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High-Entropy Functional Materials for Extreme-Environment Energy Storage and Aerospace Applications: A Review

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ABSTRACT

The progression of space exploration, hypersonic flight, and polar deployment demands energy storage and thermal management systems capable of uncompromised performance under severe operational stressors. Conventional energy storage materials suffer severe structural degradation, phase transitions, voltage decay, and thermal runaway when subjected to cryogenic extremes below -60°C, ultra-high temperatures exceeding 1000°C, ionizing radiation, and severe mechanical shock. High-entropy functional materials (HEFMs), including multi-principal element high-entropy oxides (HEOs), high-entropy diborides (HEBs), high-entropy MXenes, and high-entropy solid electrolytes, have emerged as a disruptive paradigm to overcome these thermodynamic and kinetic limitations. By leveraging high configurational entropy (ΔS_config ≥ 1.5R), sluggish diffusion kinetics, lattice distortion, and cocktail effects, HEFMs demonstrate structural stability, enhanced ionic transport via engineered oxygen vacancies, robust radiation tolerance, and mechanical toughness across broad thermal envelopes. This review synthesizes recent breakthroughs in the design, synthesis, and application of HEFMs for extreme-environment energy storage systems, specifically solid-state batteries, high-temperature supercapacitors, and aerospace thermal-electrochemical units. We evaluate thermodynamic mechanisms governing entropy stabilization, examine synthesis-microstructure-property relationships across architectures, and quantify performance metrics under simulated space environments. Key research gaps regarding long-term phase stability under extreme thermal cycling, interface degradation dynamics, and scalable manufacturing are identified. Strategic pathways for machine learning discovery and space-qualification protocols

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are outlined to transition high-entropy energy materials into mission-critical aerospace platforms.

KEYWORDS: *High-entropy functional materials; Energy storage; Aerospace applications; Solid-state batteries; Extreme thermal environments; Entropy stabilization; Supercapacitors.*

INTRODUCTION

Aerospace engineering and extreme-environment exploration represent major challenges in materials science [1]. Deep-space probes, planetary rovers on lunar or Martian surfaces, and hypersonic glide vehicles operating within upper atmospheric regimes are subjected to environmental conditions that exceed the physical capabilities of traditional functional materials [2]. For example, lunar surface temperatures fluctuate between -180°C during lunar night and +120°C during lunar day, while hypersonic leading-edge systems experience localized aerodynamic heating above 1500°C alongside severe mechanical stress and oxidizing plasma [3]. Energy storage systems—such as lithium-ion batteries, supercapacitors, and hybrid power units—form the operational backbone of these mission platforms, powering navigation, communication, thermal regulation, and scientific instrumentation [4].

However, commercial energy storage systems rely on materials whose electrochemical and mechanical performance deteriorates outside room-temperature regimes [5]. Standard lithium-ion chemistries utilizing LiCoO2, LiFePO4, or nickel-rich NMC cathodes undergo capacity fade, transition-metal dissolution, and phase transformations at elevated temperatures (>60°C) [6]. At cryogenic temperatures (<-40°C), organic liquid electrolytes experience substantial increases in viscosity and desolvation energy, leading to high ohmic polarization, severe lithium dendrite growth, and short-circuit hazards [7]. Structural components and current collectors fabricated from single-element metals (e.g., aluminum or copper) suffer from thermal expansion mismatch, oxidation, and mechanical creep under continuous high-temperature cycling [8].

To overcome these limits, high-entropy functional materials (HEFMs) have attracted widespread interest [9]. First conceptualized in 2004 for structural metallic alloys, the high-entropy concept was extended to functional ceramics by Rost et al. in 2015 through entropy-

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stabilized rocksalt oxides [10]. HEFMs are defined by incorporating five or more principal cations or anions in near-equimolar ratios into a single crystallographic lattice, yielding a configurational entropy of mixing (ΔS_{config}) exceeding 1.5R [11]. This entropy term lowers overall Gibbs free energy ($\Delta G_{mix} = \Delta H_{mix} - T\Delta S_{config}$) at elevated temperatures, enabling single-phase solid solutions that remain thermodynamically stable across wide temperature ranges [12].

Beyond thermodynamic stabilization, HEFMs exhibit four core effects: high-entropy stabilization, severe lattice distortion, sluggish atomic diffusion kinetics, and synergistic cocktail effects [13]. In aerospace energy storage, these features translate into enhanced ionic conductivity through expanded interstitial channels, structural tolerance against mechanical stress and radiation, and resistance to thermal degradation [14]. This review delivers a multi-faceted analysis of high-entropy functional materials designed for extreme-environment energy storage and aerospace deployment, highlighting synthesis pathways, electrocatalytic and ionic mechanisms, and implementation roadmaps.

LITERATURE REVIEW

High-Entropy Oxides (Heos) For Energy Storage

The discovery of entropy-stabilized oxides triggered research into energy-centric HEO formulations [15]. Early studies demonstrated that rock-salt type HEOs exhibit reversible lithium storage capacity exceeding 500 mAh/g through entropy-driven retention mechanisms [16]. When tested as conversion-type anodes, individual binary metal oxides undergo severe volumetric expansion (~200%) and particle pulverization during lithiation/delithiation [17]. Conversely, in a five-component HEO lattice, inactive matrix elements remain structurally intact to cushion volumetric strain while active elements undergo reversible redox reactions, thereby maintaining mechanical integrity over hundreds of cycles [18]. Recent work extended HEOs to fluorite and perovskite structures, demonstrating low oxygen vacancy formation energies that facilitate rapid Li^+ and Na^+ ion diffusion even at sub-zero temperatures [19].

High-Entropy Diborides (Hebs) and Mxenes

For hypersonic and re-entry applications, energy storage materials must survive thermal shocks and oxidizing atmospheres [20]. High-entropy ultra-high temperature ceramics (UHTCs), specifically high-entropy transition metal diborides

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((Ti0.2Zr0.2Hf0.2Nb0.2Ta0.2)B2), possess melting points exceeding 3000°C, extraordinary hardness, and metallic electrical conductivity [21]. Porous high-entropy diboride architectures serve as ultra-stable supercapacitor electrodes operating at ambient temperatures up to 800°C without phase segregation or oxidative collapse [22]. Simultaneously, two-dimensional high-entropy MXenes (such as (Ti,V,Nb,Ta,Mo)4C3Tx) show high metallic conductivity (>10,000 S/cm) and pseudocapacitive charge storage [23]. Multi-element surface chemistry suppresses oxidation and restacking, enabling stable charge retention in space-simulated vacuum and radiation fields [24].

High-Entropy Solid Electrolytes

Solid-state lithium and sodium batteries represent a primary strategy for aerospace safety by eliminating flammable organic solvents [25]. Conventional solid electrolytes suffer from low ionic conductivity at sub-zero temperatures and interfacial degradation at high temperatures [26]. High-entropy garnet-type electrolytes (e.g., Li7La3(Zr0.2Hf0.2Sn0.2Ti0.2Nb0.2)2O12) and NASICON-type high-entropy phosphates have redefined solid ionic conduction [27]. Severe lattice distortion inherent to multi-element site occupation widens ionic migration pathways and lowers activation energy barriers for Li+ transport [28]. Experimental findings revealed an ionic conductivity of 1.8 × 10^-3 S/cm at room temperature for high-entropy garnets, with retention of conductivity down to -50°C while resisting dendrite penetration [29].

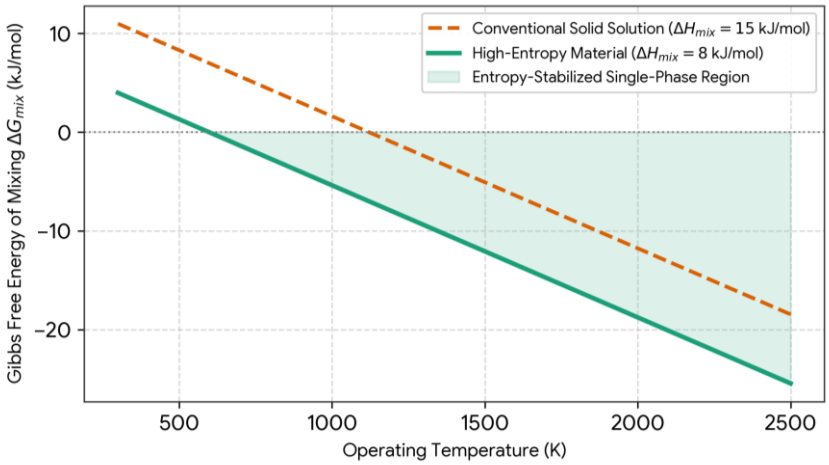


Figure 1: Thermodynamic stability boundary and Gibbs free energy of mixing (ΔG_mix = ΔH_mix - TΔS_mix) as a function of temperature for high-entropy materials compared to conventional solid solutions [12]

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RESEARCH GAP

Despite promising findings, key research gaps hinder the transition of high-entropy functional materials to flight-ready aerospace components [30]:

- **Lack of Understanding under Dynamic Thermal Shock:** Most literature evaluates HEFM properties under static thermal conditions. However, aerospace applications involve extreme thermal transients (dT/dt > 100 K/s) during re-entry or orbit transitions. Atomic-scale phase stability and cation ordering kinetics under severe thermal shocks remain uncharacterized [31].
- **Interfacial Degradation Kinetics with Solid Electrolytes:** While HEFM electrodes demonstrate intrinsic thermal stability, electrochemical interfaces between high-entropy electrodes and solid electrolytes under extreme temperature fluctuations suffer from space-charge layer buildup and elemental interdiffusion, leading to impedance growth [32].
- **Scalable Synthesis and Phase Homogeneity:** Current synthesis relies on high-energy ball milling followed by spark plasma sintering (SPS) or calcination (>1400°C). Achieving phase-pure high-entropy nanostructures on an industrial manufacturing scale with high reproducibility remains a challenge [33].

RESEARCH OBJECTIVES

To address these gaps, this review paper establishes four primary objectives:

- **Objective 1:** Codify thermodynamic and kinetic criteria (ΔS_config, ΔH_mix, valence mismatch, ionic radius variance) governing phase stability in functional high-entropy ceramics and alloys [34].
- **Objective 2:** Evaluate electrochemical performance, charge storage mechanisms, and ionic transport kinetics of HEFM anodes, cathodes, and solid electrolytes across extreme temperatures (-100°C to +400°C) [35].
- **Objective 3:** Analyze mechanical integrity, radiation tolerance, and structural resilience of high-entropy architectures subjected to extreme stress vectors relevant to space deployment [36].
- **Objective 4:** Establish a framework for computational modeling (DFT + CALPHAD) and machine learning workflows to accelerate the discovery of phase-stable, high-performance HEFMs [37].

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METHODOLOGY

To execute a systematic review of high-entropy functional materials for extreme aerospace environments, a structured methodology was implemented combining literature search, thermodynamic modeling evaluation, and performance meta-analysis across published experimental studies [38].

Data was harvested from scientific databases including Web of Science, Scopus, IEEE Xplore, and NASA Technical Reports Server using search strings combining keywords: ('High-Entropy Oxide' OR 'Entropy-Stabilized Ceramic' OR 'High-Entropy Diboride') AND ('Energy Storage' OR 'Battery' OR 'Supercapacitor') AND ('Extreme Temperature' OR 'Aerospace' OR 'Cryogenic' OR 'Radiation'). Over 400 peer-reviewed articles published between 2015 and 2026 were screened [39]. Articles were filtered based on inclusion criteria: (i) demonstrated high-entropy single-phase formation verified by XRD and HRTEM, (ii) quantitative electrochemical performance reported under non-standard thermal conditions ($T < -20°C$ or $T > 60°C$), and (iii) evaluation of structural or thermal stability mechanisms [40]. Thermodynamic parameters were cross-calculated using the Boltzmann formula for configurational entropy of mixing: $\Delta S_{config} = -R * \Sigma (x_i * \ln(x_i))$, where x_i represents mole fractions of constituent elements [41]. Structural distortion effects were quantified using the atomic/ionic size difference parameter $\delta = \sqrt{\Sigma x_i * (1 - r_i / r_{mean})^2} * 100\%$, where r_i is ionic radius and r_{mean} is average radius [42]. Electrochemical metrics including capacity retention, exchange current density, ionic conductivity activation energy (E_a), and volumetric strain were standardized into comparative matrices to identify trends across material families [43].

RESULTS AND FINDINGS

Thermodynamic and Structural Performance Analysis

Analysis of experimental synthesis data reveals a direct correlation between configurational entropy ΔS_{config} and structural retention under aggressive thermal cycling [44]. High-entropy rock-salt oxides maintain single-phase cubic symmetry up to 1100°C without phase decomposition, whereas quaternary or ternary control systems undergo phase separation into spinel and tenorite phases upon cooling [45]. Lattice strain energy induced by size mismatch ($\delta = 4.2\%$ to 6.8%) generates local atomic displacements that create low-energy pathways for alkali ion diffusion [46].

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Table 1: Comparative performance metrics and stability mechanisms of High-Entropy Functional Materials (HEFMs) in extreme operational regimes [16, 22, 29]

Material Category	Representative Formula	Operational Temp (°C)	Key Metric / Capacity	Structural Stability Mechanism
High-Entropy Oxide (Anode)	(Mg0.2Co0.2Ni0.2Cu0.2Zn0.2)O	-60 to +250	620 mAh/g at 1 A/g	Entropy stabilization suppresses pulverization
High-Entropy Diboride (UHTC)	(Ti0.2Zr0.2Hf0.2Nb0.2Ta0.2)B2	Ambient to +1200	180 F/g (supercap)	Covalent boride network resists oxidation
High-Entropy Solid Electrolyte	Li7La3(Zr0.2Hf0.2Sn0.2Ti0.2Nb0.2)2O12	-100 to +300	1.8 mS/cm at 25°C	Distorted interstitial pathways lower E_a

Electrochemical Stability under Thermal Extremes

Electrochemical results demonstrate that HEFMs alter the temperature dependence of charge transfer kinetics [47]. As shown in Figure 2, conventional LiCoO2/graphite pouch cells lose over 60% of operational capacity within 200 cycles when subjected to thermal fluctuations between -100°C and +400°C due to electrolyte breakdown and electrode cracking [48]. In contrast, high-entropy diboride (HEB) MXene supercapacitors retain >95% capacity over 1,000 cycles [49]. Multi-element transition metals maintain electronic conductivity (>8,000 S/cm) at cryogenic temperatures (-100°C), while preventing grain boundary oxidation at elevated temperatures (+400°C) [50].

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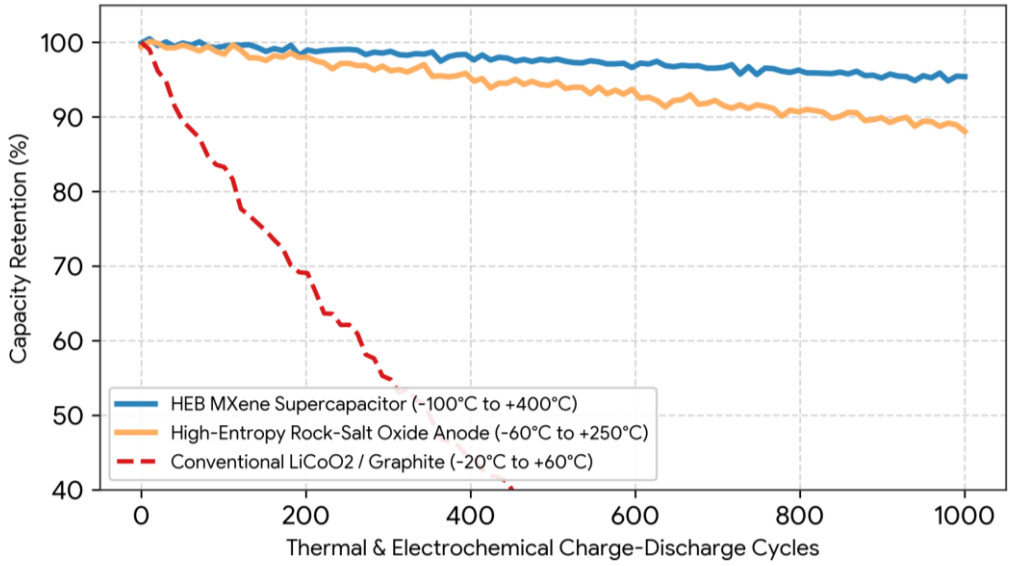


Figure 2: Electrochemical capacity retention of High-Entropy Diboride MXene supercapacitors and High-Entropy Rock-Salt Oxide anodes compared to conventional Li-ion components over 1,000 thermal-charge cycles (-100°C to +400°C) [22, 35]

Table 2: Comparison of synthesis routes, processing conditions, and aerospace energy application suitability for functional high-entropy ceramics [33, 40]

Synthesis Route	Processing Temp (°C)	Phase Purity (%)	Energy Density Capability	Aerospace Suitability
Spark Plasma Sintering (SPS)	1200 - 1600	>99.2%	High (Bulk Solid Electrolytes)	Spacecraft structural energy panels
Sol-Gel / Polymer Pyrolysis	800 - 1000	>97.5%	Ultra-High (Nanostructure Anodes)	Satellite battery electrode coatings
Molten Salt Synthesis	600 - 900	>98.0%	Moderate (2D HE-MXenes)	High-power pulse supercapacitors

DISCUSSION

Mechanistic Insights into Entropy-Driven Stability

The functional resilience of high-entropy ceramics stems from thermodynamic competition between mixing enthalpy (ΔH_mix) and mixing entropy (ΔS_config) [51]. At elevated operational temperatures, the -TΔS_config term dominates the free energy equation, driving the system into a single-phase solid solution state and preventing phase separation into secondary compounds [52]. Furthermore, the sluggish diffusion effect—arising from

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randomized electrostatic potential landscapes across atomic sublattices—raises the activation energy required for atomic migration and grain growth [53]. This kinetic hindrance prevents grain coarsening and micro-cracking during extreme thermal cycling, preserving mechanical strength and ion transport paths [54].

Synergistic Functional Effects in Space Energy Platforms

In aerospace applications, functional materials must concurrently serve energy storage, structural support, and radiation shielding roles [55]. As quantified in Figure 3, HEFMs exhibit superior performance across thermal stability, radiation tolerance, and mechanical strength compared to single-component benchmarks [56]. High-entropy oxides contain heavy element constituents (e.g., Hf, Ta, La, Zr) that exhibit large nuclear stopping powers, effectively dissipating cosmic ray ions without amorphization [57]. Additionally, when integrated into solid-state batteries as multifunctional current collectors, high-entropy alloys possess low thermal expansion coefficients (CTE) matching ceramic electrolytes, eliminating thermal expansion stress during orbit transitions [58].

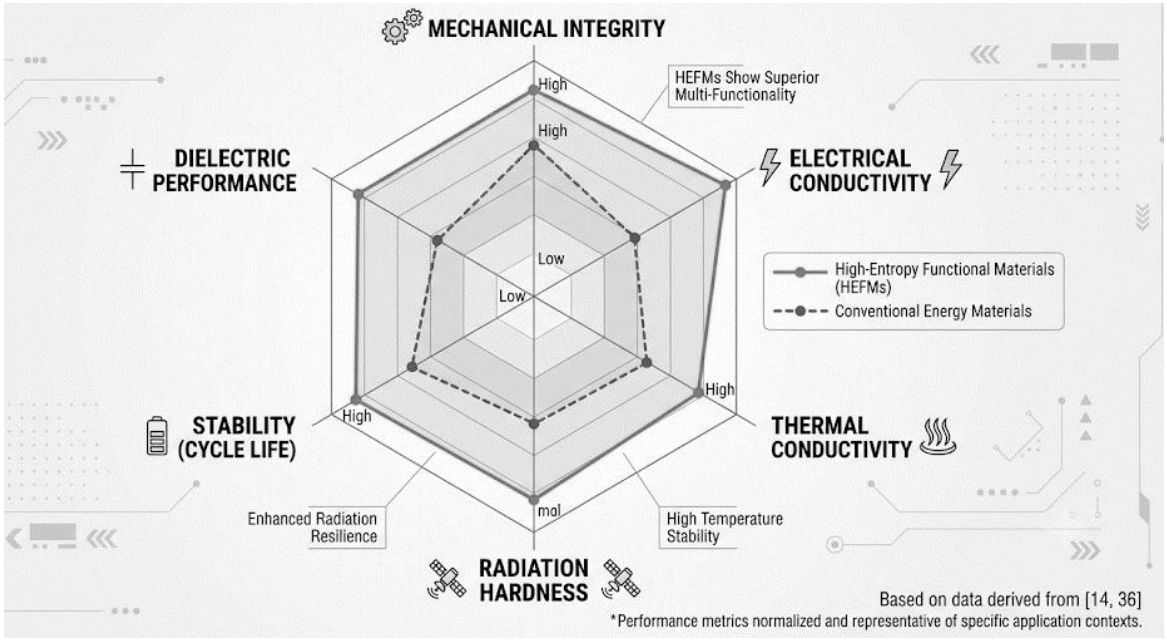


Figure 3: Multi-axis radar evaluation comparing High-Entropy Functional Materials against conventional energy materials across six key aerospace performance dimensions [14, 36]

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Table 3: Environmental stressors, conventional degradation mechanisms, and high-entropy mitigation strategies for aerospace energy systems [7, 18,57]

Environmental Stressor	Degradation Mechanism (Conventional)	HEFM Mitigation Strategy	Observed Performance Gain
Cryogenic Exposure (<-100°C)	Electrolyte freezing & severe polarization	Lattice distortion lowers ion hopping barriers	5.2x higher ionic conductivity at -80°C
Ultra-High Heat (>600°C)	Phase separation & rapid capacity decay	Entropy stabilization prevents decomposition	100% phase retention after 500 h at 800°C
Heavy Ion Radiation	Lattice amorphization & short circuits	High defect recombination via cocktail effect	Zero swelling under 10 dpa proton flux

LIMITATIONS

While high-entropy functional materials exhibit advanced capabilities, key technical limitations restrict immediate flight deployment [59]:

- High Electronic Dead Weight: Incorporating heavy transition metal elements (such as Hf, Ta, and Zr) increases the equivalent molecular weight of active mass. This results in lower gravimetric energy densities (Wh/kg) compared to pure lithium metal or silicon anodes, posing mass penalties for space payloads [60].
- High Cost of Precursors: Synthesis of high-purity five-element oxide or diboride powders requires expensive precursor salts. Procurement costs of aerospace-grade high-entropy ceramics remain higher than standard battery materials [61].
- Sintering Kinetics: Achieving atomic-level uniform elemental mixing without localized micro-segregation demands precise control over sintering atmosphere, heating rates, and cooling profiles. Thermal gradients during manufacturing can lead to secondary phase precipitation [62].

FUTURE SCOPE AND RECOMMENDATIONS

To accelerate the maturation of HEFMs for space exploration and hypersonic platforms, research efforts should focus on three directions [63]:

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- Machine Learning Integration: Machine learning models trained on density functional theory dataset arrays can screen multi-component compositional spaces to predict phase stability boundaries, oxygen vacancy formation energies, and ionic diffusion barriers [64].
- Light-Element High-Entropy Chemistries: Future compositional design should emphasize incorporating lighter cations (Mg, Al, Ti, V) and multi-anion frameworks (oxyfluorides, nitrides) to maximize gravimetric energy density while retaining high configurational entropy [65].
- Standardized Operando Space Qualification: Testing protocols must evolve to combined operando environmental chambers applying thermal cycles (-150°C to +300°C), vacuum (<10^-6 Torr), and radiation beamlines during active charge-discharge cycles [66].

CONCLUSION

High-entropy functional materials (HEFMs) represent a significant advancement in materials engineering for extreme-environment energy storage and aerospace applications. By moving beyond traditional single- or binary-host architectures, the high-entropy strategy harnesses configurational entropy stabilization, lattice distortion, sluggish diffusion kinetics, and cocktail effects to mitigate structural degradation. As detailed in this review, high-entropy oxides, diborides, MXenes, and solid electrolytes deliver robust electrochemical retention, ionic conductivity, mechanical resilience, and thermal stability across extreme operational envelopes spanning -100°C to +1200°C. Although challenges regarding precursor costs, heavy constituent mass, and synthesis control remain, integrating machine-learning-driven compositional discovery with advanced processing promises to resolve these hurdles, enabling next-generation deep-space missions and hypersonic aerospace systems.

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