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A Minimal Information Set To Enable Verifiable Theoretical Battery Research

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Batteries are an enabling technology for addressing sustainability through the electrification of various forms of transportation[1] and grid storage.[2] Batteries are truly multi-scale, multi-physics devices, and accordingly various theoretical descriptions exist to understand their behavior[3−5] ranging from atomistic details to techno-economic trends. As we explore advanced battery chemistries[6,7] or previously inaccessible aspects of existing ones,[8−10] new theories are required to drive decisions.[11−13] The decisions are influenced by the limitations of the underlying theory. Advanced theories used to understand battery phenomena are complicated and require substantial effort to reproduce. However, such constraints should not limit the insights from these theories. We can strive to make the theoretical research *verifiable* such that any battery stakeholder can assess the veracity of new theories, sophisticated simulations or elaborate analyses. We distinguish *verifiability*, which amounts to "Can I trust the results, conclusions and insights and identify the context where they are relevant?", from *reproducibility*, which ensures "Would I get the same results if I followed the same steps?" With this motivation, we propose a checklist to guide future reports of theoretical battery research in Table 1. We hereafter discuss our thoughts leading to this and how it helps to consistently document necessary details while allowing complete freedom for creativity of individual researchers. Given the differences between experimental and theoretical studies, the proposed checklist differs from its experimental counterparts.[14,15] This checklist covers all flavors of theoretical battery research, ranging from atomic/molecular calculations[16−19] to mesoscale[20,21] and continuum-scale interactions,[9,22] and techno-economic analysis.[23,24] Also, as more and more experimental studies analyze raw data,[25] we feel this checklist would be broadly relevant.

Fundamentally, any theory makes predictions based on assumptions about the system and appropriate inputs characterizing its response. *Theory* is used here as a catch-all term to include theories, analyses, models and simulations—be it physics-based or data-driven or a combination of the two. Of all possible theories, *a useful theory tells us something that we do not already know from the raw data* (experimental or otherwise). As shown in Figure 1, any theory can be expressed as a function with specific physicochemical context as inputs and corresponding predictions as an output. Most advanced theories do no afford analytical solutions and we invariably resort to numerical computations (which introduces additional information that has to be parsed appropriately). Every reliably computed behavior exhibits negligible dependence on numerical parameters. This is ensured via independence tests in solutions of differential equations, e.g., mesh independence in finite element calculations,[26] or suitably correcting for numerical parameters, e.g., finite domain size corrections in molecular dynamics,[27,28] or other method-specific practices such as bias-variance trade-off in (statistical) machine learning models.[5,29] These aspects of computer simulation are equivalent to instrument calibration in experiments. They have to be performed to trust the results but are not necessarily reported explicitly. *What are the necessary computational details to ensure verifiability*? is the aspect we debated the most as we formulated this checklist. While domain experts are used to assessing the "reliability" in terms of aforementioned independence tests and the numerical solution steps, these tests and algorithms do not succinctly convey the information to the rest of the battery stakeholders. For instance, a continuum-scale modeler solving for the porous electrode theory does not typically understand the ion diffusivity predictions using molecular dynamics but does care if those predictions provide the continuum-scale diffusivities that can be used in the porous electrode theory. Essentially, the requisite information is the error introduced in the predictions related to the numerical parameters, and is included via Q4 in Table 1. In addition to being helpful to a broader battery community, such information is also straightforward to provide irrespective of using *in-house* or *open-source* codes or software packages for computations.

Open-source codes do play an important role in accelerating progress and reusability of simulations.[20] However, we are mindful of various constraints related to funding, trade, intellectual property, logistics, etc. that oftentimes require researchers to choose closed-source software. Open-source codes are, by themselves, neither necessary nor sufficient to ensure verifiable predictions. In order to accommodate a wider range of theoretical battery research, open-source codes are not required as a part of the checklist (Table 1).

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Table 1. Checklist To Report Theoretical Battery Studies

Manuscript Title:	
Submitting Author*:	
Question:	Y/N/NA[a]
1. Have you provided all assumptions, theory, governing equations, initial and boundary conditions, material properties (e.g., open-circuit potential) with appropriate precision and literature sources, constant states (e.g., temperature), etc.? **Remarks:**	
2. If the calculations have a probabilistic component (e.g., Monte Carlo, initial configuration in Molecular Dynamics, etc.), did you provide statistics (mean, standard deviation, confidence interval, etc.) from multiple (≥3) runs of a representative case? **Remarks:**	
3. If data-driven calculations are performed (e.g., machine learning), did you specify dataset origin, the rationale behind choosing it, what information it contains, and the specific portion of it being utilized? Have you described the thought process for choosing a specific modeling paradigm? **Remarks:**	
4. Have you discussed all sources of potential uncertainty, variability, and errors in the modeling results and their impact on quantitative results and qualitative trends? Have you discussed the sensitivity of modeling (and numerical) inputs such as material properties, time step, domain size, neural network architecture, etc. where they are variable or uncertain? **Remarks:**	
5. Have you sufficiently discussed new or not widely familiar terminology and descriptors for clarity? Did you use these terms in their appropriate context to avoid misinterpretation? Enumerate these terms in the "Remarks". **Remarks:**	

*I verify that this form is completed accurately in agreement with all co-authors, to the best of my knowledge. [a]Y ≡ the question is answered completely. Discuss any N or NA response in "Remarks".

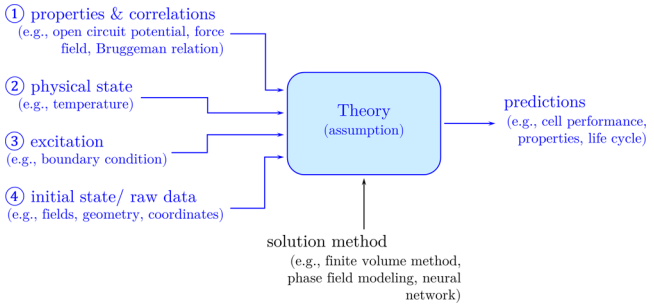

Figure 1. Any theoretical analysis can be expressed as a function that offers predictions specific to the physicochemical context, i.e., ①–④. Any reliable prediction is independent of the numerical details of the solution method.

The overarching goal of this checklist is to *maximize the utility of theoretical studies by clearly articulating the results as well as their scope of application*. A theory can be useful to

- a stakeholder using the generated insights to make decisions, e.g., an experimentalist choosing a material to synthesize, a program manager identifying a new research direction, a venture capitalist making investment decisions, etc., or
- a theoretician using the published theory, in part or in whole.

Except for a theoretician wholly using a published theory, its utility can be guaranteed by ensuring verifiability. As this is the most common use of any published theory, we focus on a *minimal information set* highlighting the critical details that strongly influences the theoretical predictions. For example, in a porous intercalation electrode study, if the ion diffusivity in the electrolyte is assumed to be smaller than the ion diffusivity in the active particles, the predicted electrode behavior would be very different compared to when the ion diffusivity in the active particles were more sluggish (as is usually the case). Accordingly, all material properties that appear in the theory (① in Figure 1) should be reported. Equivalent analogies can be drawn to discuss calculations at other scales. One should particularly justify unconventional inputs and assumptions in the manuscript rather than in the supporting text. Other relevant information is about the system's physical state ②, e.g., constant pressure versus constant temperature ensembles in molecular dynamics. Additionally, the initial configuration ④ and the specific type of excitation ③ are equally important to interpret the results, e.g., AC or DC resistance of an operating or non-operating battery examines very different aspects of the intricate battery response. These details also act to circumvent misinterpretation of the reported results. Depending on the theoretical context, not all the details on Table 1 or Figure 1 are necessarily relevant. For example, to interpret the data-driven models, it is the most important to report the details of the raw data that is used to build these models as well as model selection steps.[5] If the raw data attributes and assumptions of the analysis are sufficiently explained, it is straightforward for others to interpret the predictions, and specifically to answer, *What can this model predict?* Equivalently, if the theory contains probabilistic components, it is necessary to understand the statistical attributes of the predictions to identify pertinent insights. The checklist (Table 1) is merely a textual version of Figure 1. We acknowledge that researchers sometimes report just enough to build confidence in their results, and maintain competitive advantage in terms of proprietary models. We believe the proposed checklist accounts for this scenario and gives out enough details to be helpful without sacrificing proprietary interests.

An enticing thought is to require comparison with suitable experiments to bolster the relevance of theoretical predictions. We do agree that often the advances in modeling are motivated by a discrepancy between experimental observation and existing theory. Researchers should make efforts to compare their predictions with relevant experimental data, particularly when the two disagree. However, this is not always

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straightforward and often not at the same length and time scales. Experimental measurements can vary widely even when characterizing identical materials, for example, cation transference number in PEO electrolyte (Figure 1 in Rosenwinkel and Schönhoff[30]). Alternatively, for detailed models, often not all fields are accessible experimentally. For instance, a porous electrode theory predicts concentrations, potentials and current density distributions within the cells; while typically only the cell voltage is measured.[8] We also run into the risk of overfitting models just to show good comparison with experiments. Thus, *comparison with experiments* is useful in identifying the missing understanding, but is not necessary to report *verifiable* models.

Essentially, all theoretical models have their own limitations. Every model offers prediction given the assumptions and uncertainty in inputs. Our checklist is designed to clearly articulate this context to improve transparency and discourage misinterpretation. Also, we should be mindful of model utility beyond experimental comparison. In many cases, the theories are meant to offer insights and guidelines. The desired accuracy of these guidelines also differs widely and in turn, we have multiple models. For example, reduced-order models are more relevant for battery state estimation and controls, while porous electrode theory is meant to design porous electrodes. Thus, the verifiable model reporting is concerned with contextualizing model predictions.

How To Populate the Checklist. We envision authors of every new manuscript with theoretical elements to fill out this checklist (Table 1). This will also help the authors to report all relevant details in the manuscript. Additionally, the editors and reviewers can assess the completeness of the work using the corresponding checklist. It is worth noting that answering 'N' to any of the questions can be justified through an explanation in the "Remarks". Once published, we suggest that the filled-out checklist be a part of the Supporting Information and provide the necessary background to the readers. To give examples of filled-out checklists for different theoretical studies, each author populated a checklist for at least one of their published articles.[8,21,25,31−61] We aimed to cover many different types of battery modeling paradigms[4] in the author-populated checklists. It also serves as a good starting reference for battery modeling best practices and shortcomings. These are documented in the Supporting Information of this paper and should be helpful to future authors filling out new checklists. The readers are especially encouraged to read the "Remarks" on these examples.

Outlook. Thus, instead of an exhaustive, *nice-to-have*, reporting, for our checklist we choose the most influential, *need-to-have*, information concerning theoretical predictions. We believe this *minimal information set* will enable the broader battery community to verify theoretical results and make informed decisions. As an added benefit, forgetful battery researchers (present company included) no longer have to worry if we missed conveying something important as we pursue advanced theories and build more complex models.

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■ ASSOCIATED CONTENT

Supporting Information

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Filled-out example checklists covering different modeling types across scales (Figure 1 in Howey et al.[4]) and a summary table (PDF)

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Author Contributions

A.V. initiated the idea for the checklist. V.V. provided an initial framework and issued an open solicitation for feedback.[63] A.M., A.V., S.S., and V.V. developed the first version of the checklist. S.A.R., D.H., V.S., F.B.P., S.A., R.C., E.K., S.D., and V.R.S. provided detailed critiques, and S.A.R. proposed a new formatting for the checklist; all of the contributors listed here collectively reached a consensus on the checklist. R.T., R.K., Y.Z., P.D., W.L., S.G., Z.A., D.K., A.M.F., K.T., P.P., D.J.R., P.G, A.C., A.B., and C.D.S. filled out a checklist for their papers. All authors recognize the outsized role played by A.M. in coordinating the many challenging discussions to arrive at the final checklist.

Notes

Views expressed in this Energy Focus are those of the authors and not necessarily the views of the ACS.
The authors declare no competing financial interest.

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