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OUT-OF-THE-BOX

Lattice battery solar cells: A new paradigm for exceeding the Shockley–Queisser limit

Mehri Ghasemi,[1] Dongchen Lan,[2] Baohua Jia,[1,*] and Xiaoming Wen[1,*]

[1]Centre for Atomaterials and Nanomanufacturing (CAN), RMIT University, Melbourne, VIC 3000, Australia

[2]College of Electrical Engineering, Zhejiang University, Hangzhou 310027, China

*Correspondence: baohua.jia@rmit.edu.au (B. J.); xiaoming.wen@rmit.edu.au (X. W.)

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The development of sustainable energy technologies remains a defining challenge of the 21st century. Despite extensive advancements in photovoltaics, solar cell efficiency remains inherently constrained by the Shockley-Queisser limit, which dictates a theoretical maximum efficiency of approximately 33% for single-junction solar cells (Figure 1A). This fundamental limitation arises primarily from two major energy losses: the thermalization of hot carriers, where excess energy from high-energy photons is dissipated as heat, and the inability to harvest sub-bandgap photons, particularly in the near-infrared (NIR) range.

To overcome these bottlenecks, we introduce the lattice battery solar cell (LBSC), a concept that fundamentally redefines energy conversion in solar cells by utilizing a lattice energy reservoir (LER) to capture and redistribute phonon energy.[1] Unlike conventional semiconductors, where excess carrier energy is lost to lattice vibrations, the unique properties of metal halide perovskites allow for the formation of dynamic nanodomains as energy reservoir, where phonon energy can be stored and later used to drive subgap carrier upconversion. This ability to harness and recycle phonon energy opens the door to significantly exceeding the Shockley-Queisser limit, with theoretical efficiencies projected beyond 70%. This article explores the scientific foundation of LERs, the operational principles of LBSCs, and a roadmap for their experimental realization and commercialization.

The concept of a LER is built upon the unique physical characteristics of halide perovskites, which differ fundamentally from conventional semiconductors.[2] These materials exhibit an intrinsically soft lattice structure, where phonon-lattice interactions are far more pronounced than in rigid crystalline systems.[3] As a result, when photogenerated hot carriers transfer the extra energy to the lattice, instead of dissipating rapidly as heat, a portion of this energy can be retained within localized nanodomains, forming what we define as hot LERs (Figure 1B). LERs emerge from the interplay of dynamic lattice distortions, suppressed thermal transport due to strain interface as phonon cavity, thus prolonged LER lifetime up to seconds.[4-5] Within these nanodomains, phonon energy is effectively trapped and stored due to local strain-induced barriers that reflect acoustic phonon transport. This energy will eventually feedback as electricity output by driving subgap carriers upconversion to the conduction band, while the subgap carriers will be photogenerated to the MHP-NIR composition by NIR solar emission. This unique property leads to several critical effects that distinguish LBSCs from traditional solar cells. First, hot phonon emission from hot carriers will be stored in LER, rather than dissipating for lattice heating. Second, the stored energy in LERs enables carrier upconversion, where subgap electrons gain sufficient energy to transition into the conduction band, effectively broadening the spectral harvesting of the solar cell.

The existence of LERs has been supported by a range of experimental observations in halide perovskites, including anomalous carrier lifetimes, efficient optical-acoustic phonon upconversion, persistent photobrightening, and dynamic defect tolerance.[5] Additionally, the presence of spontaneous upconversion fluorescence in halide perovskite nanocrystals further substantiates the ability of LERs to facilitate non-equilibrium carrier dynamics. These findings provide strong evidence that LERs represent a previously unrecognized but fundamental energy storage mechanism in halide perovskites, with profound implications for solar energy conversion.

At the core of LBSC operation is the ability to simultaneously mitigate hot carrier losses and utilize NIR solar photons, two of the most significant limitations in conventional photovoltaics. This is achieved through a perovskite-NIR composite (PNC) as the active layer in the device. The operational mechanism of LBSCs is fundamentally distinct from that of traditional solar cells and follows a unique sequence of energy conversion processes. When incident solar photons interact with the LBSC absorber layer, two key processes take place. First, high-energy photons generate hot carriers, which would normally undergo rapid cooling through phonon emission. In LBSCs, however, this phonon energy is captured by LERs, preventing its dissipation and allowing it to remain stored within LERs (Figure 1C & D). Simultaneously, NIR photons, which are typically not absorbed in conventional solar cells, are efficiently captured by the NIR component of the PNC. The resulting photogenerated carriers are transferred into metastable subgap states within the perovskite, where they can be upconverted driven by the hot LER. As these subgap carriers migrate through the lattice, they encounter hot LERs, which provide the additional energy needed to upconvert them to the conduction band, eventually output as electricity (output 2, Figure 1D). This energy feedback mechanism, driven by hot LER, enables LBSCs to effectively generate

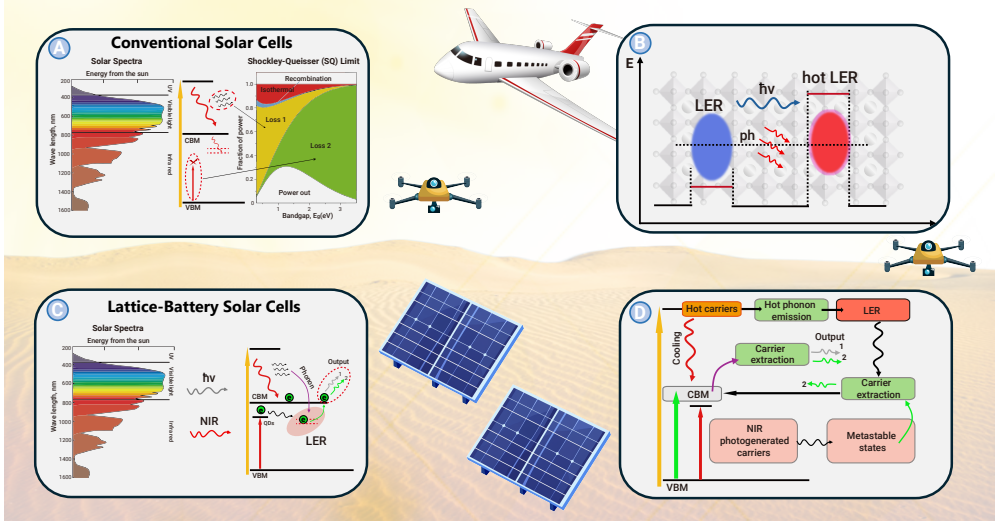

Figure 1. (A) Illustration of losses within the SQ model as a function of bandgap. (B) Scheme of Lattice energy reservoir as dynamic nanodomain in halide perovskites. Blue LER: before energy storage, red LER: energy accumulation by phonon-lattice coupling, higher potential energy is established over the surround. (C) Operational mechanism and architecture of a LBSC. (D) Energy conversion and output processes in LBSC under solar emission.

electricity from otherwise unusable NIR photons. Moreover, because LERs have an extremely long lifetime, on the order of seconds to hours, this upconversion process occurs with remarkable efficiency, making it significantly more effective than conventional multi-photon or rare-earth-based upconversion schemes. An additional benefit of this

approach is that LBSCs inherently recycle the hot phonon emission and therefore operate at lower temperatures than conventional solar cells. By storing hot phonon energy instead of allowing it to dissipate as heat, LBSCs avoid the significant thermal degradation that limits the stability of perovskite based solar cells. This reduction in operational temperature contributes to enhanced device longevity and represents a crucial step towards commercial viability. The theoretical efficiency of LBSCs is estimated to exceed 70%, significantly surpassing the Shockley–Queisser limit.[1] This improvement stems from eliminating two major energy losses in conventional solar cells: hot carrier thermalization and non-absorbed NIR photons. In detail, it comes from the contribution of: i) Extended Solar Absorption (85%), where the perovskite-NIR composite (PNC) absorbs photons across a broader spectrum, capturing ~85% of solar energy, compared to ~33% in single-junction solar cells. ii) Hot Phonon Energy Storage (95%) – Instead of dissipating as heat, excess carrier energy is retained in the LER, minimizing energy loss. iii) Efficient Electron Transfer (95%) – Well-aligned energy levels between the perovskite and NIR absorber ensure minimal recombination losses. iv) Carrier Upconversion (95%) – Stored phonon energy enables sub-bandgap electrons to transition into the conduction band, further enhancing energy conversion.

The overall theoretical efficiency can be estimated as:

$$\eta_{\mathrm{LBSC}} = \eta_{\text{solar absorption}} \times \eta_{\text{phonon storage}} \times \eta_{\text{electron transfer}} \times \eta_{\text{carrier upconversion}}$$

$$\eta_{\mathrm{LBSC}} = 85\% \times 95\% \times 95\% \times 95\% \approx 72\%$$

This fundamentally redefines solar energy conversion, as LBSCs utilize both hot phonon energy and sub-bandgap photons within a single-layer, cost-effective structure, eliminating the need for expensive multi-junction solar cells.

EXPANDING HORIZONS: FUTURE APPLICATIONS

The concept of LBSCs extends beyond traditional photovoltaics, offering practical and near-term applications in high-efficiency integrated solar energy systems, self-powered photodetectors, and solar-driven catalysis. The ability of LERs to retain and redistribute phonon energy can be leveraged for enhanced infrared detection, enabling high-performance night-vision and sensing technologies. Additionally, the extended carrier lifetimes in LBSCs provide a pathway for stable and efficient solar-driven water splitting and CO_2 reduction, improving the feasibility of solar-to-fuel conversion systems. The low-lost single-layer architecture of LBSCs also make them ideal for next-generation flexible and lightweight solar modules, particularly in portable and off-grid power applications. These advancements position LBSCs as a highly scalable and commercially viable alternative to conventional solar technologies, bridging the gap between efficiency, cost, and stability.

STRATEGIC ADVANCEMENTS AND EXPERIMENTAL ROADMAP

While the theoretical foundation for LBSCs is strong, the next step is to validate and optimize their performance through targeted experimental studies. A major challenge lies in the direct characterization of LERs, as these nanodomains exist in a highly dynamic and nonequilibrium state. Advanced spectroscopic techniques, such as TRPL, terahertz spectroscopy, and ultrafast transient absorption, will be crucial in mapping the energy transfer dynamics within LBSCs. Additionally, high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) and strain-mapping TEM can provide valuable structural insights into the presence of LERs, potentially revealing their spatial distribution and evolution under illumination. Parallel to this, the design and fabrication of optimized perovskite-NIR composites will be critical in maximizing LBSC efficiency. The energy level alignment between the perovskite host and the NIR absorber must be precisely controlled to facilitate efficient carrier transfer and minimize recombination losses. Advanced material engineering approaches, such as bandgap tuning via halide mixing and interface passivation strategies, will play a key role in optimizing device performance. Computational modelling using density functional theory (DFT) and molecular dynamics simulations will further elucidate the role of localized lattice distortions in energy storage and delayed carrier relaxation. Beyond fundamental research, the commercial feasibility of LBSCs will depend on the development of scalable manufacturing techniques. Given that LBSCs maintain a single-layer architecture, they are inherently compatible with low-cost solution processing methods, making them an attractive alternative to expensive multi-junction or tandem solar cells. Future efforts will focus on integrating LBSC technology into existing photovoltaic manufacturing pipelines, ensuring that its potential for high efficiency and low cost can be fully realized on an industrial scale.

The introduction of LBSCs represents a paradigm shift in solar energy conversion, offering a fundamentally new approach to surpassing the Shockley–Queisser limit. By leveraging the unique properties of LERs in MHPs, LBSCs overcome two of the most significant limitations of traditional photovoltaics-hot carrier losses and NIR non-absorption, enabling a projected efficiency exceeding 70%. While significant challenges remain, the potential impact of LBSCs on the future of renewable energy cannot be overstated. By combining novel energy storage mechanisms, and full-spectrum solar harvesting, LBSCs offer an unprecedented opportunity to redefine the landscape of next-generation photovoltaics. Continued research in LER characterization, PNC engineering, and scalable fabrication techniques will be critical in advancing this groundbreaking technology from theoretical concept to commercial reality.

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AUTHOR CONTRIBUTIONS

All authors contributed to the manuscript and approved the final version.

DECLARATION OF INTERESTS

The authors declare no competing interests.