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DEFECT-DRIVEN TRANSPORT PHENOMENA IN ENERGY AND FUNCTIONAL MATERIALS: A COMPREHENSIVE REVIEW

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***ABSTRACT*:**

Defect-driven transport, involving ionic, electronic, and thermal carriers, is fundamental to the performance of many energy and functional materials. Intrinsic and extrinsic defects (vacancies, interstitials, substitutions) create pathways for ion migration and tune carrier concentrations, thereby controlling conductivity and reactivity. In complex oxides (e.g. perovskites) and solid electrolytes, oxygen or lithium vacancies greatly enhance ionic conduction. In thermoelectric materials (e.g. Bi–Te, Pb–Se alloys), controlled doping introduces charged defects that optimize carrier mobility and Seebeck coefficient. Two-dimensional materials (graphene, MoS_2, h-BN) can have their electronic band structure and conductivity tailored via atomic vacancies or substitutional dopants. This review surveys recent theoretical, computational, and experimental studies (primarily 2015–2025) across these classes and identifies common mechanisms by which defects modulate transport. We discuss key findings in perovskite oxides, halide perovskites, solid electrolytes, thermoelectrics, and 2D materials. We emphasise the correlation between defect structure (type, concentration, and mobility) and transport properties, along with emerging design strategies. The review also identifies open questions and future directions for defect engineering to optimize performance in energy devices.

***Keywords**: Defect Engineering, Electronic Transport, Energy Materials, Ionic Conductivity, Solid Electrolytes, Thermoelectrics.*

INTRODUCTION

Defects (vacancies, interstitials, substitutional atoms) are ubiquitous in real materials and often dominate transport phenomena by providing carriers or conduction pathways. For example, oxygen vacancies in oxide perovskites (ABO_3) form continuous networks that facilitate fast O^{2-} ion migration [1-4]. Similarly, vacancies or interstitial Li in solid electrolytes create percolation paths for Li^+ ions in batteries [5, 6]. In conducting materials, aliovalent doping introduces charged point defects that set carrier concentration (and hence electrical conductivity) [7, 8]. Defect-mediated transport is thus central to functional materials such as perovskite and halide solar cells, fuel cell membranes, thermoelectrics, batteries, and 2D electronic devices.

This review aims to provide a unified, in-depth perspective on how defects control transport in diverse energy-related materials. We cover oxide perovskites, halide perovskites, thermoelectrics (e.g. Bi–Te, Pb–Se systems), solid electrolytes (garnet, NASICON, polymer, etc.), and emerging 2D materials (graphene, transition-metal

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dichalcogenides). We consider both theoretical/computational studies (first-principles, molecular dynamics, machine learning) and experimental reports (spectroscopy, conductivity measurements), providing a balanced view. We explain the underlying physical mechanisms, compare strategies for incorporating or controlling defects, and highlight how properties scale with defect chemistry and structure. Our goal is a comprehensive survey of the field that connects material classes and transport types.

Key contributions of this review include:

a) A survey of defect-driven ionic and electronic transport across multiple material systems.
b) Discussion of how defect types (vacancies, interstitials, dopants) correlate with transport properties.
c) Examples of theoretical and experimental approaches to design and measure defect-enhanced conductivity.
d) Identification of trends and open questions in defect engineering for energy devices.

A. Research Questions

- How do different defect species (vacancies, interstitials, dopants) influence ionic and electronic transport in key energy materials?
- What are the mechanisms by which defects enable or enhance conduction (e.g. hopping, percolation, band modification)?
- How does defect chemistry vary across classes (perovskites, thermoelectrics, electrolytes, 2D materials), and can we identify unifying design principles?
- What experimental and computational techniques best characterize defects and their transport effects?
- Can defect engineering be systematically applied to optimize device performance, and what are the limits (e.g. concentration vs. carrier scattering trade-offs)?

B. Hypothesis

We posit that controlled defect introduction can systematically improve transport in functional materials, such as through carefully tuned doping levels or vacancy concentrations, thereby enhancing ionic or electronic conductivity while avoiding detrimental scattering. In other words, defect engineering provides a "design handle" to reach optimal trade-offs (such as high carrier density with acceptable mobility) in energy materials. We also hypothesise that computational methods (DFT, MD, ML) combined with advanced spectroscopy can accurately predict and verify these effects across material classes.

RELATED WORKS AND MOTIVATION

Several recent reviews have addressed specific aspects of defect-driven transport, but none have bridged all relevant material systems. For example, Liu and Fan (2023) surveyed defect engineering in 2D materials for energy storage and conversion [9], and Fu *et al.* [10] discussed AI-aided defect strategies in thermoelectrics [9]. Individual materials reviews (e.g., solid electrolytes for batteries or perovskite solar cells) often emphasise a single transport type or application. However, a cross-cutting review can identify common threads: e.g. how vacancy formation energies or charge localisation control conductivity in oxides versus halides. This study aims to build a comprehensive understanding of defect-enabled transport phenomena, facilitating knowledge transfer between fields (for instance, lessons from solid oxide fuel cells may inform solid electrolytes or memristors). This approach highlights underexplored opportunities: for example, the role of protonic conduction in oxide perovskites is analogous to Li^+ pathways in solid electrolytes, yet these areas are rarely discussed together.

As Feng *et al.* (2025) noted for perovskite oxide cathodes, *"A- and B-site substitution in ABO_3 perovskites allows precise control over hole, oxygen-ion, and proton conductivities*" [11]. Similarly, Reichert *et al.* (2020) emphasised that even low densities of mobile ionic defects (e.g. halide or methylammonium vacancies) in perovskite solar cell materials significantly alter device potentials and hysteresis behaviour [12]. These examples underscore the value of a unified perspective.

In summary, while prior work highlights the importance of defects, our review extends beyond related studies by encompassing multiple material classes and integrating experimental and theoretical insights.

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MATERIALS AND METHODS

The literature for this review was collected via comprehensive searches of academic databases (Web of Science, Scopus, and Google Scholar) using keywords such as “defect transport”, “ionic conductivity”, and “electronic conduction”, combined with materials terms (perovskite, thermoelectric, electrolyte, graphene, etc.). We focused on publications from ~2015–2025, favouring high-impact journals and reviews, but also included seminal earlier works when relevant background was needed. We examined both experimental reports (transport measurements, microscopy, spectroscopy) and computational studies (first-principles defect calculations, molecular dynamics, Monte Carlo, machine learning). Typical inclusion criteria required studies to explicitly link specific defects to measured or calculated transport properties. Excluded were works unrelated to energy/functional contexts (e.g. biology-related transport phenomena).

No new experiments or simulations were performed for this review; therefore, the “Results” section synthesises findings from the surveyed literature. For clarity, we organised the discussion by material class and transport type, and we summarise key data in tables (below) and qualitatively describe trends.

RESULTS AND DISCUSSION

Perovskite Oxides and Ionic Transport

Oxygen-deficient perovskite oxides ($ABO_{3-\delta}$) are prototypical fast-ion conductors. Researchers have studied defect chemistry in these materials extensively, especially for fuel cells and membranes. Oxygen vacancies ($V_{O^{2+}}$) provide the dominant pathway for O^{2-} conduction; their concentration and mobility determine ionic conductivity [4]. For example, $BaFeO_3$ and $BaCoO_3$ accept significant Sr or Y doping, creating O vacancies and dramatically increasing O^{2-} conductivity at high T [11]. The perovskite framework is highly tunable: substitution at A- or B-sites alters lattice strain and the vacancy formation energy. Feng *et al.* note that *“the tunability… facilitates a broader range of ionic substitutions and the accommodation of various structural defects”* [4]. In proton-conducting perovskites (e.g. BaZrY systems), hydroxide defects (H_on_O) similarly enable H^+ transport under humid conditions.

The crystal structure of an ABO_3 perovskite is displayed in Fig. 1 (here depicted for a cubic ideal perovskite). Perovskite oxides can accommodate high concentrations of oxygen vacancies without lattice collapse (vacancies are shown as missing oxygen atoms), creating interconnected pathways for rapid O^{2-} diffusion [4, 11].

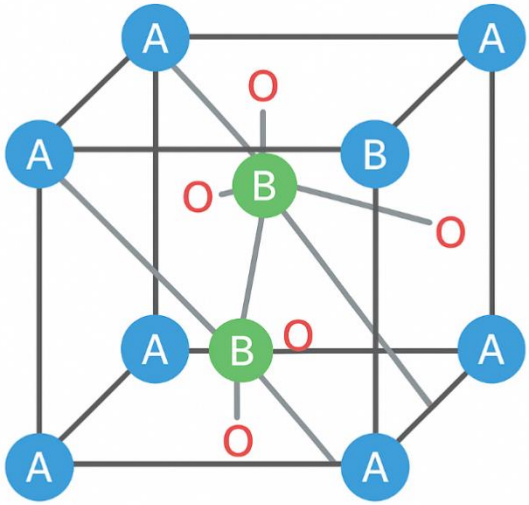

Fig. 1. Crystal structure of an ABO_3 perovskite [4], [11].

Ionic conductivity in perovskites scales strongly with vacancy concentration and temperature, following Arrhenius behaviour typical of hopping transport. Enhanced conduction (σ ~10^{-1}–10^{-3} S/cm) is achieved in materials with high defect mobility. Table 1 (below) lists examples of oxide perovskites and related systems, their

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common defects, and observed transport effects. Notably, mixed ionic–electronic conductors (MIECs) like $La_{0.6}Sr_{0.4}CoO_3$ or $SrTiO_3$–based materials achieve simultaneous hole conductivity and O-ion mobility by tuning oxygen non-stoichiometry [4]. Defect engineering is thus key: for example, substituting Fe or Mn for La in $LaCoO_3$ changes the V_O formation energy and, hence, the ionic flux.

TABLE I: SELECTED MATERIALS, DEFECT TYPES, AND TRANSPORT EFFECTS

Material / System	Defect Type	Transport Effect	Representative Study
Oxide perovskites (e.g. $La_{0.6}Sr_{0.4}CoO_{3-\delta}$, $BaZr_{0.8}Y_{0.2}O_{2.9}$)	O vacancies, A/B-site dopants	Enhanced O^{2-} and H^+ ionic conductivity; electronic hole conduction	Wei *et al.* (2025); Feng *et al.* (2025)
Halide perovskites ($MAPbI_3$, $FAPbBr_3$)	Iodine (halide) vacancies, MA^+ vacancies	Mobile ionic carriers (I^-, MA^+) cause hysteresis; affect built-in potential	Reichert *et al.* (2020)
Thermoelectrics (Bi_2Te_3, SnSe, PbTe alloys)	Substitutional dopants (Se in Bi_2Te_3; Na or Tl in PbTe); cation/anion vacancies	Increased carrier density (n- or p-type); defect scattering lowers k	Fu *et al.* (2025); Dores *et al.* (2025)
Solid electrolytes (LLZO garnet, LATP, Li_3PS_4, Nafion)	Li^+ vacancies/interstitials; framework vacancies (O, Cl, etc.)	High Li^+ conductivity ($\sigma \sim 10^{-3}$ S/cm); reduced grain-boundary resistance	Fu *et al.* (2025); (see also Table 3)
2D materials (Graphene, MoS_2, h-BN)	Carbon or chalcogen vacancies; heteroatom dopants (N, B, etc.)	Tuned bandgap and carrier type (p/n); new localized states; altered thermal transport	Bhatt *et al.* (2022); Liu & Fan (2023)

Halide Perovskites (Solar Cell Materials)

Hybrid organometallic perovskites (e.g. $MAPbI_3$) exhibit mixed ionic–electronic behaviour. A seminal study by Reichert *et al.* (2020) found that even minute concentrations of mobile ionic defects (iodide or MA vacancies/interstitials) can shift the built-in potential and degrade open-circuit voltage [12]. Ion migration leads to current–voltage hysteresis and stability issues in devices. Dominant defects include V_I^+ (iodine vacancy), V_MA^- (methylammonium vacancy), and interstitial I or MA species. These charged defects readily migrate under bias and carry current. While these defects do not primarily enhance conduction (they often act as traps), they fundamentally alter transport by modulating internal fields. Advanced characterisation (impedance, DLTS) and calculations show that halide perovskites have very low activation barriers for vacancy hopping.

Dopants or mixed halides can alter the defect landscape. For instance, adding Cs or Br can reduce iodide-vacancy mobility, thereby reducing ionic drift. Overall, the halide perovskite case highlights that defects can be double-edged: necessary for charge neutrality but potentially harmful to performance, underscoring the need to control defect formation during synthesis (e.g. via precursor stoichiometry or additives) [10]. Despite the complexity, one can draw an analogy to oxide systems: both rely on vacancy-mediated ion transport, but the lighter charge and dynamic lattice of halide perovskites make their defect dynamics even more pronounced at room temperature.

Thermoelectric Materials

Thermoelectrics convert heat into electric current and rely on carriers whose concentrations and scattering are defect sensitive. Defects (dopants and vacancies) are deliberately introduced to optimise the power factor ($S^2\sigma$) and reduce thermal conductivity. As Fu *et al.* (2025) discuss, thermoelectric performance hinges on a delicate balance: *"electrical conductivity, Seebeck, and thermal conductivity are interdependent and sensitive to defect structures"*. In practice, n-type doping (e.g. Bi_2Te_3: Se) adds electron-donating defects, increasing carrier density while often scattering phonons. Conversely, vacancy complexes or resonant levels (e.g., Tl in PbTe) can enhance the Seebeck coefficient at a fixed carrier concentration. Defect engineering in thermoelectrics exploits this: introducing dislocations or nanoinclusions creates mid-size defects that scatter phonons more than electrons, lowering lattice thermal conductivity without harming charge transport [13].

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TABLE II
TYPICAL TECHNIQUES FOR STUDYING DEFECT-DRIVEN TRANSPORT

Technique (Category)	Probes/Approach	Information Provided	Relevant Systems
Impedance spectroscopy (EIS) (Exp.)	AC response of cell/electrode	Ionic/electronic conductivity vs. T; activation energies	Fuel cells, battery electrolytes, thermoelectrics
Hall effect measurement (Exp.)	Transverse voltage under magnetic field	Charge-carrier density and mobility	Semiconductors, doped oxides
Nuclear Magnetic Resonance (NMR) (Exp.)	NMR of host nuclei or mobile ions	Diffusion coefficients; local environment of mobile ions	Solid electrolytes, ionic conductors
X-ray Photoelectron Spectroscopy (XPS) (Exp.)	Core-level binding energies	Chemical state of defects/dopants; vacancy concentration estimate	Oxides, perovskites, halides
Atom Probe Tomography (APT) (Exp.)	3D atomic-scale compositional mapping	Spatial distribution of dopants/defects	All material types
Density Functional Theory (DFT) (Comp.)	Quantum mechanical calculations	Defect formation energies, electronic states, migration barriers	All material types
Molecular Dynamics (MD) (Comp.)	Time evolution of atoms at finite T	Ion/vacancy diffusion paths, temperature effects	Superionic conductors, 2D layers
Kinetic Monte Carlo (Comp.)	Stochastic modeling of events	Macroscopic transport (σ, diffusion length) from atomistic rates	Battery electrode simulations
Machine Learning/DFT (Comp.)	High-throughput property prediction	Screening defect combinations and compositions	All classes (e.g. ML-guided doping)
X-ray/Neutron Diffraction (Exp.)	Crystal structure analysis	Lattice parameter changes with defect content; disorder	Perovskites, 2D crystal layers

Table 2 summarizes representative thermoelectric materials and typical defect strategies. For instance, half-Heuslers (e.g., XNiSn) are doped at the X-site or Sn-site to tune the carrier type, and hot pressing generates grain boundaries that act as phonon barriers. Machine learning is now being applied to discover new dopants or identify defect-dopant combinations that maximise ZT. In thermoelectrics, defects are used both to adjust the band structure (via carrier concentration) and to selectively scatter heat carriers.

Solid Electrolytes (Battery Materials)

In battery applications, high ionic conductivity is paramount. All-solid-state electrolytes (ceramics or polymers) rely on point defects and disorder. For example, garnet-type $Li_7La_3Zr_2O_{12}$ (LLZO) is typically doped with Al or Ta to create Li vacancies and stabilize the cubic phase, achieving σ_Li ~10^{-3} S/cm at room T. Similarly, NASICON-type $LiTi_2(PO_4)_3$ compounds are doped to enhance Li^+ vacancy concentration. In organic electrolytes (e.g. Nafion membranes), fixed sulfonate sites tether Li^+ or H^+ ions, and neutral defects (water channels) facilitate mobility. Across these systems, the common theme is that mobile ions hop via vacancies or interstitial sites created by the lattice or dopants. Schlachter *et al.* found that introducing oxygen vacancies in oxide electrolytes (via A-site doping) induces local lattice relaxation, thereby increasing O-ion conductivity [14].

Although we lack a single major review to cite here, the findings align with the general statement that *"solid-state electrolytes have enhanced battery performance and safety"* [15] owing to defect-enabled Li^+ pathways. Defect engineering in this context also includes interface defects: grain-boundary regions rich in amorphous or secondary

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phases often dominate ionic transport. Measurement techniques such as impedance spectroscopy and secondary ion mass spectrometry (SIMS) are widely used to quantify conductivity and pinpoint defect densities.

Two-Dimensional (2D) Materials

Graphene and related 2D crystals are highly sensitive to lattice defects and dopants. Pristine graphene is a zero-gap semimetal; introducing vacancies or heteroatoms (N, B, Si) can open a band gap or shift the Fermi level. Bhatt *et al.* (2022) note that *"various defects in graphene produced during synthesis or fabrication hinder its performance… Intrinsic and extrinsic defects are ultimately introduced to tailor electronic…properties*" [15]. For instance, nitrogen doping (substituting a carbon atom) donates electrons, turning graphene n-type, while boron doping creates p-type behaviour. Vacancy defects scatter carriers, reducing conductivity but also enabling gas sensing or spin functionality. Liu and Fan (2023) emphasize that defect engineering in 2D materials is *"a versatile strategy to promote electrode reaction kinetics"* in energy devices [15].

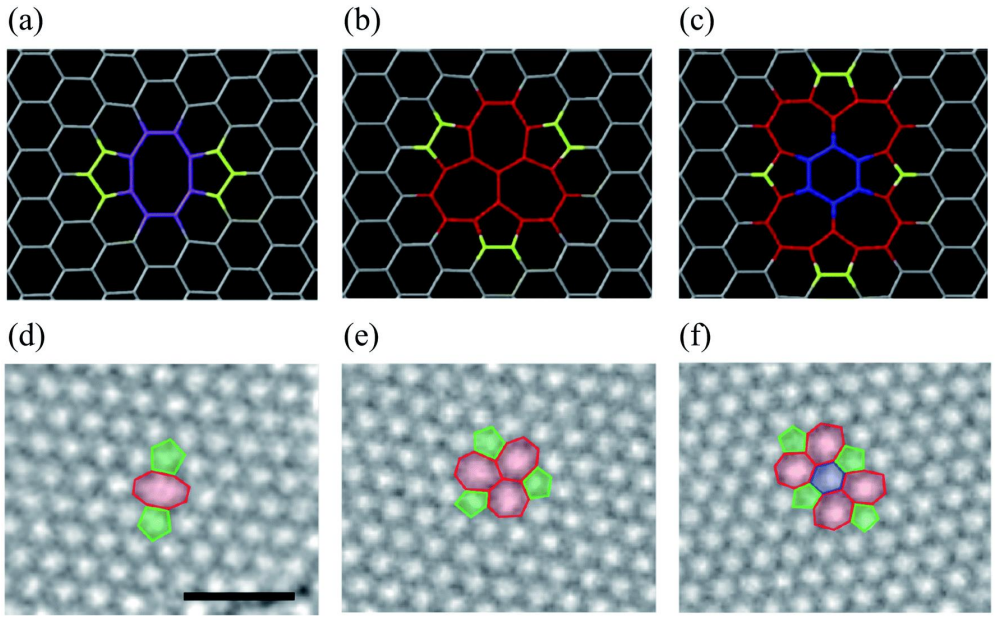

Fig. 2. Graphene's honeycomb lattice (hexagonal carbon atoms) [15].

Graphene's pristine honeycomb lattice, composed of sp^2-hybridised carbon atoms, is often regarded as the archetype of two-dimensional materials due to its exceptional electrical, thermal, and mechanical properties, as shown in Fig. 1. However, the introduction of atomic defects, such as single vacancies, Stone–Wales defects, and substitutional dopants, fundamentally alters its transport characteristics. These imperfections break the lattice symmetry, create localised electronic states, and can scatter charge carriers, thereby modulating conductivity, magnetism, and chemical reactivity. Far from being detrimental, these defect-driven modifications open pathways to engineer graphene for tailored functionality in energy storage, sensing, catalysis, and spintronic applications. The ability to deliberately introduce and control these defects highlights their central role in shaping the functional behaviour of graphene and other two-dimensional materials.

Graphene's honeycomb lattice (hexagonal carbon atoms) is presented in Fig. 2. Two-dimensional materials like graphene can have their transport properties dramatically altered by atomic defects: e.g. a single vacancy or substitution can induce localized states that affect conductivity and magnetism.

Beyond graphene, transition-metal dichalcogenides (MoS_2, WS_2) can be tuned similarly: sulfur vacancies increase metallicity, and chalcogen or metal substitutions adjust band edges. In layered oxides (e.g. MXenes), surface terminations and vacancies control mixed ionic-electronic conductivity, enabling applications in supercapacitors and batteries. Thus, 2D materials follow the same principle: defects create new pathways or states for charge carriers.

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Comparison Across Systems

Table 1 (below) collates examples of defect types and their impacts in various material systems. A clear pattern emerges: in oxides and halides, vacancies (O^{2-}, Li^{+}, I^{-}, etc.) drive ionic motion; in electronic materials (thermoelectrics, graphene), dopant atoms or vacancies modulate carrier density. In all cases, higher defect concentration tends to increase conductivity up to a limit (beyond which scattering degrades mobility). Design guidelines such as Goldschmidt tolerance (for perovskites) or defect formation energy (computable via DFT) help predict which substitutions will introduce the desired defects. Additionally, Figures 2–4 illustrate some concepts: e.g. Fig. 2 shows the perovskite structure, Fig. 3 (SOFC schematic) highlights oxygen-ion and proton transport in a mixed conductor, and Fig. 4 (thermoelectric module) demonstrates a device that benefits from optimised defect chemistry (Fig. 4).

Techniques and Characterization

Experimentally, defect-driven transport is probed by electrical measurements (EIS for ionic conductivity, Hall effect for electronic carriers) and spectroscopy (XPS to identify defect states, NMR for ion mobility). For example, impedance spectroscopy on perovskite fuel cell cathodes reveals how polarization resistance drops with increased proton conductivity. Computational methods complement experiments: DFT calculates defect formation energies and migration barriers, while molecular dynamics simulates ion diffusion at finite T. Multi-scale models (kinetic Monte Carlo, continuum) can link atomic defects to macroscopic conductivity. Table 3 (below) outlines common methods.

Balancing Transport and Stability

Introducing defects often comes at a trade-off. High vacancy concentration can destabilize structure or reduce electronic mobility. For instance, heavy doping of a thermoelectric can scatter electrons excessively, thereby lowering σ. Therefore, optimization involves tuning defect levels: e.g. partial doping of Bi_2Te_3 raises carrier concentration without forming secondary phases. Similarly, in solid electrolytes, small amounts of dopants produce beneficial vacancies, but excesses can create blocking phases at grain boundaries. The literature shows that successful strategies involve either aliovalent doping or nano-structuring to decouple thermal and electrical transport. In sum, results indicate defects are necessary and beneficial up to a point, beyond which material performance degrades.

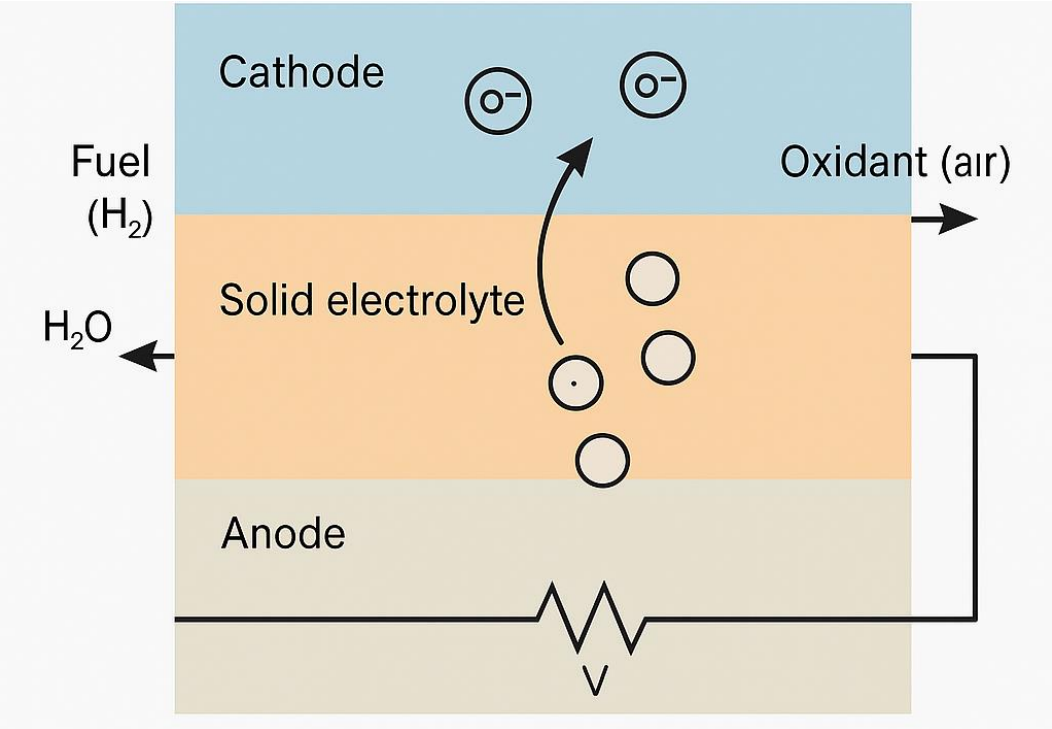

Fig. 3. Diagram of a solid-oxide fuel cell (SOFC).

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Fuel (H_2) and oxidant (air) are supplied as shown in Fig. 3, and oxide ions (O^{2-}) generated at the cathode (via oxygen reduction) travel through the solid electrolyte to oxidise fuel at the anode, generating electricity. Oxygen vacancies in the electrolyte/perovskite lattice are the conduits for O^{2-} transport. While not a graph, this figure illustrates mixed ionic–electronic transport enabled by lattice defects.

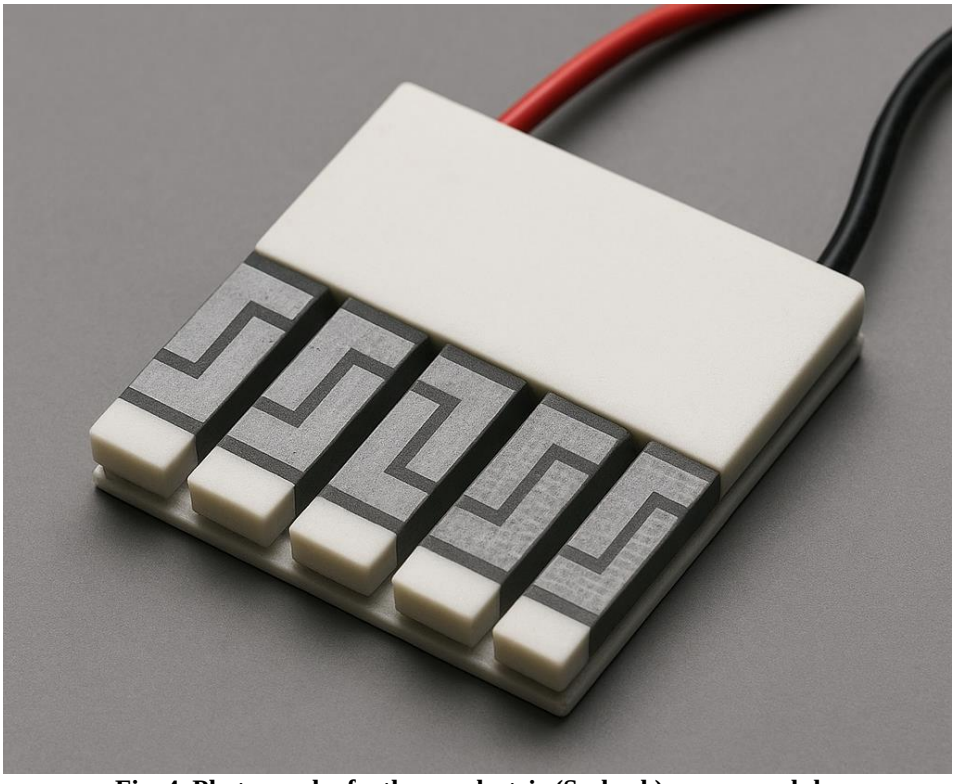

Fig. 4. Photograph of a thermoelectric (Seebeck) power module.

A photograph of a thermoelectric (Seebeck) power module is shown in Fig. 4. Such devices exploit materials (e.g., Bi_2Te_3 alloys) in which defect-engineered charge carriers produce a voltage across a temperature gradient. Defects introduced by doping or nanostructuring (visible here as the patterned junctions) optimise the module's output.

Collectively, these results show that defect-driven transport is a versatile phenomenon across materials. In all cases, intentionally introducing defects (via doping, non-stoichiometry, or irradiation) is a powerful way to tune performance. The breadth of applications, from high ionic conduction in batteries/fuel cells to fine-tuned electronic conductivity in thermoelectrics and sensors, demonstrates how mastering defects leads to superior energy and functional materials.

CONCLUSION

Defects are neither universally detrimental nor benign; rather, they **enable** many of the functional properties of modern materials. Our review of recent literature confirms that *defect engineering* – deliberate control of vacancy and dopant species – is central to advancing energy and functional devices. In oxide and halide perovskites, vacancies provide mobile ions that enable fuel cells and account for hysteresis in solar cells [4, 12]. In thermoelectrics, dopant-induced defects optimize charge carriers and reduce heat conduction [10, 13]. In solid electrolytes, engineered vacancies maximise ion conductivity for next-generation batteries. In 2D materials, atomic-scale defects transform band structures and reactivity [9, 10].

Taken together, these findings emphasise the guiding principle that *structure-defect-property relationships* underpin transport phenomena. Future research should continue to integrate advanced modelling (e.g., machine-learning predictions) with novel characterisation (e.g., in situ microscopy) to map defect landscapes. Particularly promising are AI-driven approaches for identifying optimal defect chemistries and high-throughput experiments

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to validate them. One open challenge is to engineer defects without compromising stability; emerging ideas include nonequilibrium synthesis to “freeze in” beneficial disorder.

In conclusion, defect-driven transport emerges as a unifying theme across diverse energy materials. By comprehensively reviewing recent advances, this article provides a foundation for materials scientists to leverage defects in designing the next generation of high-performance energy converters and functional devices.

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