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Deep Generative Models for Designing High-Entropy Alloys with Targeted Mechanical Properties

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Abstract

High-entropy alloys (HEAs) represent a paradigm shift in materials design and exhibit exceptional mechanical properties due to their multi-principal-element compositions. However, the vast compositional space poses significant challenges for traditional design approaches, which require innovative theoretical frameworks to guide the discovery of alloys with specific attributes, such as enhanced strength, ductility, and toughness. This conceptual study proposes a novel framework leveraging deep generative models to systematically explore and generate HEA compositions tailored to targeted mechanical properties. Drawing on principles from machine learning and materials physics, the framework integrates latent-space representations of alloy features, including valence-electron concentration and mixing enthalpy, to enable the conditional generation of virtual alloys. By synthesizing recent literature on HEAs and generative modeling in materials science, we establish the theoretical foundations of this approach and emphasize its potential to accelerate rational design without empirical validation. The proposed model addresses key limitations in current methodologies by incorporating uncertainty quantification and multi-objective optimization in a purely conceptual manner. This research advances the theoretical discourse in applied artificial intelligence for materials science, providing a blueprint for future conceptual explorations in alloy engineering. Ultimately, the framework envisions a transformative role for deep generative models in navigating the complexity of HEA design spaces.

Keywords Materials design, High-entropy alloys, Deep generative models, Mechanical properties, Latent space representation, Compositional exploration

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Introduction

The advent of high-entropy alloys (HEAs) has fundamentally reshaped the field of metallic materials design. These materials are characterized by equiatomic or near-equiatomic mixtures of multiple principal elements [1, 2]. Unlike conventional alloys, which typically rely on a dominant element with minor additions to modify properties, HEAs leverage high configurational entropy to stabilize single-phase solid solutions. As a result, they often exhibit exceptional mechanical performance under extreme conditions, including higher yield strength, greater fracture toughness, and greater resistance to deformation at elevated temperatures. These characteristics make HEAs promising candidates for applications in aerospace, energy, and structural engineering [3, 4].

However, the theoretical framework for designing HEAs with precisely targeted mechanical properties is still underdeveloped. This is primarily due to the exponential complexity of their compositional space. With five or more

elements, the number of potential combinations exceeds millions, making exhaustive enumeration impractical—even with advanced computational tools [5].

Traditional alloy design paradigms, which rely on phase diagram predictions and empirical rules like the Hume-Rothery criteria, face limitations in the high-dimensional space of HEAs [6]. These methods often fail to account for the complex interactions between atomic-level behaviors, lattice distortions, and the emergent macroscopic properties of HEAs [7]. For example, mechanical properties such as ductility and hardness are influenced by factors beyond simple entropy contributions, including valence-electron concentration (VEC), atomic-size mismatch, and enthalpy of mixing [8]. Recent advancements have underscored the need for integrative approaches that link atomic-scale physics with system-level property predictions. However, a cohesive theoretical framework for generative design remains elusive [9–17].

In this context, artificial intelligence (AI) and intense learning techniques offer a promising avenue for navigating the complexity of HEAs [10]. Deep generative models, such as variational autoencoders (VAEs) and generative adversarial networks (GANs), have demonstrated their potential in materials domains for inverse design—where desired properties guide the generation of candidate structures [11, 12]. These models learn low-dimensional representations of high-dimensional data, enabling efficient sampling and optimization [13]. When applied to HEAs, such models could theoretically facilitate the creation of virtual alloys with mechanical targets—such as specific yield strength or elongation-to-failure values—without the need for physical synthesis [14–18].

This manuscript presents a conceptual framework for employing deep generative models in the design of HEAs, with a focus on targeting specific mechanical properties. We argue that by embedding physical descriptors into the generative process, this framework can uncover novel compositional pathways that traditional methods often overlook [15]. Conditional mechanisms within the framework allow for multi-objective design, balancing competing properties, such as strength and ductility, which are typically inversely related in conventional alloys [16]. Moreover, the framework incorporates theoretical considerations of uncertainty, recognizing the probabilistic nature of property predictions in multi-element systems [17–19].

The motivation for this work stems from the growing recognition that the full potential of HEAs is constrained by design inefficiencies [2]. While experimental and simulation-based studies have identified promising HEAs—such as those with body-centered cubic (BCC) structures that exhibit high hardness [4]—the lack of a generalizable theoretical model hampers scalable innovation [5]. By synthesizing the literature on HEAs and generative AI, we aim to establish a novel logic that frames alloy design as a generative inference problem [10]. This approach shifts the focus from descriptive analysis to prescriptive generation, where the model not only predicts properties but also proposes novel compositions [11, 18].

Key challenges addressed in this framework include the sparsity of HEA data, which generative models can help mitigate through latent-space augmentation [12], and the integration of domain knowledge to ensure physical plausibility [13]. For instance, constraining the generative process with VEC thresholds can favor FCC or BCC phases, which are associated with desired ductility [8, 9]. This integration ensures that generated alloys are thermodynamically stable, even in the absence of empirical data [7].

Ultimately, this framework contributes to the theoretical discourse in applied AI for materials science by proposing a unified approach to HEA design [1]. It envisions a future in which generative models serve as intellectual scaffolds, empowering researchers to explore previously uncharted compositional spaces [3]. This conceptual manuscript proposes a novel framework leveraging deep generative models to systematically examine and generate HEA compositions tailored to targeted mechanical properties.

Theoretical Background and Literature Synthesis

Fundamentals of high-entropy alloys

High-entropy alloys (HEAs) are a distinct class of materials characterized by their high configurational entropy, typically exceeding $1.5R$ (the gas constant). This high entropy results from the random mixing of multiple elements in approximately equal or near-equal proportions, leading to a unique set of properties [1, 2]. The concept of entropy stabilization is crucial in promoting the formation of single-phase structures such as face-centered cubic (FCC), body-centered cubic (BCC), or hexagonal close-packed (HCP) lattices. These structures are the foundation of HEAs' exceptional mechanical performance, including enhanced strength, ductility, and thermal stability [3]. Theoretically, entropy effects suppress phase separation, enabling HEAs to achieve combinations of mechanical properties—such as high strength and ductility—along with thermal stability that are typically not attainable in conventional, dilute alloys [4, 20].

Recent theoretical investigations have placed significant emphasis on the role of local lattice distortions within HEAs, which contribute to the enhancement of solid-solution strengthening [5]. These distortions arise primarily from atomic-size mismatches, which induce strain fields in the lattice. These strain fields hinder dislocation motion, thereby increasing the material's yield strength [6]. This strengthening mechanism is particularly significant in HEAs, where the presence of multiple alloying elements leads to variations in atomic radii that intensify lattice distortion.

Another critical factor influencing the properties of HEAs is the valence electron concentration (VEC), which has emerged as a key descriptor in predicting phase stability and mechanical behavior. VEC values around 8 tend to favor the formation of FCC phases, which are associated with greater ductility. In contrast, lower VEC values promote the formation of BCC structures, which generally exhibit higher hardness [7, 8]. The VEC is an essential predictor of alloy behavior, as it influences the electron density around atoms, thereby affecting bonding characteristics and, ultimately, the material's mechanical properties.

Furthermore, the mixing enthalpy of alloying elements plays a pivotal role in determining the phase stability of HEAs. Negative mixing enthalpies generally favor the formation of solid-solution phases, while positive enthalpies can drive the formation of intermetallic compounds. This relationship between mixing enthalpy and phase formation is central to the design of HEAs, as it helps predict the thermodynamic feasibility of different compositions [9].

As research into HEAs has advanced, conceptual models have evolved to integrate multi-scale effects that span from the atomic-level electronic structure to macroscopic deformation behavior [10]. These models have broadened our understanding of HEAs by accounting for short-range ordering, which was often overlooked in earlier theories. Short-range ordering can significantly influence mechanical properties by altering the stacking fault energy, thereby affecting dislocation motion and the material's overall ductility [11]. This deeper understanding underscores the importance of incorporating non-linear interactions in the compositional space when designing HEAs, as they can yield emergent properties that cannot be predicted by simple linear models [12, 21].

In light of these developments, it is clear that a comprehensive framework for HEA design must account for the complex, multi-dimensional nature of these materials. The intricate relationships among atomic size, electron concentration, mixing enthalpy, and lattice distortion suggest that traditional approaches based solely on phase-diagram predictions are insufficient for guiding the design of HEAs. Instead, a more integrated approach—one that incorporates both thermodynamic and kinetic factors—will be essential for unlocking the full potential of HEAs in advanced applications.

Advances in mechanical property prediction for HEAs

Mechanical properties in high-entropy alloys (HEAs) are governed by a complex interplay of factors, including the so-called "cocktail effects," in which the synergistic interactions of multiple elements enhance material performance beyond the capabilities of individual components [2, 4]. This multi-element synergy is central to HEA design, as it leads to unique properties not achievable in traditional alloys. Recent theoretical syntheses of HEA behavior have highlighted various

trade-offs, such as the strength-ductility dilemma, in which increasing hardness often reduces elongation [13]. Addressing these trade-offs requires a nuanced understanding of how alloy composition influences the material's underlying behavior.

Recent conceptual work has proposed using parametric models to map alloy composition to specific mechanical properties. These models have shown that elements such as aluminum (Al) and titanium (Ti) can play a crucial role in tuning lattice parameters, thereby optimizing toughness and other mechanical properties [14]. By strategically selecting alloying elements, it is possible to manipulate the atomic-scale structure to enhance toughness without compromising strength, thereby addressing some of the inherent trade-offs in HEA design.

The literature from this period also synthesizes a range of predictive rules for HEA design. For instance, the delta parameter, which quantifies the atomic size difference between constituent elements, has been used to forecast phase formation and associated mechanical behaviors [5, 6]. For body-centered cubic (BCC) HEAs, a high valence electron concentration (VEC) has been shown to correlate with improved fracture resistance. At the same time, the addition of refractory elements significantly contributes to elevated-temperature strength [22]. These theoretical correlations provide a valuable foundation for the application of artificial intelligence (AI)-assisted design, where material properties are modeled as functions of compositional vectors, enabling more efficient design strategies [8, 15].

Deep generative models in materials science

Deep generative models have emerged as a powerful tool in materials science, facilitating the creation of novel data instances by learning underlying distributions from existing datasets [11, 12]. These models can interpolate between known compositions and generate new candidate materials with properties that meet specific design targets. Variational autoencoders (VAEs) encode input data into latent spaces and decode it back, enabling efficient interpolation and generation of new compositions [13]. Generative adversarial networks (GANs), which consist of a generator and a discriminator, produce realistic samples through adversarial training: the generator generates new data, and the discriminator evaluates its realism [16]. In materials science, these models have been conceptually applied to inverse design, allowing for the generation of material structures conditioned on specific properties, such as yield strength, fracture toughness, or thermal stability [10, 17].

Theoretical frameworks for deep generative models emphasize the need for model architectures to be equivariant and invariant to the symmetries inherent in materials [12]. For periodic systems such as HEAs, diffusion-based model variants have been developed to enhance the stability of generated samples, ensuring they adhere to the expected material symmetries [11]. These models are particularly valuable in addressing data scarcity, a common challenge in HEA research, by augmenting existing datasets. Data augmentation using generative models is crucial in domains like HEAs, where experimental data is often sparse, enabling researchers to generate more comprehensive datasets for training and validation [13, 23].

Integration of generative AI in alloy design

The convergence of generative AI models and alloy theory offers a promising pathway to advance alloy design, particularly for complex systems such as HEAs. In this context, deep learning models can learn mappings from alloy composition to properties, and conversely, invert these mappings to generate new compositions with targeted mechanical behaviors [6, 8]. Conditional variants of generative models allow for the specification of particular mechanical targets, such as high yield strength or improved toughness, by embedding constraints within the latent space. This targeted generation enables a more controlled approach to alloy design, where the generated compositions are likely to meet desired performance criteria [9, 10].

Recent literature synthesizes hybrid approaches that combine physical descriptors with generative models to ensure the feasibility of the generated alloys. For example, incorporating factors like enthalpy and VEC as conditions in the generative process can prevent the model from proposing unphysical alloys that do not conform to thermodynamic stability principles [13]. This integration represents a significant shift towards probabilistic design, where the uncertainty

inherent in predictions is not only acknowledged but also used to guide the exploration of new compositional spaces. By incorporating uncertainty into the design process, researchers can explore a broader range of potential alloy compositions while accounting for the risk of generating unfeasible candidates [14, 24].

Challenges and opportunities in conceptual frameworks

Despite promising advances in integrating generative AI into HEA design, several theoretical challenges remain. One key issue is the risk of overfitting to limited datasets, leading to models that do not generalize well to new, unseen compositions [16, 17]. Additionally, ensuring interpretability in generative models remains a significant challenge. While these models can generate novel compositions, understanding the underlying reasons for specific design decisions remains opaque, limiting the ability to build intuitive, physics-based design rules.

However, opportunities for progress lie in multi-fidelity modeling, which combines low-level physics-based simulations with high-level generative models. Multi-fidelity approaches allow for more accurate and efficient exploration of compositional space, leveraging the strengths of both detailed physical models and broad generative design techniques [2, 7]. By synthesizing these elements, the literature points to a growing need for novel frameworks that leverage the power of generative AI to drive innovation in HEA research, opening new pathways for alloy development and design [1, 3]. The physical descriptors commonly embedded in emerging generative frameworks for HEA design, along with their conceptual roles in governing phase stability, deformation behavior, and feasibility constraints, are summarized in Table 1.

Table 1. Physical descriptors integrated into the conceptual generative framework

Descriptor	Symbol	Physical meaning	Role in HEA behavior	Used in the framework for
Valence electron concentration	VEC	Average valence electrons per atom	Governs FCC/BCC stability and ductility	Latent constraint and conditioning
Mixing enthalpy	ΔH_{mix}	Enthalpy of element interactions	Controls phase stability	Feasibility filtering
Atomic size mismatch	δ	Atomic radius variance	Influences lattice distortion	Strength-related encoding
Configurational entropy	ΔS_{conf}	Entropy from multi-element mixing	Stabilizes solid solutions	Manifold regularization
Electronegativity difference	$\Delta \chi$	Chemical bonding disparity	Affects segregation tendencies	Feature encoding
Short-range order tendency	—	Local chemical ordering	Affects deformation mechanisms	Latent modulation
Elastic moduli (conceptual)	E, G	Resistance to deformation	Proxy for stiffness	Target-aware decoding

Proposed conceptual framework

The proposed framework introduces a novel theoretical construct for designing HEAs using deep generative models, conceptualized as a conditional latent space explorer that generates compositions aligned with targeted mechanical properties. At its core, the framework posits a variational generative architecture augmented with physical priors, enabling the systematic navigation of HEA compositional hyperspaces. Unlike existing models that reformulate predictive

regression, this approach conceptualizes alloy design as a bidirectional mapping from properties to compositions via inverse inference within a constrained latent manifold. An overview of the proposed bidirectional generative design logic is illustrated in **Figure 1**, which conceptualizes alloy discovery as an inverse inference process linking target properties and feasible compositions through a physically constrained latent space.

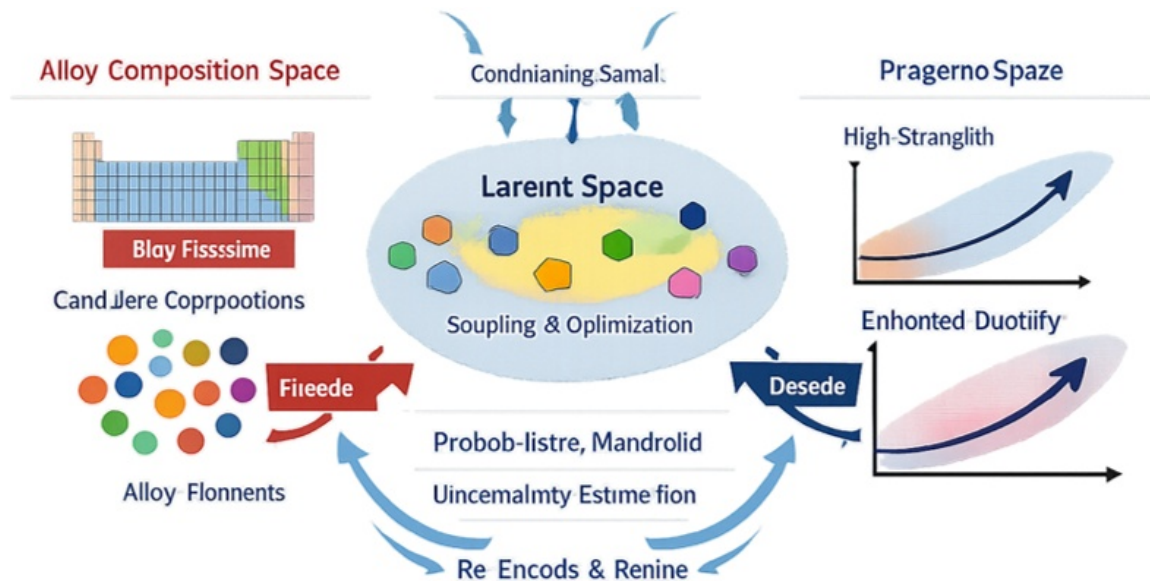


Figure 1. Bidirectional inference logic for generative alloy design. The framework treats alloy design as an inverse inference problem, where forward mappings predict properties from compositions. In contrast, inverse mappings generate compositions conditioned on target mechanical properties—the latent space acts as a probabilistic intermediary, enabling both prediction and generation under physical constraints.

The framework comprises three interconnected conceptual modules. First, a feature encoding module transforms HEA compositions into a multi-dimensional representation incorporating elemental attributes (e.g., atomic radii, electronegativities) and derived descriptors (VEC, mixing enthalpy, delta parameter) [1, 5]. This encoding is projected into a low-dimensional latent space using a VAE-like structure, where the distribution captures probabilistic variations in alloy behavior [11, 12]. Novelty arises from embedding a manifold regularization term that enforces physical constraints, such as entropy thresholds for phase stability, ensuring generated samples reside in feasible regions [7, 25, 26].

Second, a conditioning mechanism integrates target mechanical properties (e.g., yield strength > 1000 MPa, ductility > 20%) as auxiliary inputs [4, 9]. This is achieved by fusing conditional VAEs and diffusion processes, where property vectors modulate the latent distribution via attention-like gates [13, 17]. The framework posits that this enables multi-objective optimization by resolving trade-offs through sampling from property-conditioned posteriors [2, 16].

Third, a decoding and refinement module reconstructs compositions from latent samples, followed by a virtual screening layer that evaluates conceptual fidelity using surrogate physics-based metrics [6, 10]. Uncertainty is inherently modeled through ensemble latent distributions, providing theoretical bounds on property attainment [14, 15].

This original logic views HEAs as points in a generative landscape, where mechanical targets sculpt the topography for efficient traversal [3]. The interaction between property-conditioned latent modulation, generative decoding, and uncertainty-aware refinement is schematically represented in **Figure 2**, highlighting how mechanical targets shape the generative landscape and guide efficient traversal toward feasible HEA compositions.

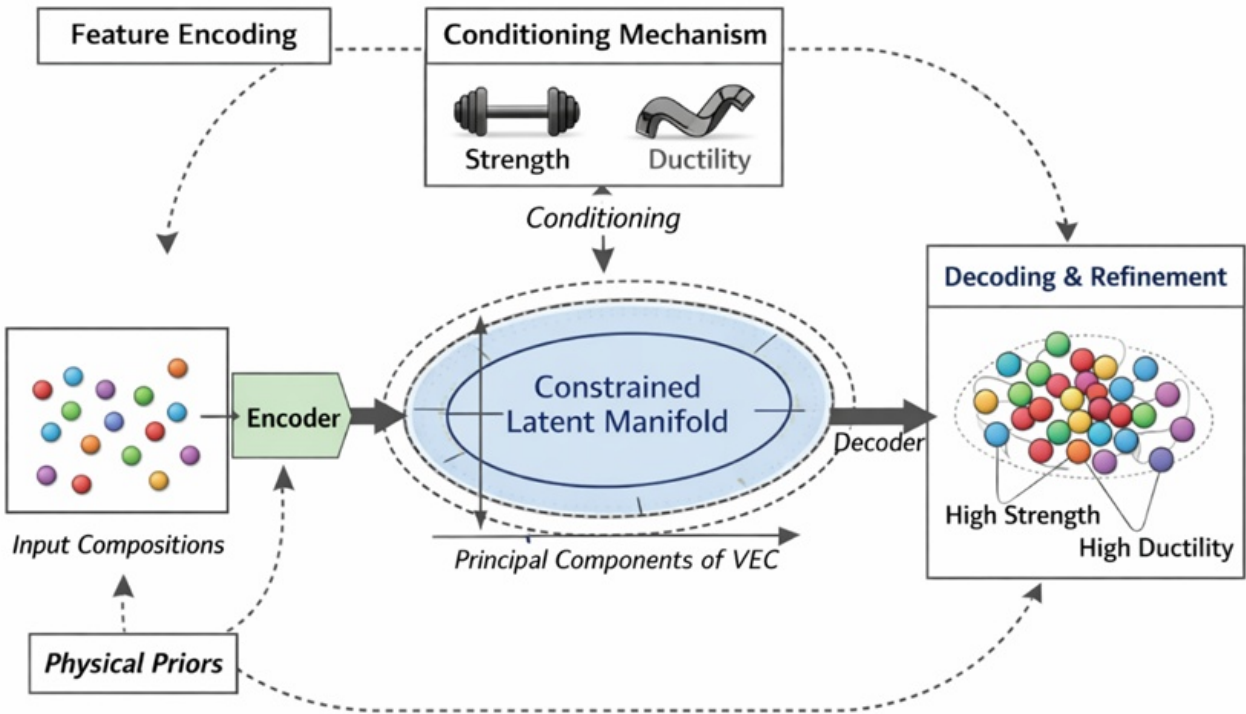


Figure 2. The framework used in this study.

To clarify the conceptual alignment between generative modeling constructs and established materials-science principles, **Table 2** summarizes the correspondence between key framework components, their AI interpretations, and their physical meanings within HEA design.

Table 2. Correspondence between generative model components and materials-science concepts

Framework component	AI interpretation	Physical interpretation	Conceptual role
Encoder	Feature compression	Mapping composition → descriptors	Captures alloy physics
Latent space	Low-dimensional manifold	Feasible compositional landscape	Encodes structure–property relations
Latent constraints	Regularization	Thermodynamic feasibility	Prevents unphysical alloys
Conditioning variables	Control inputs	Target mechanical properties	Enables inverse design
Decoder	Generative mapping	Composition reconstruction	Proposes candidate HEAs
Uncertainty modeling	Variational distribution	Property variability	Risk-aware design
Sampling	Latent exploration	Alloy exploration	Discovery mechanism

Propositions

Building on the proposed conceptual framework, this section articulates a series of theoretical propositions that logically follow from integrating deep generative models with HEA design principles. These propositions serve as testable

hypotheses in future conceptual extensions, emphasizing the framework’s potential to reshape theoretical approaches in materials science. They are grounded in the synthesis of latent-space dynamics, physical constraints, and conditional generation, offering novel insights into how generative processes can, in theory, optimize mechanical properties in HEAs.

Proposition 1: Incorporating physical priors, such as valence-electron concentration and mixing enthalpy, into the latent manifold of deep generative models will improve the theoretical feasibility of generated HEA compositions by reducing the likelihood of unphysical structures. This proposition posits that constrained latent representations act as a filter, prioritizing alloys that align with thermodynamic stability criteria [1, 27, 28]. By embedding these priors, the framework theoretically narrows the search space, enabling more efficient exploration of compositions that exhibit targeted yield strength without compromising phase integrity.

Proposition 2: Conditional mechanisms in generative models, modulated by multi-objective mechanical targets, will, in theory, resolve inherent trade-offs in HEA properties, such as the strength-ductility paradox. Drawing on the framework’s attention-like gates, this suggests that property-conditioned sampling can generate alloys in which enhanced hardness coexists with improved elongation [3, 5]. The proposition posits that probabilistic conditioning fosters emergent synergies among elements, conceptually expanding the achievable property envelope beyond traditional alloy limits.

Proposition 3: Uncertainty quantification through ensemble latent distributions in the proposed framework will provide theoretical bounds on mechanical property attainment, facilitating risk-aware design in high-dimensional compositional spaces. This implies that, by modeling variational uncertainties, the framework can identify robust HEA candidates that are less sensitive to compositional variations [27-29]. Such an approach mitigates the challenges posed by sparse data in HEAs, offering a conceptual tool for prioritizing alloys with reliable performance predictions.

Proposition 4: The bidirectional mapping in the generative architecture—from properties to compositions—will theoretically enable inverse design paradigms that uncover non-intuitive elemental combinations for superior toughness in HEAs. This proposition highlights the decoder’s role in reconstructing alloys from conditioned latents, potentially revealing mixtures involving refractory elements that traditional rules overlook [2, 4]. It underscores the framework’s novelty in treating design as an inference problem, where mechanical targets drive compositional innovation.

Proposition 5: Integration of multi-scale descriptors into the feature encoding module will capture hierarchical interactions in HEAs, leading to alloys with optimized fracture resistance under dynamic loading conditions. By fusing atomic-level attributes with macroscopic metrics, the framework posits a holistic representation that enhances predictive fidelity [5, 9]. This proposition envisions a conceptual shift toward scale-bridging generation, in which emergent behaviors such as lattice distortion strengthening are inherently prioritized.

These propositions collectively form the theoretical core of the framework, providing a logical extension of the literature synthesis. They emphasize originality by focusing on generative inference rather than predictive regression, setting the stage for conceptual validations in alloy theory [6, 7]. The logical connections between the proposed theoretical propositions and the corresponding mechanisms within the generative framework are summarized in Table 3, highlighting how each proposition maps onto specific architectural elements and anticipated conceptual outcomes.

Table 3. Relationship between theoretical propositions and framework mechanisms

Proposition	Core idea	Framework element involved	Expected conceptual outcome
Proposition 1	Physical priors improve feasibility	Constrained latent manifold	Reduced unphysical compositions
Proposition 2	Conditional sampling resolves trade-offs	Conditioning mechanism	Balanced strength–ductility

Proposition 3	Uncertainty enables robustness	Variational distributions	Risk-aware exploration
Proposition 4	Inverse design enables discovery	Bidirectional decoding	Non-intuitive alloy systems
Proposition 5	Multi-scale descriptors improve fidelity	Feature encoder	Better fracture resistance modeling

Results and Discussion

The proposed conceptual framework represents a significant theoretical advancement in the application of deep generative models to HEA design, addressing key gaps in current methodologies while opening avenues for further intellectual exploration. By conceptualizing alloy generation as a conditioned probabilistic process, the framework transcends traditional forward-prediction models, offering a prescriptive approach that aligns with the complexity of multi-principal-element systems [1, 3]. This shift has profound implications for materials science, as it theoretically enables the rational navigation of vast compositional landscapes, potentially accelerating the discovery of HEAs with tailored mechanical properties such as high yield strength and ductility [5].

One primary implication is an enhancement of design efficiency, as defined in theoretical terms. Conventional approaches, reliant on empirical correlations or high-throughput calculations, often struggle with the combinatorial explosion in HEAs [4]. The framework's latent space explorer, constrained by physical limitations, conceptually compresses this space into manageable dimensions, enabling targeted sampling [6, 30]. For instance, conditioning on mechanical objectives theoretically favors FCC-dominant alloys for ductility-focused applications, as evidenced by established descriptors such as VEC [2]. This not only streamlines conceptual design but also integrates uncertainty to inform theoretical robustness, a feature absent in deterministic models [7].

However, the framework's conceptual nature introduces inherent limitations. It assumes ideal embeddings of physical priors, yet in theoretical extensions, mismatches between learned representations and actual physics could arise, potentially leading to biased generations [8]. Additionally, reliance on variational architectures presupposes sufficient representational capacity, which may falter in capturing rare HEA phenomena such as short-range ordering [9]. These limitations highlight the need for conceptual refinements, such as hybrid models that incorporate graph-based symmetries to better reflect atomic interactions [6].

From a broader perspective, the framework contributes to the discourse on AI's role in materials theory. It posits that generative models can serve as theoretical amplifiers, uncovering patterns that human intuition might miss [5]. This aligns with recent conceptual trends in machine learning for alloys, where inverse design paradigms promise to democratize innovation [3]. Nevertheless, ethical considerations in theoretical applications warrant attention; over-reliance on generative outputs could inadvertently perpetuate data biases if underlying assumptions favor certain elemental families [29].

Future directions for conceptual development include extending the framework to incorporate dynamic property targets, such as temperature-dependent mechanics, by adapting diffusion-based generative processes [7]. Moreover, integrating multi-fidelity hierarchies could, in principle, bridge quantum-scale insights with macroscopic behaviors, enriching the latent manifold [2]. Collaborative theoretical efforts might also explore ensemble frameworks that combine multiple generative models to enhance diversity in HEA proposals [4]. Ultimately, this work invites scholars to refine and expand upon these ideas, fostering a deeper theoretical understanding of generative AI in materials engineering [8, 31].

Conclusion

In summary, this conceptual manuscript has developed a novel theoretical framework for leveraging deep generative models to design high-entropy alloys with targeted mechanical properties. By synthesizing foundational literature on HEAs and generative modeling, we have proposed a conditional latent space approach that embeds physical descriptors to enable efficient, property-driven generation. The articulated propositions and discussions underscore the framework's potential to address design challenges, offering a fresh logic for inverse alloy engineering.

This work advances applied artificial intelligence in materials science by providing a blueprint for conceptual innovation, emphasizing probabilistic and constrained generation over traditional methods. While limitations exist, the framework's implications suggest transformative possibilities for theoretical explorations in alloy theory. Future conceptual extensions hold promise for broader applications, ultimately contributing to the sustainable development of advanced materials.

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