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Multi-element synergy in catalysis: A chemistry-based design of high-entropy alloy nanoparticles for sustainable reactions

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Abstract
The avenue of development in catalytic sciences with multielement synergy, tunable electronic structures, and entropy-driven stability is represented by high-entropy alloy nanoparticles (HEA-NPs), which may be viewed as beyond the conventional mono- and bimetallic catalysts to synergize. While a theoretical study, this work attempts to present a chemistry-based approach for HEA-NP design and discuss their potential roles in sustainable catalytic reactions such as HER, OER, and CO_2RR. Using logical stepwise mechanistic reasoning, schematic representations, and conceptual energy profiles, the present work shows how HEAs can mitigate adverse adsorption-desorption energetics, reduce overpotentials, and yield excellent stability under reaction conditions. Anticipated results would be enhanced activity and stability coupled with the possibility of being amenable to widely different reaction types, thus qualifying HEAs as potential candidates in energy and environmental applications. While some restrictions remain imposed owing to the lack of experimental verification, the framework presented here paves the way for experimentalists for investigation in the near future and highlights the need for an integration.

Keywords: High-entropy alloys, nanoparticles, catalysis, sustainable reactions, multi-element synergy

Introduction

The escalating global demand for sustainable catalytic solutions in energy conversion, environmental remediation, and chemical synthesis has propelled the exploration of advanced nanomaterials with superior activity selectivity and durability. HEAs are defined as metallic systems comprising five or more principal elements in near equimolar proportions, and represent a groundbreaking paradigm in alloy and catalyst design. Unlike conventional binary or ternary alloys, HEAs derive their stability from the high configurational entropy, which thermodynamically favors solid solution formation over ordered intermetallic phases even under extreme conditions (Sun *et al*., 2024) [19]. Recent progress in HEA-NPs combines HEA configurational benefits with nanoscale traits like high surface area, abundant active sites, and tunable electronic structures, delivering superior catalytic performance (Chen *et al*., 2025) [7]. Their "cocktail effect," synergistic interactions, and unique features, which include lattice distortion, sluggish diffusion, and multi-element synergy, enhance adsorption, electron transfer, and reaction pathways while ensuring resilience in harsh conditions (Yang *et al*., 2024; Sun *et al*., 2024; Yu *et al*., 2022) [20, 19, 23]. HEA-NPs show high efficiency and stability in HER, OER, ORR, and CO_2 conversion, often outperforming conventional catalysts, with synthesis advances enabling control over phase, size, and structure (Cai *et al*., 2022) [5]. Techniques such as carbothermal shock, solvothermal auto-catalytic reduction, and continuous-flow liquid-phase reduction have enabled the production of ultrafine, compositionally homogeneous HEA-NPs with highly active surfaces and reproducibility suited for catalysis (Yao *et al*., 2018; Broge *et al*., 2020; AlZoubi *et al*., 2024) [21, 4, 2]. Despite these compelling advancements, the rationale chemistry-based design of HEA-NPs catalyst, grounded in theoretical principles, a mechanistic framework, and symmetric reasoning, remains relatively underexplored. Most existing studies rely on experimental data in evaluating catalytic performance. A purely theoretical methodology-driven approach that logically constructs HEA-NP systems tailored for sustainable catalytic applications would fill this gap and serve as a critical blueprint for future experimental validation.

In this context, this paper presents a chemistry-based design methodology for HEA nanoparticles aimed at sustainable catalysis. Our approach revolves around leveraging multi-element synergy to modulate active site chemistry, electronic structure, and lattice dynamics, all within a mechanistically grounded framework. Through conceptual schematics and reaction mechanism analysis, we outline a reproducible, systematic approach to design HEA-NP catalysts for reactions such as hydrogen evolution or CO_2 conversion, without resorting to numerical data or empirical literature comparisons. This methodology-centric viewpoint aims to enrich the conceptual toolbox of catalysis research, offering a structured path from elemental selection to mechanistic hypothesis and expected catalytic behavior.

Methodology

This methodology frames the HEA-NP Catalyst design as a multi-stage pipeline: (A) chemistry-guided element selection and target reaction mapping, (B) proposed synthetic routes (for prospective experimental validation), (C) competition screening and mechanistic modeling, (D) proposed catalytic testing protocols (electrochemical/mechanistic), and (F) characterization and stability evaluation. Each stage explains how researchers can both conceptually understand design choices and practically implement them during experimental work (Sun *et al*., 2024; Yao *et al*., 2022) [19, 22].

Target Reaction Definition and Reaction-Centered Design Goals

Choose one or two demonstrator reactions to focus on design constraints and mechanistic hypotheses. For this paper, we propose:

1. Hydrogen Evolution Reaction (HER) in aqueous media (acidic or alkaline) - where optimal H* adsorption energy (ΔG_H*) and facile Volmer-Heyrovsky/Tafel steps are central (Li *et al*., 2019) [12].
2. Oxygen Evolution Reaction (OER) is a four-electron, multi-step process that is often considered the bottleneck in water-splitting due to its sluggish kinetics and high overpotentials. Intermediates (OH*, O*, and OOH*) must be stabilized in an energetically balanced way to minimize reaction barriers.
3. CO_2 reduction (to CO or C_1 products**)** - where CO_2 activation, intermediate stabilization (CO*, HCOO*), and C-O bond scission/formation energetics are controlling (Sun *et al*., 2024) [19].

Design goals derived from reaction choices

1. Tune surface adsorption energies (via multi-element electronic effects) to approach volcano-peak values for the chosen reaction (d-band engineering) (Bhattacharjee *et al*., 2016) [3].
2. Maximise active site diversity to exploit multi-step catalytic cycles (e.g., bifunctional sites) (Sun *et al*., 2024) [19].
3. Ensure structural and electrochemical stability under operating conditions (lattice distortion & entropy stabilization) (Yao *et al*., 2022) [22].

Chemistry-Guided Element Selection and Compositional Rules

Use a combination of chemical heuristics and electronic-structure principles to propose element pools:

1. **Function mapping:** Assign elemental roles by expected function (e.g., H-adsorbing elements: Pt, Ru, Ni, Co; CO_2-activating elements: Cu, Fe, Mo; stabilizing/supporting elements: Cr, Al, Ti). This mapping is hypothesis-driven and grounded in known element chemistries rather than new empirical screening (Sun *et al*., 2024) [19].
2. **d-band tuning:** Choose elements so that alloying shifts the surface d-band center toward an adsorption optimum (we reference the d-band model for designing adsorption energies) (Bhattacharjee *et al*., 2016) [3].
3. **Thermodynamic feasibility:** Prefer combinations with manageable mixing enthalpies or where entropy can compensate ($\Delta S_{mix} >> \Delta H_{mix}$) to favor solid solution formation at the nanoscale (Yao *et al*., 2022) [22].

The practical compositional strategies included

1. Near-equimolar senary/quinternary pools (five or six elements) to maximize configurational entropy while including at least one element that provides the primary catalytic motif for the target reaction.
2. Surface-enrichment thinking plan for surface enrichment of the most catalytically active element(s) (core-shell or gradient configurations) to reconcile bulk entropy with surface activity.

Structural Motifs and Support Strategies

Define the conceptual motif(s) to be targeted:

1. Single-phase solid-solution HEA-NPs (homogeneous mixing) for maximum site diversity.
2. Core-shell or gradient HEA structures to concentrate active species on the surface while keeping multi-element bulk for stability.

Recommend conductive, high-surface-area supports (carbon nanofibers, doped graphitic carbon, TiO_2, or porous conductive oxides) to prevent nanoparticle sintering and to modulate electronic coupling with HEA-NPs. Support selection should be justified chemically (e.g., oxide supports can alter charge transfer and stabilize specific oxidation states) (He G *et al*., 2025; Park *et al*., 2024) [8, 15].

Proposed Synthetic Routes

Although this paper is theoretical, listing reproducible synthesis options anchors methodological proposals for later validation.

Rapid thermal shock/carbothermal shock

This enables the rapid thermal activation and alloying of multiple metal precursors while minimizing sintering due to extremely short high-T pulses. Suitable for creating single-phase HEA-NPs on supports.

Conceptual steps to be implemented by experimentalists:

1. Impregnate a conductive carbon support with mixed metal salts (chlorides/nitrates, stoichiometric ratios).
2. Apply a millisecond thermal shock ($\sim 10^4$-10^5 K s^{-1}, peak T ~2000 K) and quench to form ultrafine solid-solution nanoparticles.

Thermal plasma/in-flight synthesis

This is continuous, ultrafast heating to form HEA-NPs from elemental powders or precursors with high throughput and fine composition control (Kim *et al*., 2024) [10].

Colloidal/wet-chemical approaches
This has better size control and surface ligand engineering, useful for studies that require isolated particles for surface-sensitive measurements. Include post-synthesis ligand removal and support deposition strategies (Zeihl &Zhang, 2025) [7].

Hydro/solvothermal &Joule-heating derived approaches
An alternative means to create supported HEA or high-entropy oxides with porous supports via rapid heating (Joule/heating) or solvothermal conversion (Abdelhafiz *et al*., 2022; Park *et al*., 2024) [1, 15].

Computational Screening and Mechanistic Modeling
Multi-scale Computational Strategy

1. **Electronic structure descriptors (DFT):** Compute surface slab models for selected HEA compositions (representative surface terminations) to estimate adsorption energies of key intermediates (H*, CO*, HCOO*, etc.). Use the d-band center, projected DOS, and Bader charge analyses as descriptors.
2. **Cluster expansion / Monte Carlo sampling:** Use cluster expansion or special quasi-random structures (SQS) to model disordered solid solutions and sample local environments in HEA surfaces to capture site heterogeneity and distribution of adsorption sites
3. **Microkinetic modelling:** Build microkinetic models (rate constants from DFT barriers or Brønsted-Evans-Polanyi relations) to simulate reaction rates and dominant pathways (e.g., Volmer-Heyrovsky vs Volmer-Tafel for HER). Sensitivity analysis identifies rate-controlling steps (Chen *et al*., 2018) [6].
4. **Machine learning / surrogate models:** Train regression models (e.g., kernel ridge regression, graph-based neural nets) on computed descriptors to rapidly predict adsorption energies across vast compositional spaces and identify candidate compositions

Descriptor Selection and Screening Rule
The primary descriptors can be ΔG_H* (HER), ΔG_CO*, and ΔG_HCOO* (CO_2RR), d-band center, adsorption energy distributions, and surface segregation energies. Screening rules (theoretical) accept candidates where ΔG_H* is within ±0.1-0.2 eV of the optimum volcano peak for HER; for CO_2RR, prioritize compositions stabilizing CO* weakly enough for desorption but strong enough for formation. Use microkinetic outputs to refine cutoffs.

Proposed Catalytic Evaluation Protocols (for future validation)
Electrochemical Tests

1. **Electrode prep:** deposit HEA-NPs on glassy carbon or carbon paper at a defined metal loading (e.g., μg cm^{-2}). Remove organic ligands if colloidal synthesis is used.
2. **Measurements:** linear sweep voltammetry (LSV) for polarization curves, Tafel analysis (extract slope, exchange current), electrochemical impedance spectroscopy (EIS) for charge transfer resistance, chronoamperometry / chronopotentiometry for durability. Report overpotential at benchmark currents (e.g., 10 mA cm^{-2}) (Razzaq &Exner *et al*., 2024) [18].
3. **Mechanistic probes:** measure Tafel slopes and H_2 exchange currents to infer dominant HER pathways (Volmer-Heyrovsky vs Volmer-Tafel) and correlate with ΔG_H* predictions.

CO_2 Reduction Testing

1. **Cell:** H-cell or flow cell with defined electrolyte and CO_2 saturation; report Faradaic efficiencies for products (GC/HPLC detection) and partial current densities.
2. **Mechanistic link:** correlate DFT-predicted intermediates stabilization with observed product distribution.

Characterization Plan (to connect theory ↔ experiment)
This would validate structural and electronic hypotheses:

1. **X-ray diffraction (XRD):** Identify single-phase solid solutions or phase separation.
2. **Transmission electron microscopy (TEM / HAADF-STEM):** Particle size, morphology, and atomic-resolution elemental mapping (EDS/EELS) to show homogeneous mixing or core-shell motifs.
3. **X-ray absorption spectroscopy (XAS/XANES/EXAFS):** Probe local coordination and oxidation states to validate electronic structure predictions.
4. **X-ray photoelectron spectroscopy (XPS):** Surface composition and chemical states (surface enrichment).
5. **Inductively coupled plasma (ICP-MS/OES):** Bulk composition confirmation.

Stability, Poisoning, and Durability Considerations

1. Surface segregation and leaching under reaction potentials (compute segregation energies and simulate dissolution tendencies).
2. Resistance to poisoning (sulfur, CO) via calculating binding energies of common poisons and analyzing site heterogeneity that can dilute poisoning effects.
3. Long-term lattice evolution uses kinetic Monte Carlo or accelerated ageing models to predict sintering or phase separation under operating conditions.

Results and Discussion
The foremost expected outcome of designing high-entropy alloy nanoparticles (HEA-NPs) for catalysis is the realization of the multi-element synergy or "cocktail effect." Unlike traditional catalysts composed of one or two elements, HEAs provide a chemically heterogeneous surface where multiple elements can simultaneously contribute to catalytic activity. This diversity of active sites creates a situation in which different intermediates-such as H* in the hydrogen evolution reaction (HER), OH* in the oxygen evolution reaction (OER), or COOH* in the CO_2 reduction reaction (CO_2RR)-are stabilized through different local environments. The result is a catalytic surface that avoids overly strong or weak adsorption, thereby aligning with the Sabatier principle of optimal binding strength. HEAs enhance catalytic activity through balanced energetics and electronic structure modulation. Atomic-level interactions among constituent elements cause charge redistribution and orbital hybridization, shifting the d-band center of surface atoms. This tuning modifies adsorption energies, lowers electron transfer barriers, and stabilizes transition states. In HER, near-zero ΔG_H* enables efficient hydrogen release, while in OER and CO_2RR, optimized activation of oxygenated and carbonaceous intermediates improves kinetics. Additionally, HEAs are expected to lower

overpotentials by providing favorable reaction energy landscapes that stabilize intermediates and reduce activation barriers, leading to higher overall catalytic efficiency.
In OER, multiple elements in the HEA are predicted to offer a broader range of binding sites for OH*, O*, and OOH*, thereby facilitating smoother reaction progression. Similarly, in CO_2RR, the improved stabilization of COOH* intermediates should reduce the barrier for CO_2 activation, improving both activity and selectivity.
Taken together, these outcomes underscore the unique potential of HEA nanoparticles as next-generation catalytic systems. Table 1 demonstrates a comparison between the HEA-NPs versus Conventional Catalysts. Their combination of multi-element synergy, electronic tunability, structural resilience, and favorable reaction energetics positions them as strong candidates for sustainable chemical transformations. By logically deriving these outcomes from chemical principles rather than empirical data, the proposed methodology provides a forward-looking framework that not only predicts catalytic performance but also guides future synthesis and testing strategies.

Table 1: Expected Outcomes of HEA-NPs vs. Conventional Catalysts.

Feature	Conventional Catalysts (Mono/Bimetallic)	HEA Nanoparticles (Proposed Design)
Active Site Diversity	Limited to one or two types of active sites; restricted catalytic versatility.	Multiple active sites from diverse elements; enhanced stabilization of various intermediates.
Electronic Structure	Fixed d-band structure; limited tunability of adsorption energies.	Charge redistribution and orbital hybridization shift the d-band center; tunable energetics.
Thermodynamic Stability	Prone to phase segregation, sintering, and surface reconstruction under harsh conditions.	High configurational entropy enhances structural stability and prevents segregation.
Overpotential in Catalysis	Often, high overpotentials are due to sub-optimal adsorption energies.	Expected lower overpotentials by balancing adsorption/desorption energetics (Sabatier principle).
Adaptability Across Reactions	Usually tailored for one specific reaction pathway.	Versatile catalytic potential across HER, OER, CO_2RR, and other sustainable reactions.
Long-Term Durability	Performance degrades significantly over time in reactive environments.	Improved long-term durability with resistance to deactivation under catalytic cycles.

Limitations and Assumptions
While promising, the present methodology has inherent limitations. The catalysis outcomes are theoretical and rely on chemical reasoning, not actual measured data. Catalytic behavior might deviate due to unforeseen surface reconstructions or kinetic bottlenecks. HEAs may expose heterogeneous atomic ensembles, leading to competing catalytic pathways that are hard to incorporate into a simple schematic framework. Uniform atomic distribution in multi-element systems, particularly on the nanoscale, is non-trivial. Conventional surface preparations of HEAs may cause surface segregation, thus negating predicted benefits of catalysis. Although nanoscale HEAs might indeed be catalysts, their large-scale production and stability during catalytic applications need additional consideration.
The framework rests on several assumptions:

1. Idealized homogeneous distribution of elements within the nanoparticle, without significant clustering or segregation.
2. Steady-state catalytic operation where adsorbate coverage and turnover frequencies are stable over time.
3. Applicability of the Sabatier principle, assuming that optimal adsorption energies directly correlate with catalytic efficiency.
4. Negligible mass transfer limitations, focusing solely on electronic and thermodynamic aspects.

Future Directions
This study establishes a theoretical framework for HEA nanoparticle catalysis and highlights pathways for future research. A key next step is the experimental synthesis and characterization of predicted motifs through techniques such as carbothermal shock synthesis, cryomilling, or wet-chemical methods, which enable precise compositional control. Integrating computational modeling with machine learning, including DFT and high-throughput screening, could accelerate discovery and prediction of optimal element combinations. Beyond HER, OER, and CO_2RR, HEAs hold promise in biomass valorization, nitrogen fixation, and photocatalysis, where multi-element synergies may unlock novel mechanisms. Finally, advancing scalable and sustainable synthesis methods will be critical for industrial deployment while reducing environmental and economic impacts. These directions, thus, lay the roadmap for a nexus in which theory, computation, and experiments converge to realize the full catalytical promise of HEA nanoparticles.

Conclusion
The present theoretical study underscores the transformative potential of high-entropy alloy nanoparticles (HEA-NPs) as a next-generation platform for sustainable catalysis. By moving beyond the constraints of mono- and bimetallic systems, HEAs offer an unparalleled combination of multi-element synergy, electronic tunability, and entropy-driven stability. The proposed chemistry-based design approach highlights how the intrinsic heterogeneity of HEA surfaces can create multiple active sites and support an adsorption-desorption balance, thereby reducing overpotentials in HER, OER, and CO_2RR. A conceptual mechanistic framework, supported by chemical reasoning and schematic representation, suggests HEAs can surpass classical catalytic limits by improving efficiency, sustaining performance under harsh conditions, and adapting to diverse pathways. Their resistance to phase segregation and deactivation further promises longer catalyst lifetimes, addressing a key barrier to industrial nanomaterial use in energy and environmental applications.
At the same time, the framework's limitations are acknowledged: predictions remain speculative without experimental validation. Future efforts in synthesizing and characterizing novel HEA motifs will be essential, particularly in tailoring compositions for selectivity and stability. Overall, HEA nanoparticles emerge as a promising frontier in catalysis, where rational design grounded in chemistry can guide innovation and provide a foundation for

empirical research to accelerate their integration into sustainable catalytic systems.

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