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PERSPECTIVE

The emergence of quantum energy science

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Florian Metzler^{1,*} , Jorge I Sandoval¹  and Nicola Galvanetto^{1,2,*} RECEIVED
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* Authors to whom any correspondence should be addressed.

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**Abstract**

Quantum engineering seeks to create novel technologies based on the exploitation of distinctly nonclassical behaviors such as quantum coherence. The vast majority of currently pursued applications fall into the domain of quantum information science, with quantum computing as the most visible subdomain. However, other applications of quantum engineering are fast emerging. Here, we review the deployment of quantum engineering principles in the fields of solar energy, batteries, and nuclear energy. We identify commonalities across quantum engineering approaches in those apparently disparate fields and draw direct parallels to quantum information science. We find that a shared knowledge base is forming, which de facto corresponds to a new domain that we refer to as ‘quantum energy science’. Quantum energy science bears the promise of substantial performance improvements across energy technologies such as organic solar cells, batteries, and nuclear fusion. The recognition of this emerging domain may be of great relevance to actors concerned with energy innovation. It may also benefit active researchers in this domain by increasing visibility and motivating the deployment of resources and institutional support.

1. Introduction

Improving the performance of energy technologies is a key objective of many ongoing innovation efforts. However, prevalent energy technologies frequently run up against physical limits. An example is the ionization energy of atoms and molecules with an upper bound of around 15 eV. This number defines a hard theoretical upper limit for the achievable energy density of prevalent energy storage technologies. In actual implementations of technology, the practical limits are often much lower. Electrochemical batteries, for instance, are based on electronic redox reactions and ion migration, which constrains achievable energy density to below 10 kWh kg⁻¹ (Zhou *et al* 2022). Equivalent physical constraints apply to charging and discharging rates of batteries as well as minimum material requirements of solar cells.

Such limits can be overcome by more radically reconsidering the physics that underlie sought energy technologies. Here, we lay out how quantum engineering informs novel approaches to solar, battery and nuclear engineering—promising to overcome certain physical limitations that stifled energy technology development for decades. Such opportunities may be of interest to those in pursuit of disruptive innovation in the energy space, seeking improvements of 10× and more across key metrics. The presented approaches include high-efficiency organic solar cells with much reduced material requirements, below 10 g m⁻² (>30× reduction compared to present levels); quantum batteries with enhanced charging through superabsorption (>60× acceleration); and high-capacity nuclear batteries that use atomic nuclei as energy reservoirs (>1000× increase). See supplementary note S1 for supporting calculations.

While implementations may look different across domains, there is a common denominator to quantum-engineering-based energy technologies: in each case, energy is deliberately moved into and out of energetic states of quantum systems, which can comprise molecules, atoms, and nuclei. Control over this process is achieved by selectively activating or suppressing couplings between and to such quantum systems.

As a result of such deliberate control, new fundamental building blocks become available to be utilized in energy technologies; and collective quantum effects can be employed to greatly accelerate desirable dynamics. The employed theoretical and practical toolsets are closely related to those of other quantum engineering domains, providing ample opportunities for spillover of knowledge and human resources.

Quantum computing as well as quantum simulation, quantum sensing, and quantum communication are the most visible applications of quantum engineering today. Around the globe, large programs are forming to systematically support and foster emerging quantum engineering ecosystems (Thew *et al* 2019). However, direct energy applications are typically missing from such programs. We argue that the vast potential of quantum engineering for energy applications warrants greater attention to that domain and suggest its inclusion in major quantum initiatives.

In the remainder of this article, we provide an overview of quantum engineering for energy applications. We introduce key principles, lay out the possibilities that researchers have envisioned in different application areas, and summarize what has been accomplished to date.

2. Background and key principles

Most properties and behaviors of materials are governed by quantum principles. These insights, first recognized during the early 20th century, led to the first quantum revolution, which revolved around aggregate effects of quantum principles such as the electronic band structure of materials. During the 1970s, a second quantum revolution emerged and is today in full swing. The new wave of quantum engineering associated with it—sometimes referred to as *Quantum 2.0*—focuses on the precise control of quantum properties and on the exploitation of distinctly nonclassical behaviors such as superposition and entanglement (Pritchard and Till 2014, Awschalom *et al* 2017, Rapp and Schneider 2021). Quantum computing is perhaps the most visible manifestation of Quantum 2.0. In quantum computing, quantum systems with discrete energetic states such as atoms and small superconducting circuits are deliberately excited and then allowed to time-evolve in probabilistically predictable ways.

The storage and manipulation of information entails the storage and manipulation of energy—a principle that applies to classical physics and quantum physics alike (Szilard 1929). Consider a memory chip where the information content of a binary bit is represented through a small amount of charge. For information applications, engineers seek to minimize the amount of charge required while maximizing the fidelity with which it can be retrieved. Priorities differ for energy applications: consider a bank of capacitors which can be either empty (0) or charged (1). Here, engineers care more about the capacity of the system than about fidelity. The same shift of perspective applies to quantum science. Two-level quantum systems, widely known as *quantum bits* or *qubits*, can be in a higher energetic state or in a lower energetic state—which can be interpreted as $|1\rangle$ and $|0\rangle$ when viewed from an information perspective, or as ‘charged’ and ‘uncharged’ when viewed from an energy perspective (Hübner and Osuagwu 2010). Quantum systems that are optimized for energy storage, transfer and conversion rather than for information storage, transfer and conversion have been referred to as *work qubits* (Binder *et al* 2015).

What both information and energy perspectives have in common is that quantum systems can be manipulated by temporarily enhancing interactions between them (Majer *et al* 2007). This allows for energy to redistribute and energetic states to change. As a result of enhanced interactions, quantum systems that are now coupled can no longer be seen as separate entities. Like multiple small waves forming a single larger one, energy is then—for a short period of time—held collectively in an overarching system, where it can no longer be pinpointed. This collective state is known as a state of coherent superposition (Vewinger *et al* 2003, Sillanpää *et al* 2007). It is also sometimes described as a delocalized state (Levi and Mintert 2014). Eventually, the superposition state ends—often within nanoseconds—due to disturbances from the environment. Energy may then end up redistributed compared to the system’s initial state. This redistribution effectively represents an energy transfer or an energy conversion event. The same process can also be interpreted as an information transfer or information conversion event—as is the case in quantum state transfer between qubits (figure 1(a)). Figure 1(b) shows two coupled qubits and figure 1(c) shows six coupled qubits. In both cases, the interactions between the qubits can be tuned via external stimulation, so as to accelerate or decelerate their excitation and deexcitation through induced energy transfers via superposition states (Bernien *et al* 2017, Wu *et al* 2018).

Several characteristics are important here. First, this quantum mode of energy redistribution—also known as quantum energy transfer or quantum transport—can be extremely fast (Jones and Bradshaw 2019). Consequently, quantum energy transfer can preempt competing events—such as the spontaneous decay of an excited molecule. Fast dynamics are in part driven by collective quantum effects known as Dicke enhancement (also known as superradiance, superabsorption, and supertransfer—see Dicke 1954, Lloyd and Mohseni 2010, Higgins *et al* 2014). Second, the rate at which energy transfer occurs depends on the extent to

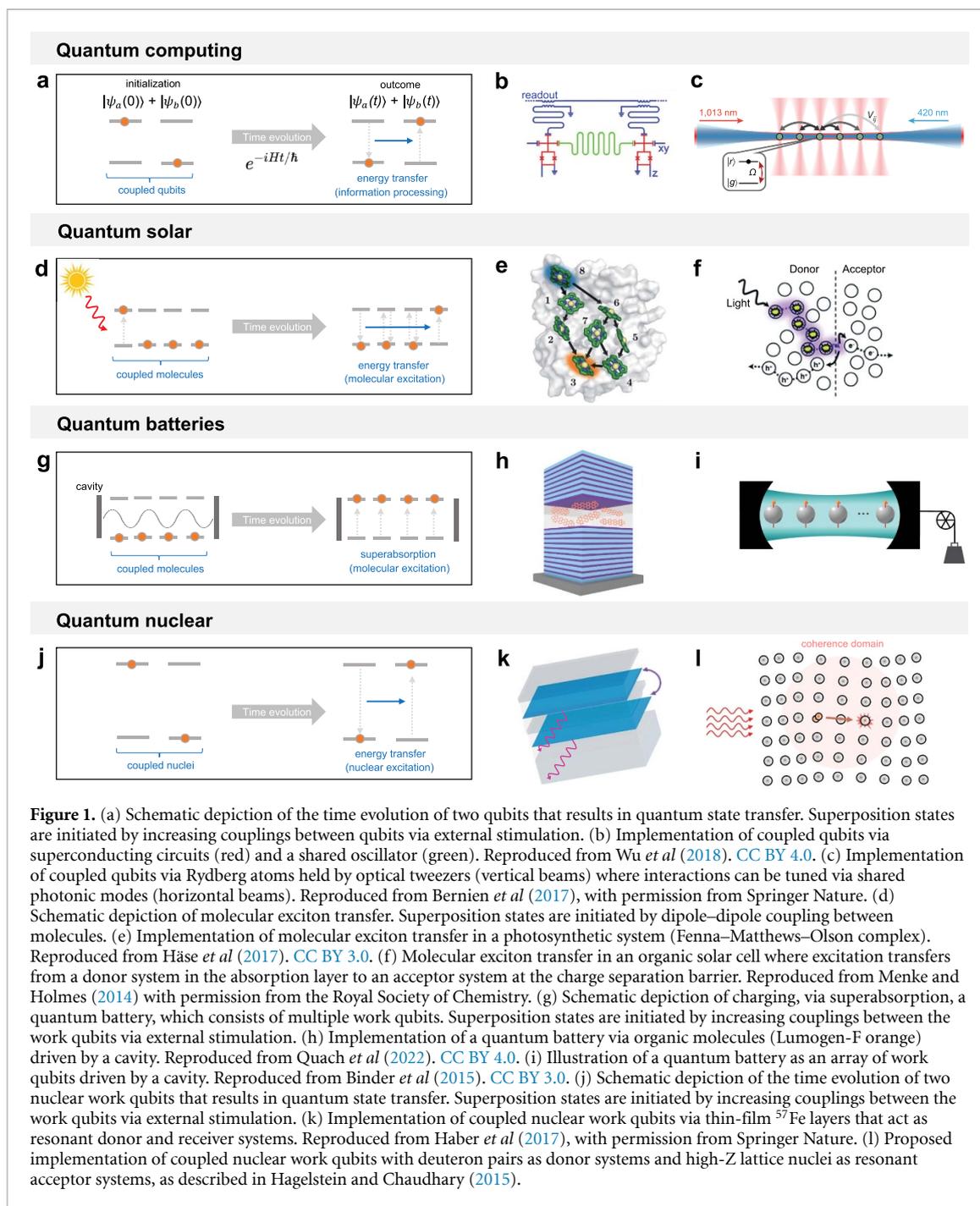


Figure 1. (a) Schematic depiction of the time evolution of two qubits that results in quantum state transfer. Superposition states are initiated by increasing couplings between qubits via external stimulation. (b) Implementation of coupled qubits via superconducting circuits (red) and a shared oscillator (green). Reproduced from Wu *et al* (2018). CC BY 4.0. (c) Implementation of coupled qubits via Rydberg atoms held by optical tweezers (vertical beams) where interactions can be tuned via shared photonic modes (horizontal beams). Reproduced from Bernien *et al* (2017), with permission from Springer Nature. (d) Schematic depiction of molecular exciton transfer. Superposition states are initiated by dipole–dipole coupling between molecules. (e) Implementation of molecular exciton transfer in a photosynthetic system (Fenna–Matthews–Olson complex). Reproduced from Häse *et al* (2017). CC BY 3.0. (f) Molecular exciton transfer in an organic solar cell where excitation transfers from a donor system in the absorption layer to an acceptor system at the charge separation barrier. Reproduced from Menke and Holmes (2014) with permission from the Royal Society of Chemistry. (g) Schematic depiction of charging, via superabsorption, in a quantum battery, which consists of multiple work qubits. Superposition states are initiated by increasing couplings between the work qubits via external stimulation. (h) Implementation of a quantum battery via organic molecules (Lumogen-F orange) driven by a cavity. Reproduced from Quach *et al* (2022). CC BY 4.0. (i) Illustration of a quantum battery as an array of work qubits driven by a cavity. Reproduced from Binder *et al* (2015). CC BY 3.0. (j) Schematic depiction of the time evolution of two nuclear work qubits that results in quantum state transfer. Superposition states are initiated by increasing couplings between the work qubits via external stimulation. (k) Implementation of coupled nuclear work qubits via thin-film ^{57}Fe layers that act as resonant donor and receiver systems. Reproduced from Haber *et al* (2017), with permission from Springer Nature. (l) Proposed implementation of coupled nuclear work qubits with deuterium pairs as donor systems and high-Z lattice nuclei as resonant acceptor systems, as described in Hagelstein and Chaudhary (2015).

which resonances exist in the coupled system (Andrews 2009). Providing resonant acceptors—matched by design or via in situ tuning—then allows for the acceleration of desirable transitions. Finally, this mode of energy redistribution through coherent superposition states is in principle lossless—the quantum of energy, understood as a discrete unit, that ends up at an acceptor system is the same quantum of energy that was originally present at the donor system (May and Kühn 2011). This stands in contrast to other, incoherent modes of energy transfer with significant energy dissipation such as electron movement.

To better understand these unique features of manipulating energy at the nanoscale, researchers have created models that describe relevant aspects of quantum systems and their interactions. Such models can then be evolved over time to study their dynamic behavior. A common way of representing these models is through Hamiltonians—equations that keep track of a system’s energy reservoirs and energy transfer pathways, along with the factors that affect them (Eisberg and Resnick 1985). As laid out in figure 1 and further described in supplementary note S2, the models—and the quantum principles that govern them—are highly similar across the different cases discussed in this article: solar energy, batteries, and nuclear energy.

Table 1. Overview of presented quantum energy subdomains.

Subdomain	Choice of work qubits	Key results to date	Promise
Quantum solar	Molecules and molecular excitons (electron–hole pairs)	Molecular exciton diffusion lengths of >300 nm demonstrated; acceleration of deexcitation (through supertransfer) by a factor of >100× simulated. See Abasto <i>et al</i> (2012), Sneyd <i>et al</i> (2021), Sneyd <i>et al</i> (2022), Varvelo <i>et al</i> (2023).	Low-cost and robust organic solar cells with high efficiency; utilization of a broader range of the light spectrum
Quantum batteries	Molecules and atoms	Acceleration of excitation of molecules (through superabsorption) demonstrated. Charging rates up to 672 kW kg ^{−1} reported. See Cruz <i>et al</i> (2022), Quach <i>et al</i> (2022).	Batteries with quasi-instantaneous charging and discharging; lossless storage through ‘dark states’
Quantum nuclear	Nuclei and nuclear excitons (collective nuclear excitations)	Deliberately induced deexcitation of nuclear states in ⁵⁷ Fe; acceleration of nuclear deexcitation (through superradiance) by 15× demonstrated; phase alignment of nuclear states across multiple nuclei via external radio frequency stimulation demonstrated. See Haber <i>et al</i> (2017), Chumakov <i>et al</i> (2018), Bocklage <i>et al</i> (2021).	Nuclear quantum batteries with high storage capacity; nuclear waste processing through accelerated nuclear decay, compact fusion technology through accelerated nuclear reactions

In the following sections, we will provide examples of emerging quantum engineering applications in each area and discuss their potential for the improvement of existing or the creation of novel energy technologies (see also table 1 for an overview).

3. Subdomains of quantum energy science

3.1. Quantum solar

Quantum engineering is now employed to apply lessons learned from photosynthesis to solar cell design to maximize the efficiency of light harvesting. The aspiration is to combine nature’s high efficiency in utilizing absorbed photons with the ability of artificial materials to absorb a greater number of photons (by making use of a wider range of the light spectrum compared to biological systems; Brédas *et al* 2017).

The extremely high efficiency in the utilization of absorbed photons in photosynthesis has startled scientists for decades (Cao *et al* 2020). Almost every photon that is absorbed by a photosynthetic system is used in the formation of chemical bonds, rather than getting reemitted and lost. Achieving photon utilization rates close to 100% is not trivial since the excited molecular-level quantum systems that result from photon absorption—known as excitons—are extremely short-lived (Dursun and Guzelturk 2021). If the energy held by an exciton is not moved within picoseconds to a reaction center molecule, where sugar production occurs, then the exciton decays and the excitation energy is reemitted in the form of a photon. If plants were to employ purely classical transfer mechanisms, e.g. where energy to be transferred is imparted onto a particle that physically moves through its environment akin to the migration of ions in batteries, then most of the initially absorbed energy would be lost due to the slowness of such a process. In actuality, it is not energetic particles that move but the excitation energy itself, in an oscillator-mediated, nonradiative transfer process, which involves the temporary superposition and delocalization of coupled molecules (Andrews *et al* 2020, Giannini *et al* 2022, Varvelo *et al* 2023; see figures 1(d) and (e)). Finally, because of boundary conditions in the photosynthetic complex, the energy in the system is more likely to end up—when the coherent superposition state is broken—at the reaction center of the complex, where it needs to be. This efficient path-finding process—known as a quantum walk—has been compared to plants engaging in a form of quantum computing (Biello 2007, Mohseni *et al* 2008). When viewed from this perspective, excitons can

be seen as excited work qubits that temporarily hold energy—energy which then transfers to other work qubits as the exciton diffuses.

Theoretical models of this energy transfer process suggest that it works so well because parameters of the surrounding environment are just right, ensuring maximum efficiency. Apparently nature has evolved ways of maintaining temporary superposition states despite the presence of noisy environments—and certain noisy environments may even contribute to the stabilization of such states (Plenio and Huelga 2008). Insights from such models can then be applied to the design of technology (see for instance Mattioni *et al* 2021). Specifically, solar cells face similar challenges as photosynthetic systems: if energy is not transferred fast enough from the sites of exciton creation (the top layer of a solar cell where photons are absorbed) to the sites where excitons generate charge carriers (the bottom layer of a solar cell), then energy is lost through reemission (Menke and Holmes 2014; also see figure 1(f)). In practice, this means that the top layer of the cell is limited in thickness to the exciton diffusion length, i.e. the distance that excitons manage to travel within their short lifetime. However, thin top layers, e.g. with thicknesses on the order of a few nm, mean that much of the incoming light is not utilized, as many photons require more than 100 nm of penetration depth to be absorbed (Sajjad *et al* 2020).

This is of particular concern with organic solar cells, one of the most promising types of emerging solar technologies. Organic solar cells—sometimes called plastic solar cells—are created from polymeric materials, making them low-cost in their fabrication and installation (Chiechi *et al* 2013). Other advantages are low material requirements ($<10 \text{ g m}^{-2}$), environmentally friendly disposal, bendability, and the possibility to create semi-transparent cells—all factors that enable diverse and broad deployment. The key drawback to date has been the comparatively low efficiency of organic solar cells—often below 10%—especially when paired with practical considerations such as large-scale production and longevity. The low efficiencies are rooted in the short lifetimes of excitons in organic materials, which correspond to short diffusion lengths (Riede *et al* 2021). When working with thick absorption layers $>10 \text{ nm}$, many excitons recombine and lose their energy to the environment before they can reach a junction where this excitation energy is converted to charge. In certain prototype cells, this issue has been addressed through the creation of special structures where junctions with charge separation barriers permeate the absorption layer, known as *bulk heterojunctions* (Rand and Richter 2014). However, such designs are not as scalable and robust as the much simpler *planar heterojunctions*, which are essentially plane layers of thin film. To achieve both high efficiency and high manufacturability as well as robustness, researchers aim for planar heterojunctions with long exciton diffusion lengths across deep absorption layers. Ideally, organic solar cells exhibit absorption layers and corresponding diffusion lengths in excess of 100 nm.

Increases of exciton diffusion lengths in organic materials have been achieved by testing different material configurations, often without fully understanding why some work better than others (Cnops *et al* 2014, Long *et al* 2016, Sneyd *et al* 2021). Sneyd *et al* (2021), for instance, report in films of oligomeric polyfluorene nanofibers an exciton diffusion length of $300 \pm 50 \text{ nm}$, estimated from pump-probe measurements. To truly optimize exciton diffusion in a variety of materials, however, researchers seek to identify ideal material configurations and morphologies based on models and simulations of the above-described energy transfer processes, which would then allow for the prediction of optimal parameters (Mattioni *et al* 2021, Ruseckas and Samuel 2021). Recent modeling efforts directly relate fast exciton diffusion with coherent dynamics, and derive lessons from resulting models for the design of efficient organic solar cells (Giannini *et al* 2022, Sneyd *et al* 2022, Varvelo *et al* 2023).

To summarize: quantum models have been developed to explain the remarkably high efficiency of energy transfer in photosynthesis. These models suggest the presence of the same coupling-induced superposition states that are used in quantum computing. The analogy becomes particularly clear when viewing excited molecules as work qubits. The interactions between such work qubits allow for fast excitation transfer across them. In quantum solar engineering, the described models inform optimal parameters for the design of new solar cell materials that seek similarly efficient energy transfer performance. Plants have an internal efficiency of close to 100%—meaning that almost all absorbed photons are utilized. However, because only small parts of the light spectrum are utilized, their overall efficiency is only about 1%—meaning most of the available photons are not absorbed. Combining the best of both worlds, namely absorbing a much larger portion of the light spectrum while engineering a high internal efficiency through fast exciton diffusion, is sought to lead to robust, scalable, and low-cost organic solar cells with overall efficiencies in excess of 20%. The 20% is the estimated threshold for large-scale adoption of organic solar cells, as estimated by Riede *et al* (2021). A discussion of an exemplary Hamiltonian that has been used by researchers to model Dicke-enhanced exciton diffusion (Lloyd and Mohseni 2010, Abasto *et al* 2012) can be found in supplementary note S3.

3.2. Quantum batteries

The equivalence of energy and information led researchers to consider whether two-level quantum systems, i.e. qubits, could be optimized for the storage and retrieval of energy instead of the storage and retrieval of information. In this case, design requirements shift: addressability of individual qubits is not required; however, the energy held per qubit ought to be high and the total number of qubits large.

In one proposed design for quantum batteries, energy is stored in excited states of dye molecules (Lumogen-F Orange) which are contained in a thin film polymer matrix (figure 1(h); Quach *et al* 2022). Data from one such experimental configuration suggest that 1.6×10^{11} molecules were successfully used as work qubits, each with an energy transition of 0.108 eV (resulting in a total capacity of the battery prototype of 2.768×10^{-9} J). Charging occurs through exciting work qubits via coherent laser light, although the authors of the study suggest that in the future, incoherent sunlight might be used as well. An alternative configuration is proposed by Cruz *et al* (2022), which uses as work qubits molecules known as metal carboxylates. These authors report the storage of 0.85 mJ of energy per mol of the molecule $\text{Cu}_2(\text{HCOO})_4(\text{HCOOH})_2(\text{C}_4\text{H}_{10}\text{N}_2)$. The above values are still far below the energy densities of common batteries (which are in the hundreds of Wh kg^{-1} range, whereas the values of Cruz *et al* correspond to about 1 $\mu\text{Wh kg}^{-1}$ and the values of Quach *et al* correspond to about 4 Wh kg^{-1}). However, these early experimental configurations already exhibit some key strengths of anticipated quantum batteries. In Quach *et al*, remarkable power densities such as 672 kW kg^{-1} are reported from experiments. This value already far exceeds the power densities of existing lithium-ion batteries, which remain below 1 kW kg^{-1} (see supplementary note S1). Even the most advanced supercapacitors do not exceed a power density of 10 kW kg^{-1} .

While such early experimental reports need to be treated with caution, they already exhibit a key principle that motivates quantum battery design: when the transfer of energy to and from the work qubits occurs through superposition states, then the process can be very fast. Specifically, the dynamics benefit from quantum speedup associated with Dicke enhancement (superradiance and its inverse mechanism, superabsorption). This means that, depending on the exact configuration, charging and discharging times can scale by a factor of \sqrt{N} , N , or N^2 , where N is the number of work qubits that participate in the intermediate superposition state (Higgins *et al* 2014, Campaioli *et al* 2018, Ferraro *et al* 2018, Gumberidze *et al* 2019). In other words, the larger the battery (and the coherence state that can form within it), the faster it can charge and discharge. Quantum battery designers then seek to optimize such configurations toward achieving both high power densities and high energy densities. Higher energy densities, compared to those demonstrated to date, are conceivable when quantum systems with larger transition energies and smaller molecular weights are utilized.

Like in quantum solar engineering, system designs are informed by Hamiltonian-based models that describe the major components and couplings in such systems (see supplementary note S4). Evaluating predicted system performance across the design space then informs the optimal composition and structure of the employed materials. As a result, key metrics such as charging rates, energy retention, and discharging rates can be optimized.

When tuned sufficiently well, charging and discharging rates for such batteries can be almost instantaneous (Alicki and Fannes 2013). Resulting technology could overcome a major limitation of existing battery technology where charging and discharging is severely rate-limited, a constraint that has to date impeded battery deployment in such mass-market applications as vehicles and airplanes as well as such specialized applications as high-power lasers and pulsed magnetic fields.

3.3. Quantum nuclear

Thus far, we have considered as relevant two-level systems—i.e. as work qubits—quantum systems at the atomic level such as molecules and atoms. Atomic nuclei, too, can absorb and emit discrete quanta of energy and therefore also fulfill the basic condition for qubits or work qubits (Boyles 2014). This prompted some researchers to consider the use of nuclei as work qubits for quantum batteries—what could then be called nuclear quantum batteries (Liao 2014).

The prospective advantage of nuclear quantum batteries is vastly increased energy density, exceeding by orders of magnitude any current storage technology. This is because nuclear excited states can typically accommodate more than 100 000 times the energy of atomic and molecular excited states (supplementary note S1). However, interactions that at the atomic level can readily cause superposition states and energy transfer pathways are much weaker at the nuclear level. Nevertheless, researchers have succeeded experimentally in creating nuclear superposition states, and in increasing and decreasing the decay rates of such nuclear excited states (Chumakov *et al* 2018, Heeg *et al* 2021)—important steps toward the coherent control of nuclei. In Chumakov *et al* (2018), for instance, the acceleration of the 14 keV $|^{57}\text{Fe}^*\rangle \rightarrow |^{57}\text{Fe}\rangle$ nuclear deexcitation by a factor of 15 is shown experimentally. Like in photosynthesis and in molecular

quantum batteries, at the nuclear scale too, conventionally slow dynamics can be accelerated through Dicke enhancement (Terhune and Baldwin 1965, Hannon and Trammell 1999). Accelerated excitation and deexcitation correspond to charging and discharging processes in quantum batteries; and delayed deexcitation corresponds to retaining stored energy.

Other research shows that relevant interactions between oscillators and nuclei and between nuclei and nuclei can be increased by external stimulation such as externally applied fields (Haber *et al* 2017, Bocklage *et al* 2021). Figure 1(j) shows an experimental configuration where nuclear excitation energy was transferred through external laser stimulation between two collective nuclear excited states (also known as nuclear excitons—note the similarity in nomenclature to molecular excitons used in solar engineering). Varying the parameters of such external stimulation can moreover be used to tune systems into and out of resonance, further accelerating or decelerating sought dynamics. Such considerations and early results motivate the nascent field of quantum nuclear engineering.

The potential scope of quantum nuclear engineering becomes even larger when considering its possible effect on nuclear reactions. Some researchers proposed that principles applied to the coherent control of nuclei may not only apply to nuclear state transitions but also to nuclear reactions³ (Schwinger 1991, Preparata 1995, Hagelstein and Chaudhary 2015). In this picture, if nuclear reactions take place in an environment where a temporary superposition of multiple nuclei is achieved—e.g. due to external stimulation—then the resulting energy redistribution within the coupled system affects the nuclear reaction parameters. For instance, if the energy release associated with one nuclear reaction can be readily absorbed by a counterpart reaction (or, more generally, a counterpart state transition) in the same coupled system—in other words, if the two complementary processes are resonant—then the rate at which respective reactions occur is expected to increase, compared to the isolated case (Hagelstein *et al* 2009, Hagelstein and Chaudhary 2015).

Specifically, Schwinger (1990) proposed to view a pair of deuterium nuclei D_2 as a four-nucleon quantum system in an excited state, i.e. as the equivalent of a work qubit in state $|1\rangle$. Transitioning to a more compact and less energetic four-nucleon configuration such as a stable ${}^4\text{He}$ nucleus then corresponds to a deexcitation step—analogue to the induced flip of a qubit from $|1\rangle$ to $|0\rangle$ (figure 1(a)). Researchers have proposed that this dynamic could be accelerated by stimulating interactions between deuteron pairs and matching heavy nuclei that exhibit excited states resonant with the 23.8 MeV $|D_2\rangle \rightarrow |{}^4\text{He}\rangle$ deexcitation process (figure 1(k)). Such a mechanism would be analogous to accelerated exciton diffusion at the atomic level (figure 1(f)) and analogous to the accelerated charging and discharging of a quantum battery's work qubits (figure 1(h)). It would represent the acceleration of nuclear reactions beyond their conventionally expected reaction rates. Researchers envision using such techniques to accelerate the decay of nuclear waste and to render desirable fusion reactions more accessible (Dumé 2021, Metzler *et al* 2022).

As in the examples above, the proposed systems and processes—from nuclear quantum batteries to accelerated nuclear reactions—can be described via Hamiltonian-based models that capture relevant features of the participating quantum systems and the interactions between them (see supplementary notes S5 and S6). The time evolution of such models then identifies dominant energy transfer pathways and rates. The dependence of such dynamics on environmental parameters such as geometric arrangements and on stimulation characteristics informs the design of materials and promises the rational engineering of corresponding technologies.

4. Conclusions

We described the application of quantum science and quantum engineering principles to energy technologies, across the domains of solar technology, battery technology, and nuclear technology. An overview is provided in table 1. In each of these domains, the quantum-based approaches described here are to date largely viewed as niche areas. However, the knowledge bases that these approaches draw on tend to have more in common with each other than with the traditional knowledge bases of each of their corresponding application domains.

We have seen that there is a common denominator across the presented cases, namely modeling different kinds of quantum systems through appropriate Hamiltonians and then studying the time evolution and energy redistribution as a function of key parameters of the respective physical configuration. This then

³ From this perspective, nuclear reactions are viewed as a subset of nuclear state transitions. Nuclear state transitions in general terms can be seen as reconfigurations of nucleons hindered by barriers that are overcome probabilistically (akin to how atomic state transitions can be seen as reconfigurations of electrons). Nuclei relaxing from excited states to lower energy states then correspond to the reconfiguration of nucleons within nuclei, whereas nuclear reactions such as fusion reactions correspond to the reconfiguration of nucleons across nuclei.

informs the design of new systems—or the deliberate modification of existing systems—and enables the optimization of relevant parameters.

Different names have been proposed to describe this kind of modeling and engineering process: ‘energy transfer editing’ (Qin *et al* 2019), ‘coherence engineering’ (Huynh *et al* 2012), and ‘transition rate engineering’ (Higgins *et al* 2014) are just a few examples. Broader terms include ‘tuning chemical reactions’ (Tan *et al* 2017) and ‘tuning nuclear reactions’ (Metzler *et al* 2022).

We posit that the shared knowledge base across the different energy applications of quantum engineering justifies the recognition as a dedicated subfield of quantum science, which may be referred to as ‘quantum energy science’ as a counterpart to ‘quantum information science’.

Research on traditional energy technologies and research on quantum information science both enjoy high public interest and high levels of investment. Recognizing quantum energy science as a dedicated field of study that emerges at the intersection of these two major domains could lead to greater awareness of its potential societal impact, and greater support in the form of human and financial resources.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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ORCID iDs

Florian Metzler  <https://orcid.org/0000-0003-1818-1332>

Jorge I Sandoval  <https://orcid.org/0000-0001-5299-9248>

Nicola Galvanetto  <https://orcid.org/0000-0002-0408-1747>

References

- Abasto D F, Mohseni M, Lloyd S and Zanardi P 2012 Exciton diffusion length in complex quantum systems: the effects of disorder and environmental fluctuations on symmetry-enhanced supertransfer *Phil. Trans. R. Soc. A.* **370** 3750–70
- Alicki R and Fannes M 2013 Entanglement boost for extractable work from ensembles of quantum batteries *Phys. Rev. E* **87** 042123
- Andrews D L 2009 Resonance energy transfer: theoretical foundations and developing applications *Tutorials in Complex Photonic Media* (SPIE Press) (<https://doi.org/10.1117/3.832717.ch14>)
- Andrews D L, Bradshaw D S, Forbes K A and Salam A 2020 Quantum electrodynamics in modern optics and photonics *J. Opt. Soc. Am.* **37** 1153
- Awschalom D, Christen H, Clerk A, Denes P, Flatté M, Freedman D, Galli G, Jesse S, Kasevich M and Monroe C 2017 *Basic Energy Sciences Roundtable: Opportunities for Basic Research for Next-Generation Quantum Systems* (USDOE Office of Science (SC))
- Bernien H *et al* 2017 Probing many-body dynamics on a 51-atom quantum simulator *Nature* **551** 579–84
- Biello D 2007 *When It Comes to Photosynthesis, Plants Perform Quantum Computation* (Scientific American) (available at: www.scientificamerican.com/article/when-it-comes-to-photosynthesis-plants-perform-quantum-computation/)
- Binder F C, Vinjanampathy S, Modi K and Goold J 2015 Quantacell: powerful charging of quantum batteries *New J. Phys.* **17** 075015
- Bocklage L, Gollwitzer J, Strohm C, Adolff C F, Schlage K, Sergeev I, Leupold O, Wille H-C, Meier G and Röhlberger R 2021 Coherent control of collective nuclear quantum states via transient magnons *Sci. Adv.* **7** eabc3991
- Boyles A 2014 Gamma-ray shaping could lead to “nuclear” quantum computers (Physics World) (available at: <https://physicsworld.com/a/gamma-ray-shaping-could-lead-to-nuclear-quantum-computers/>)
- Brédas J-L, Sargent E H and Scholes G D 2017 Photovoltaic concepts inspired by coherence effects in photosynthetic systems *Nat. Mater.* **16** 35–44
- Campaioli F, Pollock F A and Vinjanampathy S 2018 Quantum batteries *Thermodynamics in the Quantum Regime (Fundamental Theories of Physics vol 195)* (Springer) pp 207–25
- Cao J *et al* 2020 Quantum biology revisited *Sci. Adv.* **6** eaaz4888
- Chiechi R C, Havenith R W, Hummelen J C, Koster L J A and Loi M A 2013 Modern plastic solar cells: materials, mechanisms and modeling *Mater. Today* **16** 281–9
- Chumakov A I *et al* 2018 Superradiance of an ensemble of nuclei excited by a free electron laser *Nat. Phys.* **14** 261–4
- Cnops K, Rand B P, Cheyons D, Verreet B, Empl M A and Heremans P 2014 8.4% efficient fullerene-free organic solar cells exploiting long-range exciton energy transfer *Nat. Commun.* **5** 3406

- Cruz C, Anka M F, Reis M S, Bachelard R and Santos A C 2022 Quantum battery based on quantum discord at room temperature *Quantum Sci. Technol.* **7** 025020
- Dicke R H 1954 Coherence in spontaneous radiation processes *Phys. Rev.* **93** 99–110
- Dumé I 2021 Atomic nuclei go for a quantum swing (Physics World) (available at: <https://physicsworld.com/atomic-nuclei-go-for-a-quantum-swing/>)
- Dursun I and Guzelurk B 2021 Exciton diffusion exceeding 1 μm : run, exciton, run! *Light Sci. Appl.* **10** 39
- Eisberg R and Resnick R 1985 *Quantum Physics of Atoms, Molecules, Solids, Nuclei, and Particles* (Wiley) (<https://doi.org/10.1002/piuz.19760070417>)
- Ferraro D, Campisi M, Andolina G M, Pellegrini V and Polini M 2018 High-power collective charging of a solid-state quantum battery *Phys. Rev. Lett.* **120** 117702
- Giannini S, Peng W-T, Cupellini L, Padula D, Carof A and Blumberger J 2022 Exciton transport in molecular organic semiconductors boosted by transient quantum delocalization *Nat. Commun.* **13** 2755
- Gumberidge M, Kolář M and Filip R 2019 Measurement induced synthesis of coherent quantum batteries *Sci. Rep.* **9** 1–12
- Haber J, Kong X, Strohm C, Willing S, Gollwitzer J, Bocklage L, Ruffer R, Pálffy A and Röhlberger R 2017 Rabi oscillations of x-ray radiation between two nuclear ensembles *Nat. Photon.* **11** 720–5
- Hagelstein P L and Chaudhary I U 2015 Phonon models for anomalies in condensed matter nuclear science *Curr. Sci.* **108** 507–13 (available at: www.jstor.org/stable/24216595)
- Hagelstein P L, Chaudhary I U, McKubre M C H and Tanzella F 2009 Progress toward a theory for excess heat in metal deuterides *AIP Conf. Proc.* **1154** 257–71
- Hannon J P and Trammell G T 1999 Coherent γ -ray optics *Hyperfine Interact.* **123** 127–74
- Häse F, Kreisbeck C and Aspuru-Guzik A 2017 Machine learning for quantum dynamics: deep learning of excitation energy transfer properties *Chem. Sci.* **8** 8419–26
- Häse F, Roch L M, Friederich P and Aspuru-Guzik A 2020 Designing and understanding light-harvesting devices with machine learning *Nat. Commun.* **11** 4587
- Heeg K P et al 2021 Coherent x-ray—optical control of nuclear excitons *Nature* **590** 401–4
- Higgins K D B, Benjamin S C, Stace T M, Milburn G J, Lovett B W and Gauger E M 2014 Superabsorption of light via quantum engineering *Nat. Commun.* **5** 4705
- Hübler A W and Osuagwu O 2010 Digital quantum batteries: energy and information storage in nanovacuum tube arrays *Complexity* **15** 48–55
- Huynh P-A, Portier F, le Sueur H, Faini G, Gennser U, Mailly D, Pierre F, Wegscheider W and Roche P 2012 Quantum coherence engineering in the integer quantum Hall regime *Phys. Rev. Lett.* **108** 256802
- Jones G and Bradshaw D 2019 Resonance energy transfer: from fundamental theory to recent applications *Front. Phys.* **7** 100
- Levi F and Mintert F 2014 A quantitative theory of coherent delocalization *New J. Phys.* **16** 033007
- Liao W-T 2014 *Coherent Control of Nuclei and X-Rays (Springer Theses)* (Springer) (<https://doi.org/10.1007/978-3-319-02120-1>)
- Lloyd S and Mohseni M 2010 Symmetry-enhanced supertransfer of delocalized quantum states *New J. Phys.* **12** 075020
- Long G, Wu B, Solanki A, Yang X, Kan B, Liu X, Wu D, Xu Z, Wu W-R and Jeng U-S 2016 New insights into the correlation between morphology, excited state dynamics, and device performance of small molecule organic solar cells *Adv. Energy Mater.* **6** 1600961
- Majer J et al 2007 Coupling superconducting qubits via a cavity bus *Nature* **449** 443–7
- Mattioni A, Caycedo-Soler F, Huelga S F and Plenio M B 2021 Design principles for long-range energy transfer at room temperature *Phys. Rev. X* **11** 041003
- May V and Kühn O 2011 *Charge and Energy Transfer Dynamics in Molecular Systems* (Wiley) (<https://doi.org/10.1002/9783527633791>)
- Menke S M and Holmes R J 2014 Exciton diffusion in organic photovoltaic cells *Energy Environ. Sci.* **7** 499–512
- Metzler F, Hunt C and Galvanetto N 2022 Known mechanisms that increase nuclear fusion rates in the solid-state (arXiv:2208.07245)
- Mohseni M, Rebentrost P, Lloyd S and Aspuru-Guzik A 2008 Environment-assisted quantum walks in photosynthetic energy transfer *J. Chem. Phys.* **129** 174106
- Plenio M B and Huelga S F 2008 Dephasing-assisted transport: quantum networks and biomolecules *New J. Phys.* **10** 113019
- Preparata G 1995 *QED Coherence in Matter* (World Scientific) (<https://doi.org/10.1142/2738>)
- Pritchard J and Till S 2014 UK Quantum Technology Landscape 2014 (Defence Science and Technology Laboratory) DSTL/PUB75620
- Qin X, Xu J, Wu Y and Liu X 2019 Energy-transfer editing in lanthanide-activated upconversion nanocrystals: a toolbox for emerging applications *ACS Cent. Sci.* **5** 29–42
- Quach J Q, McGhee K E, Ganzer L, Rouse D M, Lovett B W, Gauger E M, Keeling J, Cerullo G, Lidzey D G and Virgili T 2022 Superabsorption in an organic microcavity: toward a quantum battery *Sci. Adv.* **8** eabk3160
- Rand B P and Richter H 2014 *Organic Solar Cells: Fundamentals, Devices, and Upscaling* (CRC Press) (<https://doi.org/10.1201/b17301>)
- Rapp H P and Schneider S 2021 Economic-technological revolution through Quantum 2.0 *Germany Monitor* (Deutsche Bank Research)
- Riede M, Spoltore D and Leo K 2021 Organic solar cells—the path to commercial success *Adv. Energy Mater.* **11** 2002653
- Ruseckas A and Samuel I D 2021 Engineering highways for excitons *Joule* **5** 2762–4
- Sajjad M T, Ruseckas A and Samuel I D 2020 Enhancing exciton diffusion length provides new opportunities for organic photovoltaics *Matter* **3** 341–54
- Schwinger J 1991 Nuclear Energy in an Atomic Lattice: Causal Order Prog. Theor. Phys. **85** 711–2
- Schwinger J 1990 Nuclear energy in an atomic lattice. 1 *Z. Phys. D: At., Mol. Clusters.* **15** 221–25
- Sillanpää M A, Park J I and Simmonds R W 2007 Coherent quantum state storage and transfer between two phase qubits via a resonant cavity *Nature* **449** 438–42
- Sneyd A J et al 2021 Efficient energy transport in an organic semiconductor mediated by transient exciton delocalization *Sci. Adv.* **7** eabh4232
- Sneyd A J, Beljonne D and Rao A 2022 A new frontier in exciton transport: transient delocalization *J. Phys. Chem. Lett.* **13** 6820–30
- Szilard L 1929 Über die Entropieverminderung in einem thermodynamischen System bei Eingriffen intelligenter Wesen *Z. Phys.* **53** 840–56
- Tan S, Xia T, Shi Y, Pfäendner J, Zhao S and He Y 2017 Enhancing the oxidation of toluene with external electric fields: a reactive molecular dynamics study *Sci. Rep.* **7** 1710
- Terhune J H and Baldwin G C 1965 Nuclear superradiance in solids *Phys. Rev. Lett.* **14** 589–91

- Thew R, Jennewein T and Sasaki M 2019 Focus on quantum science and technology initiatives around the world *Quantum Sci. Technol.* **5** 010201
- Varvelo L, Lynd J K, Citty B, Kühn O and Raccach D I G B 2023 Formally exact simulations of mesoscale exciton diffusion in a light-harvesting 2 antenna nanoarray *J. Phys. Chem. Lett.* **14** 3077–83
- Vewinger F, Heinz M, Garcia Fernandez R, Vitanov N V and Bergmann K 2003 Creation and measurement of a coherent superposition of quantum states *Phys. Rev. Lett.* **91** 213001
- Wu Y *et al* 2018 An efficient and compact switch for quantum circuits *npj Quantum Inform.* **4** 1–8
- Zhou G, Chen H and Cui Y 2022 Formulating energy density for designing practical lithium–sulfur batteries *Nat. Energy* **7** 312–9