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A mini-review on high-entropy alloy nanomaterials for electrocatalysis: advances and prospects

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High-entropy alloy nanomaterials (HEA-NMs), composed of multiple metallic elements, offer tunable electronic structures, abundant active sites, and excellent stability, making them highly promising for electrocatalysis. This mini-review summarizes their structural effects influencing electrocatalytic behavior, recent advances in synthesis strategies, and electrocatalytic applications, including the hydrogen evolution reaction (HER), oxygen evolution reaction (OER), oxygen reduction reaction (ORR), carbon dioxide reduction reaction (CO₂RR), and nitrate reduction reaction (NO₃RR). Challenges in synthesis scalability and mechanistic probing are discussed, along with future directions for atomic-level design and data-driven catalyst optimization. HEA-NMs offer a versatile platform for sustainable energy and environmental electrocatalysis.

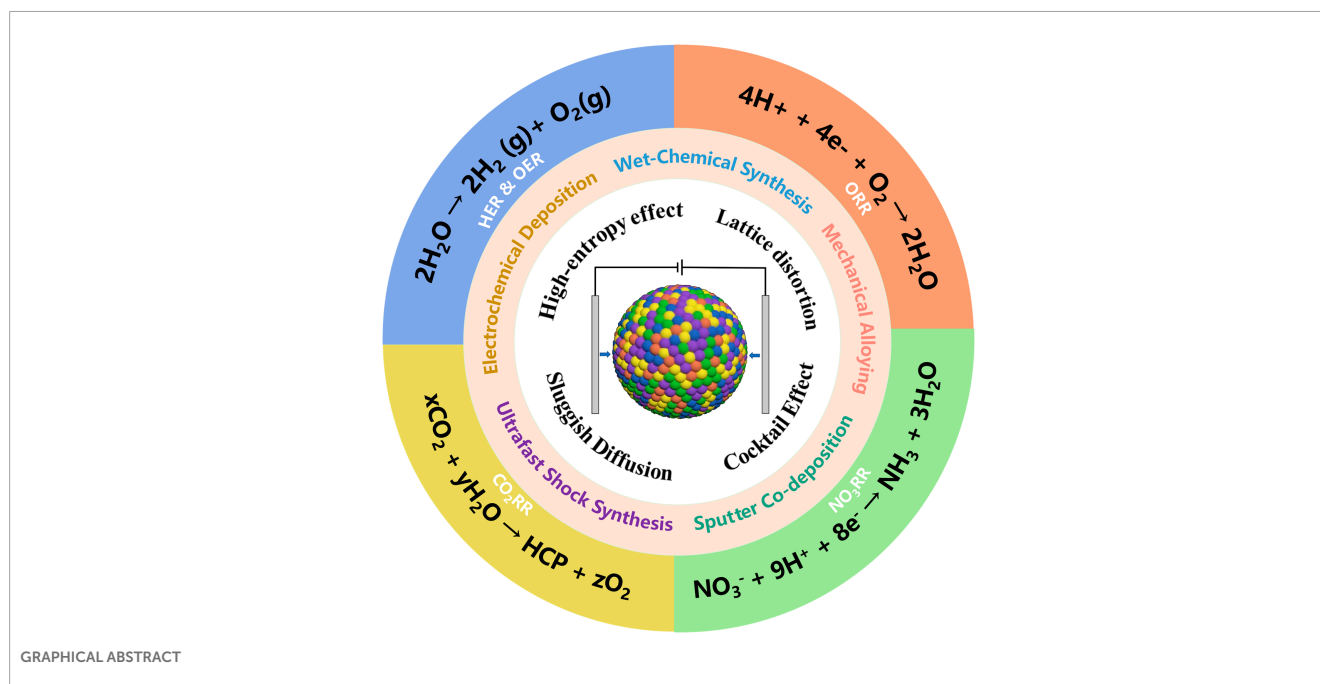
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1 Introduction

The urgent demand for sustainable energy and environmental solutions has accelerated the development of advanced electrocatalysts, which play a central role in enhancing reaction kinetics and lowering activation barriers in processes such as water splitting (Liu et al., 2025), fuel cells (Serov, 2022), and CO₂ conversion (Gandionco et al., 2024). High-entropy alloys (HEAs), composed of five or more principal elements in near-equimolar ratios, have emerged as a promising class of materials due to their high configurational entropy, which stabilizes single-phase solid solutions (Yeh et al., 2004). Their unique features including lattice distortion, sluggish diffusion, and multi-element synergy contribute to enhanced structural stability and tunable catalytic properties.

The integration of HEA concepts into the nanoscale has led to the emergence of high-entropy alloy nanomaterials (Li et al., 2024a), which further benefit from increased surface-to-volume ratios, abundant active sites, and adjustable electronic structures. These attributes enhance intermediate adsorption, accelerate reaction kinetics, and improve product selectivity. Since the first synthesis of HEA nanoparticles in 2018 (Yao et al., 2018), HEA-NMs have demonstrated impressive performance in various electrochemical reactions, including the hydrogen evolution reaction (HER), oxygen evolution reaction



(OER), oxygen reduction reaction (ORR), carbon dioxide reduction (CO₂RR), and nitrate reduction (NO₃RR).

This mini-review summarizes recent progress in HEA-NMs for electrocatalysis. We examine the mechanistic origins of their activity, current synthetic approaches for controlled nanostructure fabrication, and their applications in representative electrocatalytic reactions. Finally, we outline remaining challenges and future opportunities for advancing HEA-NMs as multifunctional electrocatalysts for next-generation energy and environmental technologies.

2 Mechanistic effects underlying the electrocatalytic behavior of HEA-NMs

2.1 High-entropy effect

The high-entropy effect, derived from the near-equiatomic incorporation of five or more elements, leads to high configurational entropy ($\Delta S_{\text{mix}} \geq 1.5 R$) (Wang et al., 2024) and low Gibbs free energy of intermetallic compounds ($\Delta G_{\text{mix}} = \Delta H_{\text{mix}} - T\Delta S_{\text{mix}}$) (Lee et al., 2023), favoring the formation of stable solid-solution phases over intermetallics. At the nanoscale, this effect is amplified by high surface energy, enabling single-phase structures and enhancing long-term stability in electrochemical environments. Homogeneous multi-element distributions further ensure consistent catalytic activity.

2.2 Lattice distortion and electronic modulation

Atomic size mismatch induces severe lattice distortion in HEA-NMs, disrupting periodic structures and modifying the local

electronic environment (Li et al., 2024b). This shifts d-band centers and tunes adsorption energies of key intermediates, boosting catalytic performance. Nanoscale effects intensify distortion and promote favorable electronic interactions for reactions such as CO₂ and NO₃[−] reduction (Shaikh et al., 2024).

2.3 Sluggish diffusion and microstructural stability

The multi-element environment introduces diverse diffusion barriers, reducing atomic mobility and suppressing grain coarsening (Lee et al., 2023). This “sluggish diffusion” helps preserve the nanostructure and compositional uniformity under harsh conditions, contributing to the thermal and electrochemical durability of HEA-NMs.

2.4 Cocktail effect and synergistic active sites

The cocktail effect describes the synergistic properties from multielemental interactions that go beyond the sum of individual elements (Kamaruddin et al., 2024). These include coexisting catalytic sites, adaptive surface reconstructions, and multi-pathway reactivity, all of which enhance charge transfer and overall catalytic versatility (Liu et al., 2024).

In addition to the above structural and electronic effects, the careful selection of elemental combinations is essential in the designation of HEA-NMs. Factors such as mixing enthalpy, atomic size, and electronegativity must be considered to ensure the formation of single-phase solid solution nanoalloys. Moreover, computational approaches such as density functional theory (DFT) and machine learning (ML) play an increasingly important role

in elucidating the microenvironment of HEA-NMs and forecasting interfacial reactions. For instance, Roy et al. (2022) demonstrated the use of ML algorithms to screen high-entropy alloy catalysts suitable for the selective hydrogenation of CO₂ to methanol. These predictive tools provide valuable insights for the rational design of HEA-NMs tailored for specific electrocatalytic applications.

3 Synthetic strategies of HEA-NMs for electrocatalysis

The synthesis of HEA-NMs requires methods that ensure compositional uniformity, structural tunability, and nanoscale stability. The main synthesis methods for HEA-NMs include five representative strategies.

3.1 Mechanical alloying

This solid-state method uses high-energy ball milling to alloy elemental powders through repeated cold welding and fracturing (Figure 1a) (Mongella et al., 2025). It enables the formation of metastable solid solutions from even immiscible elements. Post-annealing or cryomilling enhances grain refinement. Though scalable and solvent-free, it often yields irregular or aggregated particles with limited morphology control.

3.2 Sputter co-deposition

This technique allows atomic-level control by co-depositing multiple metals onto substrates (Figure 1b). Parameters like power and deposition time tune size and composition. CrMnFeCoNi HEA-NMs synthesized via ionic liquid as substrate showed exceptionally high electrocatalytic activity and phase stability (Löffler et al., 2018). This method is ideal for fabricating model electrocatalysts for fundamental studies.

3.3 Electrochemical deposition

Electrochemical methods involve co-deposition of multiple metal ions onto conductive substrates under applied potential (Figure 1c) (Bian et al., 2023). This strategy enables the direct growth of HEA-NMs with controllable thickness and crystallinity. It is energy-efficient, room-temperature, and easily scalable. However, achieving uniform deposition of elements with vastly different reduction potentials remains a challenge, often requiring pulse techniques or complexing agents to balance deposition kinetics. These issues become more pronounced during scale-up, with reduced control over composition and particle uniformity.

3.4 Ultrafast shock synthesis

Ultrafast shock synthesis enables rapid formation of HEA-NMs under non-equilibrium conditions, typically using carbothermal shock, Joule heating, or laser ablation. These

methods achieve heating rates exceeding 10⁵ K/s, promoting atomic-scale mixing and preventing phase segregation (Figure 1d). The resulting nanoparticles are ultrasmall, often below 5 nm, providing better atomic control. For instance, PtPdRhRuCe HEA-NMs synthesized via carbothermal shock showed enhanced ammonia oxidation activity and phase stability (Yao et al., 2018).

3.5 Wet-chemical synthesis

Co-reduction or polyol processes allow controlled nucleation and morphology tuning with scalability. These cost-effective methods are surfactant-compatible but require careful optimization to prevent contamination. Wei et al. synthesized PtMoPdRhNi HEA-NMs exhibiting an ultralow overpotential of 9.7 mV at 10 mA cm⁻² in the alkaline HER via this approach (Figure 1e) (Wei et al., 2023). However, during scale-up, variations in nucleation and reduction rates often lead to elemental segregation and broader particle size distributions.

Each synthesis method for HEA-NMs has specific strengths and limitations in atomic control, scalability, cost, and tunability. Mechanical alloying is inexpensive and scalable but lacks control over morphology and composition. Sputter co-deposition offers atomic precision, suited for mechanistic studies, though high cost and poor scalability limit broader use. Electrochemical deposition is energy-efficient under mild conditions, but uniform co-deposition is difficult due to reduction potential differences. Ultrafast shock synthesis rapidly produces ultrafine, mixed nanoparticles but needs specialized equipment and has limited compositional control. Wet-chemical synthesis is low-cost and flexible but prone to segregation and contamination. Thus, synthesis strategies should match the performance and scalability demands of the target application.

Despite progress, scaling HEA-NM synthesis remains difficult. During batch production, elemental segregation arises from differences in reduction kinetics and nucleation, especially in wet-chemical and electrochemical methods. These approaches also struggle to maintain uniform particle size and composition. Phase control is harder under thermal and concentration gradients at Gram scale. While mechanical alloying and ultrafast shock synthesis show gram-scale potential (e.g., Yao et al., 2018), industrial adoption is limited by reproducibility, cost, and complexity. Solving these issues is key to enabling HEA-NMs in practical electrocatalytic systems.

4 Electrocatalytic applications of HEA nanomaterials

HEA-NMs, with high surface-to-volume ratios and compositional complexity, offer abundant active sites, tunable intermediate adsorption, and robust structural stability. These characteristics make them highly promising for key electrochemical reactions, including HER, OER, ORR, CO₂RR, and NO₃RR, where they often match or surpass the performance of state-of-the-art single or bimetallic catalysts in terms of overpotential, current density, Tafel slope, conversion, selectivity, and durability (Table 1) (Hao et al., 2022; Wang et al., 2025).

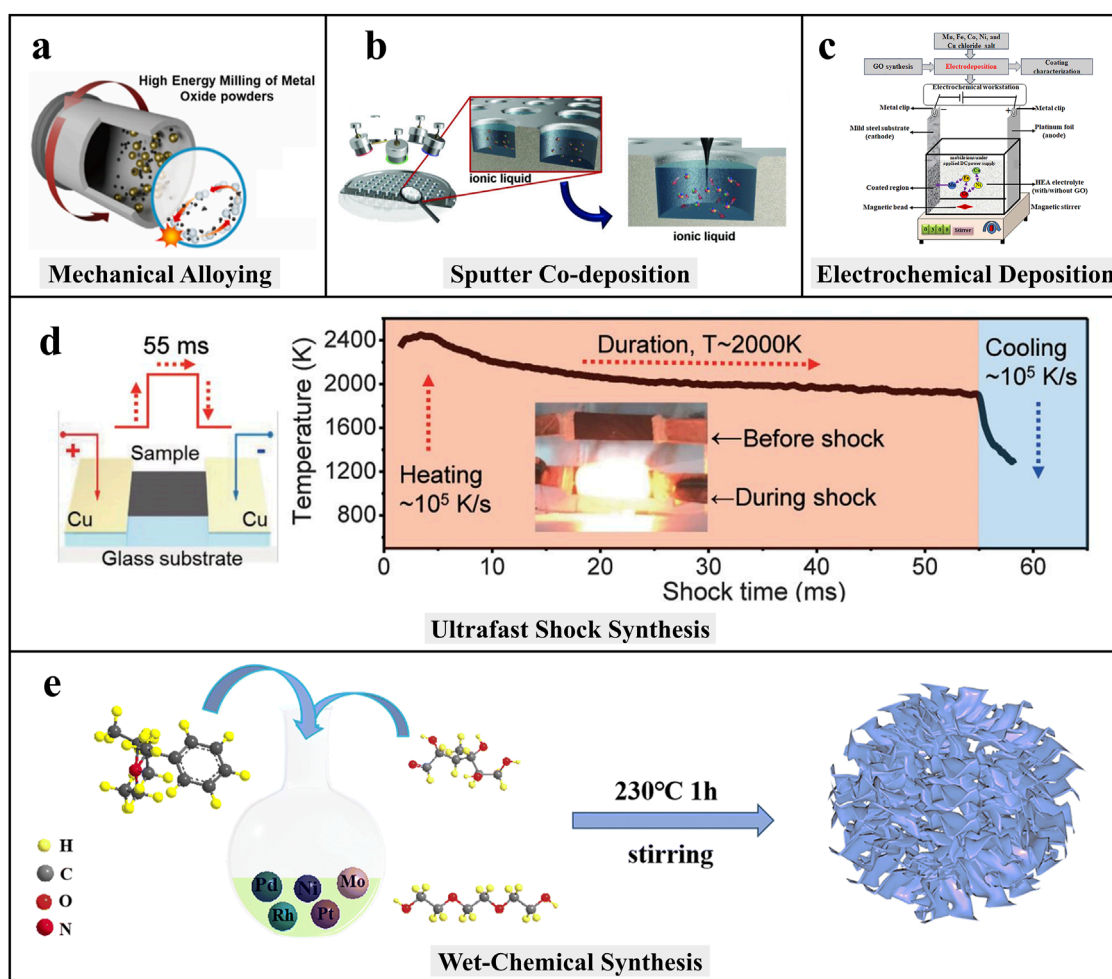


FIGURE 1

Five synthesis methods for HEA-NMs: (a) Mechanical alloying (Mongella et al., 2025); (b) Sputter co-deposition (Löfller et al., 2018); (c) Electrochemical deposition (Bian et al., 2023); (d) Ultrafast shock methods (Yao et al., 2018); and (e) Wet chemical synthesis (Wei et al., 2023).

4.1 HER and OER

HEA-NMs enhance HER and OER via d-band modulation and atomic-level disorder, promoting water dissociation and intermediate adsorption (Wei et al., 2023). In HER, tuning ΔG_{H} across heterogeneous sites improves both Volmer and Tafel steps (Huang et al., 2024). In OER, a wide distribution of $^*\text{OOH}$ binding energies enables overpotential reduction and activity enhancement (He et al., 2023). The entropy-stabilized structure and “cocktail effect” contribute to long-term durability. HEA catalysts also maintain stable performance over a broad range of loadings, enabling integration into thin-film and porous electrodes for practical water electrolysis applications.

4.2 ORR

HEA-NMs improve ORR activity by tuning electronic structures and $^*\text{OOH}$ adsorption through multi-element alloying (Zhao et al., 2024). The disordered surface provides a range of binding energies,

promoting $4e^-$ pathways and enhanced kinetics. Many HEAs surpass Pt/C in mass activity, half-wave potential, and durability (Chen et al., 2023a). Their corrosion resistance and composition flexibility allow operation across pH conditions and electrolytes (Xie et al., 2024a). HEA catalysts also deliver stable performance across various loadings, supporting their integration into cathodes for fuel cells and metal–air batteries (Figure 2b).

4.3 CO₂RR

HEA-NMs offer diverse active sites for key intermediates such as $^*\text{COOH}$, $^*\text{CO}$, and $^*\text{CHO}$, enabling tuning of adsorption energies and product selectivity (Ding et al., 2021; Nellaiappan et al., 2020). Stronger $^*\text{CO}$ binding favors CH_4 formation, while weaker binding promotes CO evolution. Multi-metallic surfaces facilitate simultaneous stabilization of intermediates and C–C coupling (Xing et al., 2025). Nanoscale features, including high surface area and short diffusion lengths, enhance conversion efficiency. HEA catalysts demonstrate low overpotentials, high current densities, and

TABLE 1 Comparison of the application performance of HEA-NM with single or bimetallic catalysts.

Reaction	Catalyst	Overpotential [V vs. RHE]	Current density [mA cm ⁻²]	Tafel slope [mV dec ⁻¹]	TOF [s ⁻¹]	ECSA normalization [cm ⁻²]	Conversion [%]	Selectivity [%]	Durability	Scalability	Electrolytes	Ref.
HER	FeNiCoCrRu	0.148	600	52.2	0.168	5767.5	—	—	3050 h@250 mA cm ⁻²	High (process maturity)	1 M KOH/1 M KOH +0.5 M NaCl	Xie et al. (2024b)
	Pt/C	—	—	84.5	—	—	—	—	—	—	—	—
	Pt ₂₁ Ni ₂₇ Fe ₁₉ Co ₁₇ Cu ₁₆ /C	0.012	10	36	—	—	—	—	—	High (process maturity)	1 M KOH	Li et al. (2020)
	Pt/C	—	—	98	—	—	—	—	—	—	—	—
	PdMoGaInNi	0.013	10	149	1.2	—	—	—	12 h	High (process maturity)	0.5 M H ₂ SO ₄	Fu et al. (2022)
	Pd/C	0.042	—	185.1	—	—	—	—	—	—	—	—
	Pt/C	0.017	—	127.6	0.5	—	—	—	—	—	—	—
	RuAu-RGO	0.056	10	113	3.87	—	—	—	10 h@0.5 mA cm ⁻²	—	1 M KOH	Khalid et al. (2021)
	RuPx@NPC	0.074	10	70	—	—	—	—	1000 CV cycles@10 mA cm ⁻²	—	1 M KOH	Chi et al. (2018)
	IrFeCoNiCu	0.302	—	58	—	—	—	—	—	Low (laboratory scale)	1 M KOH	Maulana et al. (2023)
OER	Ir	0.352	10	75.8	—	—	—	—	—	—	—	—
	IrCo	—	—	83.8	—	—	—	—	—	—	—	—
	ZnFeNiCoCr	0.305	10	76.8	—	—	—	—	240 h	Medium (requires high temperature annealing)	0.1 M KOH	Li et al. (2025a)
	RuO ₂	0.328	—	—	—	—	—	—	—	—	—	—
ORR	ZnFeNiCoCr	1.018	—	76.8	—	—	—	—	2,000 CV cycles@10 mA cm ⁻²	Medium (requires high temperature annealing)	0.1 M KOH	Li et al. (2025a)
	PNN/NC	—	—	80.5	—	—	—	—	1,200 s	—	0.1 M KOH	Chen et al. (2023b)

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TABLE 1 (Continued) Comparison of the application performance of HEA-NM with single or bimetallic catalysts.

Reaction	Catalyst	Overpotential [V vs. RHE]	Current density [mA cm ⁻²]	Tafel slope [mV dec ⁻¹]	TOF [s ⁻¹]	ECSA normalization [cm ⁻²]	Conversion [%]	Selectivity [%]	Durability	Scalability	Electrolytes	Ref.
CO ₂ RR	AuAgPtPdCu	-0.3	—	—	—	—	—	—	5 h	High (process maturity)	0.5 M K ₂ SO ₄	Nellaippan et al. (2020)
	FeCoNiMnCuAl@C	1.05	—	—	—	—	—	—	134 cycles@100 mA g ⁻¹	High (process maturity)	Li ₂ CO ₃	Yi et al. (2024)
	CuAl@C	1.50	—	—	—	—	—	—	—	—	—	—
NO ₃ RR	FeCoNiCuRu 1.5/C	—	—	—	—	—	90.2	92.2	120 h@90.0% conversion rate	High (process maturity)	100 mg N/L + 0.1 M Na ₂ SO ₄	Wu et al. (2025)
	FeCoNiCu(Zn)@MC	—	—	—	—	462.5	91.1	89	5 cycles	High (process maturity)	50 mg N/L +0.1 M Na ₂ SO ₄	Chen et al. (2025)
	FeNi	—	—	88.9	—	—	93.59	86.6	6 cycles	—	45 mg N/L +0.5 M Na ₂ SO ₄	Li et al. (2025b)
	Cu/TNTA-300	—	—	—	—	557.5	84.3	—	10 cycles	—	50 mg N/L +0.1 M Na ₂ SO ₄	Song et al. (2022)

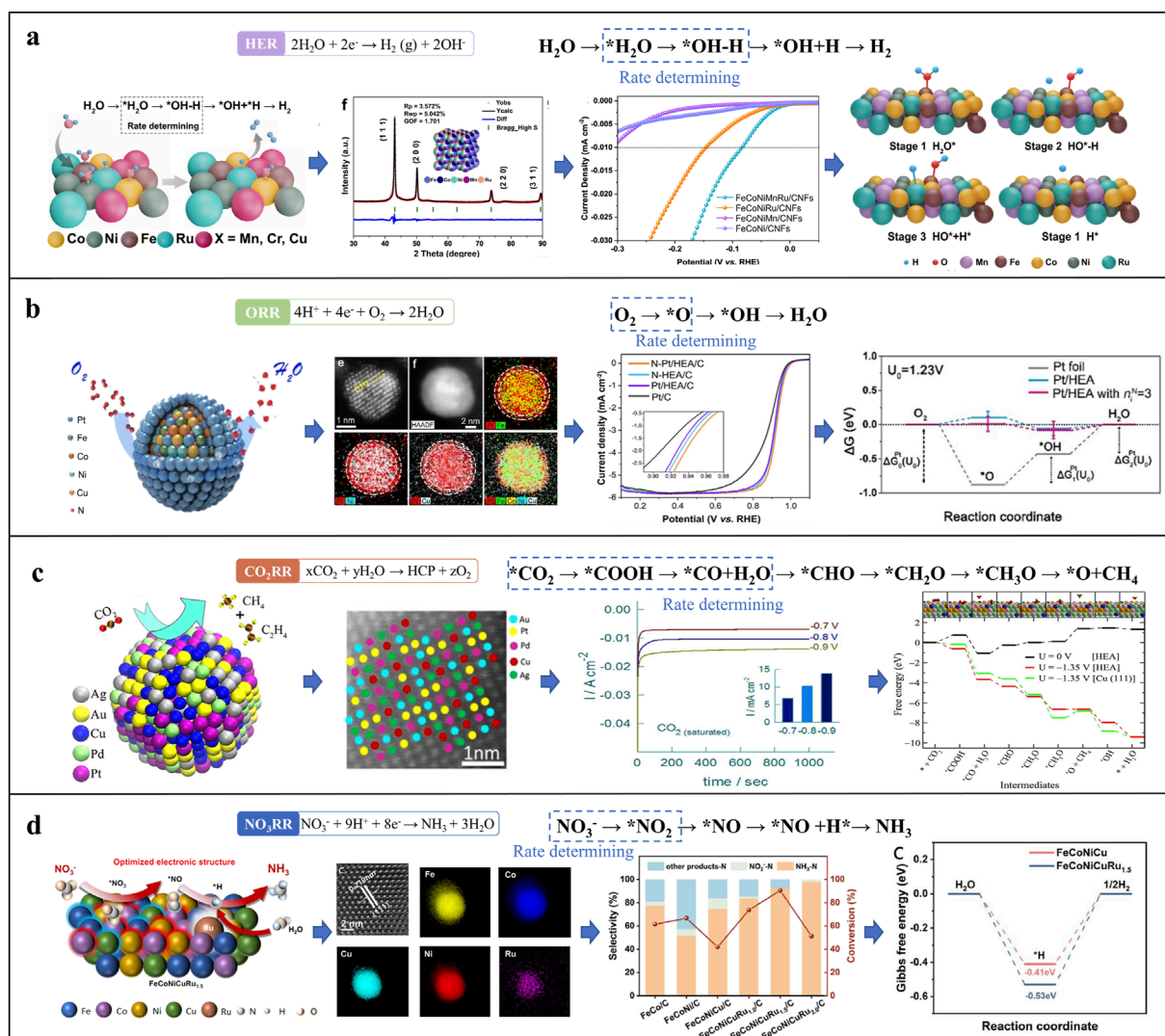


FIGURE 2

Applications of HEA-NMs in electrocatalysis: (a) HER (Hao et al., 2022), (b) ORR (Zhao et al., 2024; Chen et al., 2023a), (c) CO₂RR (Nellaippan et al., 2020), and (d) NO₃RR (Wu et al., 2025; Chen et al., 2025).

selective production of hydrocarbons and alcohols, showing strong potential for CO₂ utilization in energy devices (Figure 2c).

4.4 NO₃RR

In NO₃RR, product selectivity (N₂, NH₃, NO₂⁻) depends on both thermodynamic and kinetic factors, including $*\text{NO}$, $*\text{NH}_2$, and $*\text{N}$ adsorption strengths (Chen et al., 2025). Strong $*\text{N}$ binding favors NH₃, while weaker adsorption promotes N₂ evolution. HEA-NMs offer tunable active sites that selectively stabilize intermediates like NO₂⁻ and NH₂OH, enabling controlled electron transfer and improved selectivity (Tang et al., 2024). Local pH affects $*\text{NH}_3$ desorption and catalyst durability. Cl⁻-containing electrolytes can generate reactive chlorine species, further enhancing nitrogen selectivity by suppressing by-products (Tokazhanov et al., 2020). Our FeCoNiCu-based HEAs demonstrate

high nitrate conversion and Faradaic efficiency (Figure 2d), confirming their promise in water treatment and ammonia synthesis (Chen et al., 2025; Wu et al., 2025).

5 Support-enhanced electrocatalysis of HEA-NMs

To enhance dispersion and prevent aggregation of high-surface-energy HEA nanoparticles, HEA-NMs are commonly integrated with conductive supports such as graphene, carbon nanotubes (CNTs), and reduced graphene oxide (rGO). These supports offer anchoring sites that stabilize nanoparticles, promote effective charge transport, and improve electrochemical accessibility. For example, FeCoNiIrRu HEAs supported on carbon nanofibers showed improved OER activity due to better dispersion and

conductivity (Zhu et al., 2022). Mesoporous carbon-supported FeCoNiCu(Zn) HEAs exhibited enhanced NO₃RR performance, attributed to the accelerated mass transfer and intermediate confinement enabled by the porous architecture (Chen et al., 2025).

Beyond conductivity, interfacial charge transfer also plays a crucial role. Ling et al. (2025) demonstrated that rGO anchoring induced d-band modulation in FeCoNiCuSn HEAs, facilitating NO₃RR. Similarly, MXene-based Pt-doped HEAs exhibited enhanced HER activity through orbital hybridization with hydrogen (Shu et al., 2024).

Hydrophobic/hydrophilic tailoring of the support surface can further modulate gas–liquid–solid interfaces. For instance, controlling the hydrophobicity of a Co–Cu–Mo–Pd–Re catalyst layer enabled high-current HER by preventing H₂ bubble accumulation (Wang et al., 2024).

6 Challenges and prospects

- (1) Scalable and controllable synthesis: The scalable synthesis of phase-pure HEA-NMs remains challenging due to compositional deviation, particle size heterogeneity, and environmental risks such as metal leaching. Higher catalyst loadings can induce interfacial stress and detachment in practical electrolyzers. Recovery strategies using green separation techniques should be developed to enable sustainable application.
- (2) Mechanistic understanding of catalytic processes: The complex interactions among diverse active sites and their dynamic evolution during reactions remain poorly understood. *In-situ* and operando techniques, such as X-ray absorption spectroscopy, Raman, and TEM, combined with density functional theory (DFT), are essential for elucidating structure–activity relationships and guiding rational catalyst design.
- (3) Data-driven optimization: The vast compositional space of HEA-NMs renders traditional screening inefficient. Integrating machine learning and high-throughput computation can accelerate catalyst discovery by predicting optimal compositions and identifying key performance descriptors, enabling targeted design of HEA-NMs for specific electrochemical reactions.
- (4) Sustainability and Material Lifecycle: The long-term application of HEA-NMs requires attention to sustainability. Many systems still rely on noble metals (e.g., Pt, Pd, Ru), raising cost and supply concerns. Recent efforts toward noble-metal-free HEAs using Fe, Co, Ni, or Cu show promise. End-of-life recovery, recyclability, and lifecycle impact assessments remain underexplored and should be integrated into future HEA catalyst development strategies.

7 Conclusion

This mini-review summarizes recent advances in high-entropy alloy nanomaterials (HEA-NMs), focusing on their synthesis,

mechanistic effects, and electrocatalytic applications in key reactions such as HER, OER, ORR, CO₂RR, and NO₃RR. While the compositional complexity of HEA-NMs enables tunable catalytic properties and superior stability, it also poses challenges in achieving controlled synthesis and understanding dynamic reaction mechanisms. Future research should integrate atomic-scale structural design, *in situ*/operando characterization, and machine-learning-guided screening to accelerate rational catalyst discovery and advance HEA-NMs for clean energy and environmental technologies.

Author contributions

JC: Investigation, Writing – original draft. AW: Writing – original draft, Investigation. YZ: Investigation, Writing – original draft. YX: Investigation, Writing – original draft. HZ: Writing – review and editing, Project administration, Funding acquisition. WT: Writing – review and editing, Conceptualization, Funding acquisition.

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