sodium during the first cycle of the battery. Hard carbon anodes tend to have substantially lower initial Coulombic efficiency than graphite anodes (typically <85% compared with >90%), owing to the high material surface area and defects that lead to increased formation of the solid electrolyte interphase[62,63]. Such a low initial Coulombic efficiency causes the loss of a considerable part of the available battery capacity, as the cathode is the source of sodium in the cell, providing the necessary cations to form the solid electrolyte interphase on the hard carbon.

It is then interesting to use cost and energy density analysis to examine the impact of compensating for the initial-cycle sodium loss, specifically the effect on battery pack performance that results from improving initial Coulombic efficiency with pre-sodiation − a technique that, as described in the previous section, entails several complications during battery production.

For this case study, we selected three additional cathode materials from different classes, each with distinct physical and electrochemical properties: $Na_3Fe_2(PO_4)_3$ (NFPO), an iron-based polyanionic compound[64]; $Na_{0.95}[Ni_{0.32}Mn_{0.32}Mg_{0.16}Ti_{0.21}]O_2$ (NNMMTO), an O3-phase layered oxide[29]; and $Na_2Mn[Fe(CN)_6]$ (NMFCN), a Prussian blue analogue[65]. The detailed methodology for the simulations is provided in the Supplementary Information.

Based on the results of the simulations (Table 3), it is evident that the battery performance is consistently improved by the compensation for first-cycle sodium loss. This improvement holds true for all the cases of anode pre-sodiation in this study. In the case of sacrificial salt addition in the cathode, a decrease in pack volumetric energy density is observed for NNMMTO only.

In the best-case scenario, there is a minimum increase of 4% and 4.4% percent in volumetric and gravimetric energy density, respectively, while the cost per pack decreases by at least 5%. Because the added capacity with the pre-sodiation in this case is notably lower than the capacity increase observed in the previous case study, the improvements in relevant metrics are comparatively limited. Nevertheless, the average voltage decreases only slightly in this case, especially for NMFCN, which features a high-voltage plateau. With NMFCN, the capacity recovered with the sodium compensation lies at a relatively high voltage compared with the other two materials (Fig. 3). Consequently, it experiences a relatively greater improvement owing to the shape of its voltage profile.

NMFCN is also minimally affected by using the sacrificial salt as a pre-sodiation additive and is only marginally penalized compared with the best-case scenario provided by anode pre-sodiation. This may be attributed to its inherently low density, around 1.8 g cm^{-3}, which is even lower than the density of the sacrificial salt used (sodium oxalate, 2.34 g cm^{-3}). As a result, the space occupied in the positive electrode by the sacrificial salt is limited compared with the space occupied by the active material itself. Pre-sodiation with sacrificial salt is beneficial to all three performance metrics for NFPO, a material that also has a rather low density (3.4 g cm^{-3}). By contrast, in the case

**Table 3 | Results of simulations for case study on pre-sodiation for compensation of first-cycle sodium loss**

Material	Pre-sodiation	Lower cut-off voltage (V)	Pack volumetric energy density (Wh l^{-1})	Pack gravimetric energy density (Wh kg^{-1})	Pack cost per kWh (US$ kWh^{-1})	Capacity gain with pre-sodiation (%)	Battery average voltage (V)
$Na_3Fe_2(PO_4)_3$	No	0.70	147.5	77.1	173.1	–	2.39
	Yes (anode)	0.45	153.3	81.4	163.4	16.8	2.29
	Yes (cathode)	0.45	150.0	79.9	165.5	16.8	2.29
$Na_{0.95}[Ni_{0.32}Mn_{0.32}Mg_{0.16}Ti_{0.21}]O_2$	No	1.30	205.6	104.0	143.9	–	3.00
	Yes (anode)	0.70	211.4	108.6	137.2	15.4	2.88
	Yes (cathode)	0.70	204.2	106.0	138.9	15.4	2.88
$Na_2Mn[Fe(CN)_6]$	No	1.95	159.3	99.3	130.3	–	3.11
	Yes (anode)	0.70	168.4	105.2	121.9	14.4	3.05
	Yes (cathode)	0.70	165.7	103.6	123.2	14.4	3.05
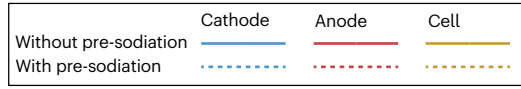
a $Na_3Fe_2(PO_4)_3$
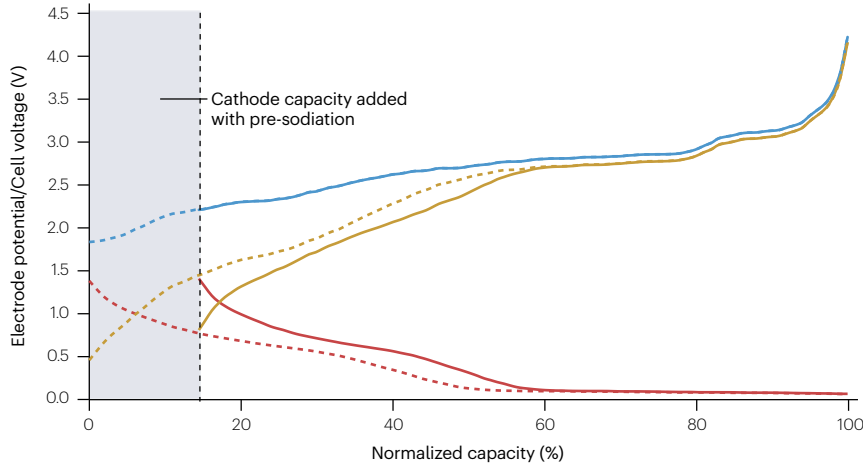
b $Na_{0.95}[Ni_{0.32}Mn_{0.32}Mg_{0.16}Ti_{0.21}]O_2$
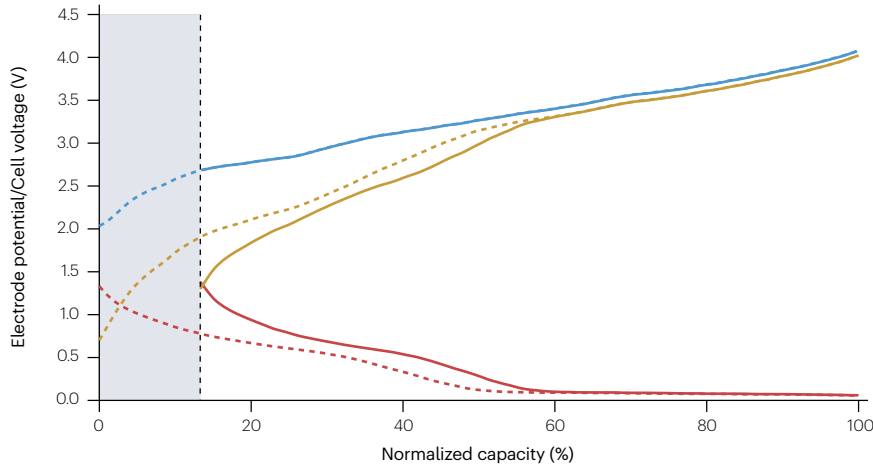
c $Na_2Mn[Fe(CN)_6]$
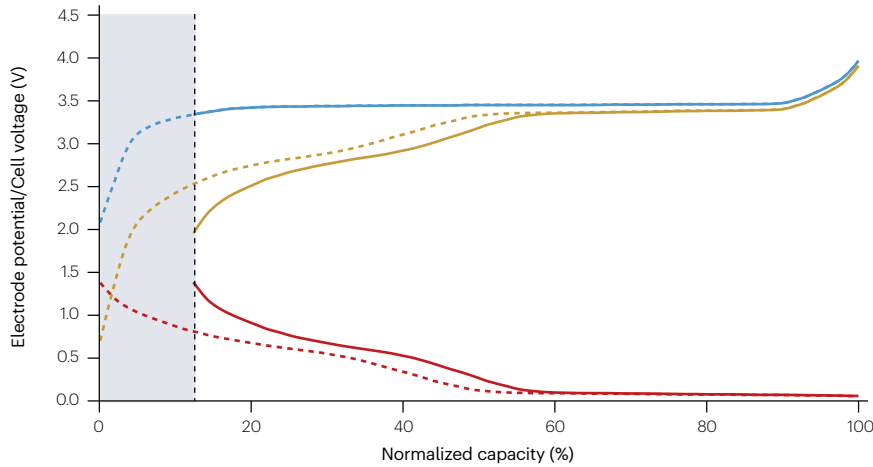
Fig. 3 | Electrode potentials of cathode and anode and resulting cell voltages of the materials analysed in the study of pre-sodiation for first-cycle sodium loss compensation. The materials analysed are $Na_3Fe_2(PO_4)_3$ (panel **a**), $Na_{0.95}[Ni_{0.32}Mn_{0.32}Mg_{0.16}Ti_{0.21}]O_2$ (panel **b**) and $Na_2Mn[Fe(CN)_6]$ (panel **c**). The light grey region represents the part of cathode capacity that is added by the pre-sodiation. The capacity is normalized by dividing by the specific capacity with pre-sodiation of the cathode material.

of NNMMTO, characterized by a density of 4.4 g cm^{-3}, the increase in porosity caused by the salt inclusion in the cathode coating outweighs the capacity gains.

In summary, the simulation of cost and energy density has provided insights into the effectiveness of compensating for the initial sodium loss through pre-sodiation. Such an analysis can be applied to determine whether it is worth conducting pre-sodiation studies on a specific active material and to quantify the actual improvements in the metrics of the final battery. If the capacity that is recovered is situated at a high voltage, the capacity increase is indeed beneficial for the final battery pack performance. The use of sacrificial salts may be more appropriate for active materials that are already characterized by low density, as, in this case, the impact of porosity increase is limited compared with the benefits of capacity recovery.

Outlook

These examples of a low-level cost and performance analysis with experimental data drawn from literature, using modelling approaches that simulate cost and energy density, show how to systematically assess the potentiality of a wide range of battery materials in rather complex scenarios such as pre-sodiation or voltage limitations. The results of the case studies underscore the importance of aligning material performance with practical application requirements, allowing the proper selection of materials suitable for battery pack integration.

This type of techno-economic modelling does not inherently account for the impact of the battery pack's cycle life, which needs a separate evaluation. However, the analysis serves as a useful starting point for comparing and assessing battery materials, assuming optimistically that stability is not a limiting factor.

The described methodologies are not restricted to the realm of sodium-ion batteries: the simulations are 'blind' to the class of the energy carrier, as they require only a voltage profile and some physical and electrochemical properties. The outlined guidelines can be adapted and extended to all types of battery chemistries, from lithium-ion batteries to multivalent cations and organic materials.

Implementing this approach consistently in laboratory-scale research could help to focus efforts on the most promising options in the vast landscape of possible battery materials, towards practical solutions for the future of energy storage.

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Author contributions
A.I. and S.P. conceived the idea. A.I. and S.B. read and summarized the relevant literature, carried out the simulations, analysed the results and visualized the data. A.I. wrote the original draft. S.P. revised the original draft, supervised the project and acquired the funding.

Competing interests
The authors declare no competing interests.