

MACHINE LEARNING FOR QUANTUM ENERGY STORAGE APPLICATIONS: A SHORT REVIEW

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Abstract

Quantum energy storage is a rapidly growing research and development arena that ranges from highly speculative quantum batteries that may harness coherence and entanglement via quantum-mechanical modeling for the control and materials design of electrochemical storage devices. This work explore a total of few areas of application like use of reinforcement learning (RL) for the control of quantum-battery recharging protocols, the employment of variational quantum algorithms in the evaluation of extractable work, a quantum-enhanced sequence model for predicting state-of-health (SOH) and state-of-charge (SOC), the quantum-influenced control of grid-connected battery energy-storage systems (BESS) and the utilization of ML and quantum-assisted tools for discovery of battery materials and electrolytes. Besides comparing these different approaches across their effectiveness, one of the results is that RL-based policies. A lot outperform heuristic charging protocols which are static and do little more than charging. Also, quantum-enhanced recurrent networks show a reduction in prediction error of ten-fold compared to baseline classical ones. The combination of quantum-chemical descriptors together with graph neural networks and generative models in materials-discovery pipelines leads to the faster screening of electrolytes and solid-conductors far beyond even conventional trial-and-error approaches.

Keywords: Machine Learning, Quantum Energy Storage, Batteries, RL method, Strategy

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1. Introduction

Energy storage is the key to the worldwide switch toward electrified transportation and renewable-power dominated electrical grid systems. Lithium-ion batteries together with other electrochemical devices are the heart of mobile electronics, electric vehicles and utility grade renewable energy integration. But their long term reliability is limited by issues of capacity fading, thermal sensitivity and the limited amount of energy they can store. The demand for storage capacity is increasing while material cost and environmental cost must be minimized, the search for electrochemical innovations has given way to computational methods that can predict and optimize storage systems more effectively[1]. Classical machine learning methods like long short-term memory (LSTM) networks, convolutional neural networks and ensemble models have already done a remarkable job in forecasting degradation trends and estimating state-of-health (SOH), state-of-charge (SOC) by using data of cycling of the battery. But limitations like difficulty in handling

huge sizes of data, the need for data for training and inability to represent the electrochemical processes which are highly nonlinear are challenges these methods face. Meanwhile, there has been a parallel and quite separate line of questioning whether at the quantum level it is possible to imagine energy storage in a different way, resulting in the idea of a quantum battery. This is a device whose charging and discharging are not driven by ion movement but by the principles of quantum thermodynamics[2,3].

Quantum battery concept is a revolutionary approach that uses quantum coherence, quantum entanglement and collective many-body effects to store and retrieve energy in an entirely new way that cannot be accomplished with classical physics principles alone. Two major theoretical model families dominate the quantum battery concept area: cavity quantum batteries that store and release energy via control of interaction between the optical resonator and the battery. Spin-chain quantum batteries make use of entanglement among a set of coupled spin states just like in the

Dicke model. In one such model, many two-level systems are coupled to a common photon and the system rapidly charges up and the maximum work which could in principle be extracted increases as well[4]. Efficiency of these systems is generally quantified by ergotropy. Yet, the energy variance that define charging precision is also a vital factor here. Crafting the control fields that yield high ergotropy and minimize charging time and losses is a complex, high-dimensional optimization problem which grows beyond analytical tractability. In particular with the increasing size of the quantum systems. When the influence of the external factors like, for example, the decoherence effects and non-Markovian noise has been taken into account this complexity can be considered as the main feature that has been a limiting factor until recently in developing such batteries. This is why machine learning and more exactly reinforcement learning has recently become one of the central tools in the field of quantum battery research. Instead of trying analytically to find the very best control that has to fulfill all of the constraints, researchers are increasingly relying on learning methods where an agent learns the strategy through simulated interactions without the researchers themselves having to explicitly program these strategies[5,6]. Machine learning has already become a central element in the real implementation of batteries apart from its quantum aspects. Nowadays, one can find such tools that by taking in the data generated from the battery operation, help estimate its degradation and time still left without replacement. They are also useful from a practical standpoint to plan battery charging and discharging such that battery life is as long as possible and batteries are bidirectionally operated to work as energy storage systems in the renewable microgrids where they must reconcile generation electric vehicle charging demand and grid stability requirements[7]. There have been many exciting applications like that of finding suitable materials in which the machine learning models used descriptors of quantum-chemical reactions like formation enthalpies and HOMO-LUMO energy gaps which can be generated through density functional theory to search candidate electrolytes and solid-state ionic conductors across vast spaces of chemicals much more speedily than conventional trial-and-error synthesis method. These include graph neural networks, generative adversarial networks, as well as Bayesian optimization. In fact, these different techniques lead to the production of a few experimentally validated candidate electrolytes with high ionic and chemical conductivities and stabilities that have also been made by the researchers. Such discovery pipelines for materials are progressively introducing quantum-mechanical calculations right into the steps where data meets models in a machine learning process as a result

classical data-based modeling on one side and quantum-computing-inspired modeling on the other are now not only adjacent but practically inseparable. So, this trend will further open up a channel of communication and integration of quantum computing with battery materials science[8–10].

Machine learning today operates research in parallel threads such that the demarcation between the two is gradually becoming blurred. On quantum battery research, reinforcement learning has been an aid to develop charging protocols which outperform static heuristic strategies, whereas a kind of variational quantum algorithm executed on a so-called noisy intermediate-scale quantum (NISQ) computer directly calculates ergotropy and because of this one is not even able to perform quantum state tomography. For traditional battery engineering QML is the term used here and it includes models that are based on quantum kernel methods as well as a hybrid quantum-classical one where the classical circuit architecture is the recurrent one containing variational quantum circuits which can act as compact and also potentially more data-efficient alternatives to entirely classical networks for degradation detection and SOH estimation[11]. In fact one cannot even talk about the results being consistent or homogenous they were reported across these papers, a reinforcement learning policy yields tangible gains in ergotropy and charging accuracy even when partial-observability conditions are taken into account in such policies prediction errors of quantum-enhanced sequence models drop by a double-digit figure compared to classical references, as far as regression quantum kernel techniques are concerned, their performance is such that they achieve comparable level of accuracy with only a few times fewer training samples[10,12]. And quantum-motivated and physically transparent control architectures like entangled reservoir computing also depict how principles of quantum have been used as design methods for classical control systems without any dependence on physical quantum hardware. A lot of research has been done in quantum batteries but many papers are scattered over different disciplines like quantum thermodynamics, quantum computing, materials science and battery engineering with rarely any attempt to put results together or determine how far the advantages obtained are when different methods baselines and datasets are used[13][14].

2. Learning approaches

2.1 Quantum batteries and quantum thermodynamics

A quantum battery is a kind of energy storage system that involves charging and discharging dynamics being determined not by the conventional electrochemistry but by quantum thermodynamics.

In fact, the two main model types in the literature are cavity quantum batteries, where energy is stored or released via the controlled interaction between the battery and a quantum cavity or optical resonator and spin-chain quantum batteries which rely on the entanglement of collective spin states, such as a Dicke model scenario in which many two-level systems are simultaneously coupled to a common photon mode to speed up the charging and increase the working capacity that can be extracted[15,16].

The open quantum-battery models go one step further and represent these systems as including dissipative and decohering processes which in physical terms are the side effects that cannot be prevented in a real-life device. A quantum battery's capability is largely determined by factors like ergotropy, charging power and energy fluctuations that affect how accurately the system can be charged. To devise fields which will control the system that would achieve maximal ergotropy and at the same time reduce charging time and energy loss, a multi-dimensional optimization is needed, a problem which has turned out to be a very suitable area for the application of machine learning as well as more to be exact reinforcement learning[17]. Table 1 represents the summary of the literature on machine learning for quantum energy storage.

Table 1. Summary of the literature on machine learning for quantum energy storage

S. No	ML / QML method	Application focus
1	Reinforcement learning	Fast-charging control of a Dicke quantum battery
2	LSTM-driven deep deterministic policy gradient RL	Charging control of an open quantum battery
3	Reinforcement learning under partial observability	Charging optimization of an inhomogeneous Dicke quantum battery
4	Variational quantum algorithm	Ergotropy / work-extraction estimation in many-body quantum batteries
5	Quantum-enhanced LSTM	State-of-health prediction for lithium-ion batteries
6	Survey of quantum machine learning (CQ / hybrid-CQ)	SOH / SOC prediction and optimization in energy-storage devices
7	Quantum neural networks	Energy management for microgrids with EVs and battery storage
8	Quantum kernel regression on NISQ hardware	Data-efficient battery-degradation prognostics

9	Quantum-inspired entangled reservoir computing (QERC)	Unified glass-box control of battery energy-storage systems
10	Quantum machine learning, quantum-assisted multiscale simulation	Discovery of electrolyte, anode and cathode materials
11	Computational + machine-learning screening, quantum computing	High-entropy material discovery for batteries and supercapacitors
12	Graph convolutional neural network + quantum-chemistry calculations	Discovery of ionic-liquid polymer electrolytes for Li-metal batteries
13	Generative adversarial network + message-passing NN + quantum calculations	Generative design of next-generation alkali-metal-battery electrolytes
14	High-throughput screening + ML surrogate classifier	Discovery of superionic solid-state electrolytes for Li-ion batteries
15	ML interatomic potentials, graph neural networks, Bayesian optimization	Review: bridging quantum-accurate simulation with ML-driven materials screening

2.2 Machine learning and quantum machine learning approaches

Reinforcement learning models the charging or control issue as a sequence of decisions where AI learns a policy that changes driving-field amplitudes or coupling parameters live as reward is defined through extractable energy or charging speed. Quantum machine learning works with parameterized quantum circuits either as a quantum kernel classifier/regressor or inserted into classical recurrent architectures, with the goal of leveraging the advantage of states superposition and entanglement to generate more compact models, which in theory can cause significant improvement in data efficiency[18,19]. Materials discovery by ML-based approach integrates quantum-chemical descriptors in graph neural networks, generative adversarial networks and Bayesian optimization to efficiently search large chemical spaces for candidate electrolytes and solid-state conductors much faster than through exhaustive synthesis and testing[20].

3. Literature review

3.1 Reinforcement learning for quantum-battery charging control

The pioneering work of Erdman et al. in which they applied reinforcement learning to charging a Dicke quantum battery demonstrates how a learned policy not only enhances ergotropy and charging precision

when compared with fixed protocols, but also mitigates the negative impacts of quantum chaos. This study preserved the collective speedup linked to simultaneous many-body charging until even when the battery is approaching its maximum capacity, it can still charge at a higher speed. Inspired by Erdman et al. Zakavati et al. tackled a more pragmatic scenario of open-system setting with the battery exchanging energy with its surrounding which leads to decoherence. Their strategy featured a combination of deep deterministic policy gradient with long short-term memory (LSTM) networks so that the policy of the agent could evolve in time reflecting the memory of non-Markovian dynamics of the reservoir[21,22]. This adaptive policy consistently outperformed fixed heuristic strategies even with suppressing the undesired energy backflow from battery to charger. The investigation of Song et al. went into another practical limitation partial observability. Since it is very unlikely to obtain the full quantum state access on an experimental level they trained the RL policies in four different observability settings from full-state access to the lowest limit of one-particle energy measurement. While a fully observable setting allowed nearly optimal performance at ergotropy extraction with low variance, adding the second order correlation measurements to single-particle observations narrowed down most of the performance gap achieving about 94-98 % of the performance of a fully observable system thereby showing quite clearly what types of sensors will be necessary for the controller of a real-life quantum battery[23,24]. **Figure 2** represents overview of quantum technologies in energy management.

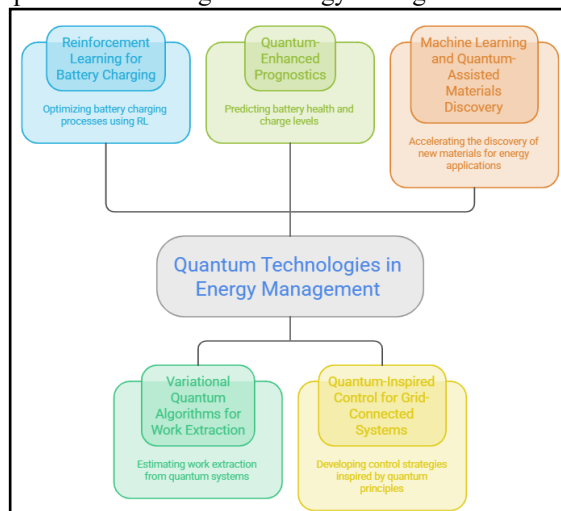


Figure 2 Overview of quantum technologies in energy management

3.2 Variational quantum algorithms for work-extraction estimation

Usually, estimating the ergotropy of many-body quantum batteries is carried out through a full state tomography. Still this turns intractable with the

increasing system size. Instead of performing tomography the team of Hoang developed a Variational Quantum Ergotropy (VQErgo) algorithm which directly finds the optimal unitary operator that maximizes extractable work. It was tested on a many-body battery driven by the transverse-field Ising dynamics after a quench. VQErgo successfully reproduced ergotropy variations for varied system sizes and charging times but the researchers highlighted that in larger systems the development of correlations of larger ranges demanded more ansatz circuits for a given accuracy pointing to scaling issues common to most near-term variational quantum algorithms[25,26].

3.3 Quantum-enhanced prognostics: state-of-health and state-of-charge prediction

The tested QML not in abstract quantum batteries, but in real lithium-ion cells to tackle prediction of health (SOH) and battery charge (SOC) levels from cycling data, a long-standing issue that remains difficult to solve. Using QLSTM, Xu et al. replaced classical affine layer operations with quantum circuit gates in a variational way by integrating them directly into the gates, of a LSTM network. In several battery datasets, QLSTM brought about a 20% reduction in mean-absolute prediction error compared with the corresponding classical LSTM models and this advantage was explained by In reality quantum operations added extra non-linearities to network recurrence[27].

3.4 Quantum-inspired control for grid-connected battery energy-storage systems

The use of single-cell prognostics is also beyond one-cell prediction. In this work quantum-inspired methods were not only used for prognostics but also applied in system-level control with two studies. One of them is a quantum neural network that aims at predicting the state of health (SOH) and state of charge (SOC) of a plug-in electric vehicle/battery combination in a renewable microgrid energy system. This is challenging because it is done in thermally stressed and highly variable environments typically found in grid operation. On a related line of research, the quantum entangled reservoir computing (QERC) system was introduced as a new way of battery energy storage systems control without using black-box deep learning models. Rather than a randomly-initialized neural network, the QERC model consists of a fixed, complex-valued reservoir consisting of unitary entanglement matrices that the authors have claimed will provide stability and energy-conserving dynamics similar to closed quantum systems, plus the interpretability that grid operators can audit[28]. [29]

3.5 Machine-learning- and quantum-assisted materials discovery

The majority of the work surveyed is focused on ML that is often paired with quantum-chemical

computations in discovering battery materials rather than being used in control or prognosis. A QunaSys team under a EU-funded consortium named FULL-MAP is modeling electrolytes, anodes and cathodes at the atomic level through quantum computing and quantum machine learning with the final goal to link quantum-mechanical aspects to continuum-level simulation for resolving electrode-electrolyte interface stability and ionic migration. As by including quantum computing are being applied in the design of high-entropy materials like high-entropy MXenes for batteries and supercapacitors with a remark that data availability and structural-parameter selection remain the key bottlenecks[30,31].

In the molecular-design level an article by Li et al. presents a combination of quantum-chemistry computations with a graph convolutional neural network to select ionic liquids suitable as polymer electrolytes in lithium-metal batteries, after which they produced thin mechanically stable electrolyte membranes with high critical current density from the top computational-screening candidates. A more recent generative work connected a generative adversarial network with a message-passing neural network that had been trained on quantum-mechanical properties to come up with new electrolyte molecule ideas for alkali-metal batteries and candidates were filtered down by formation energy prediction and also electrochemical window. In a high-throughput screening study, an ML surrogate classifier on over 20,000 lithium-containing compounds to highlight superionic solid-state electrolyte candidates, tackling the issues of ionic conductivity and interfacial stability that conventional liquid electrolytes are unable to handle[32]. **Table 2** represents comparative performance characteristics of ML/QML method families for quantum energy storage.

Table 2. Comparative performance characteristics of ML/QML method families for quantum energy storage.

Method family	Reported advantage	Key limitation
Reinforcement learning for charging control	Higher ergotropy, improved charging precision and robustness to non-Markovian noise versus fixed heuristic protocols	Performance degrades under partial observability; policies are trained in simulation, not yet on physical quantum-battery hardware

Variational quantum algorithms	Enables ergotropy estimation directly on NISQ devices without full state tomography	Accuracy falls as system size and circuit depth grow, requiring more ansatz repetitions
Quantum-enhanced sequence models	Roughly 20% lower mean-absolute-error than classical LSTM baselines on SOH benchmarks	Gains depend on dataset and are sensitive to hardware noise and qubit count
Quantum kernel methods	About 2.1% higher accuracy while needing roughly 6.6-times fewer training samples than classical models	Demonstrated at small qubit counts (tens of cells); scaling to fleet-level data unresolved
Quantum-inspired reservoir / classical surrogates	Physically interpretable, Lyapunov-stable control without opaque deep networks	Validated in simulation (MATLAB/Simulink); hardware deployment still pending
ML-guided / quantum-assisted materials discovery	Orders-of-magnitude faster screening of candidate electrolytes and solid conductors than trial-and-error synthesis	Model accuracy bounded by training-data coverage; experimental validation still required for top candidates

4.2 Quantitative performance gains

The following four results are reported quantitatively and directly from the studies and collected in the same Figure 2 shows by how much accuracy is improved and by how many fewer training samples are needed when using a quantum

kernel regression for battery prognostics. shows how much mean absolute error is reduced by a QLSTM state-of-health predictor, while reveals the ergotropy recovered through an RL charging policy only partially observed compared to the fully observed one[33–38].

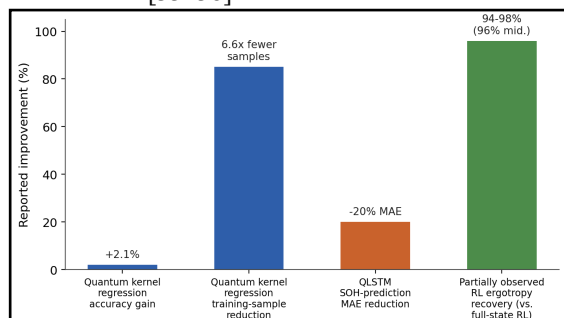


Figure 2 Selected quantitative performance gains reported for ML/QML methods across the reviewed studies.

Clearly the given representation above are not comparable with each other, as they are results from different problems data sets and baselines but altogether they clearly show the main advantage of quantum/ML combination in this paper is the use of data being more efficient[36–39].

7. Conclusion

The convergence has machine learning reshaping the two roads of quantum energy storage. First, it gives us the tools for control and estimation schemes for quantum batteries that are purely theoretically interesting since they cannot be analyzed. Then, it allows us to get the prognosis and materials discovery for conventional electrochemical storage quicker. A quantum-battery charging that uses a reinforcement learning is much better than the use of static heuristics as a tool of getting quantum states from classical ones, whereas variational quantum algorithms have a small role to play, in that they make ergotropy estimation workable on quantum hardware which is available now. Also, quantum-enhanced sequence models and kernel methods give somewhat limited improvements in accuracy and data-efficiency over their classical counterparts, but such improvements are still quite promising. Material-discovery pipelines that incorporate quantum-chemical descriptors and graph neural networks and generative models are the most developed ones of the five areas mentioned in the review and they were capable of bringing on the market electrolyte compositions made and checked experimentally.

Competing interest and declaration

The authors state that none of the research described in this analysis appears to have been impacted by any known financial conflicts of interest or intimate personal ties.

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