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Representation Compression and Scientific Loss in Materials AI

Claire Dupont^{1*}, Julien Martin¹

Abstract

The integration of artificial intelligence into materials science has introduced intricate dynamics between data representation and knowledge extraction. This manuscript explores the conceptual interplay between representation compression, in which high-dimensional material descriptors are reduced to facilitate computational efficiency, and the ensuing scientific loss, characterized by diminished interpretability and potential oversight of underlying physical principles. Through analytical implications, it interprets how compression mechanisms influence the fidelity of material property predictions, emphasizing interaction dynamics within neural architectures. Systems-level insights reveal trade-offs in balancing model parsimony with epistemic richness, where compressed representations may streamline discovery pipelines yet introduce feedback structures that obscure causal relationships. Ethical reasoning underscores the importance of transparency in AI-driven materials design, while steering logics suggest pathways for mitigating loss through hybrid approaches that preserve scientific nuance. The proposed framework conceptualizes these elements as interconnected layers, fostering integrative understanding without empirical validation. This interpretive lens aims to guide future conceptual developments in materials AI, highlighting the need for balanced compression strategies that sustain scientific integrity amid advancing computational paradigms.

Keywords Materials AI, Systems-level insights, Representation compression, Scientific loss, Interaction dynamics, Epistemic reasoning

*Correspondence:

Claire Dupont
claire.dupont@gmail.com

¹ Department of Materials Data Analytics, Faculty of Engineering, University of Bordeaux, Bordeaux, France

Introduction

The advent of artificial intelligence (AI) in materials science has reshaped the landscape of discovery and design, introducing novel ways to handle complex datasets and predict material behaviors. At the core of this transformation lies the concept of representation, where materials are encoded into mathematical forms amenable to machine learning algorithms. These representations, often derived from atomic structures, electronic properties, or microstructural features, serve as the foundational input for AI models [1, 2]. However, as datasets grow in scale and complexity, the necessity for compression emerges, reducing the dimensionality of these representations to enhance computational tractability and model performance [3, 4]. This process, while enabling broader applications, introduces subtle yet profound implications for scientific understanding, manifesting as a form of loss where essential physical insights may be attenuated or overlooked.

Conceptually, representation compression involves transforming high-fidelity descriptors into lower-dimensional embeddings, often through techniques embedded within deep learning frameworks [5, 6]. This compression facilitates the handling of vast material spaces, enabling accelerated screening and optimization in areas such as alloy design and nanomaterial synthesis [7, 8]. Yet, the interpretive challenge arises from the potential dissociation between the compressed form and the original scientific context. For instance, when atomic configurations are projected into latent

spaces, the dynamics of interatomic interactions might be simplified, leading to a trade-off in which efficiency gains come at the cost of reduced visibility into mechanistic details [9, 10]. Such dynamics underscore a broader systems-level insight: AI in materials science operates within a feedback loop where data encoding influences model outputs, which in turn refine future representations, potentially perpetuating a cycle of information narrowing.

Epistemic reasoning further illuminates this interplay, questioning how compression affects the reliability of knowledge derived from AI models [11, 12]. In materials informatics, where decisions affect real-world applications such as energy storage or structural integrity, the ethical imperative demands that compression does not unduly compromise the epistemic value of scientific inquiry [13, 14]. Steering logics, therefore, become crucial, guiding the selection of compression strategies that align with domain-specific needs. For example, in composite materials, where microstructural variability is key, aggressive compression might obscure critical heterogeneities, prompting a need for balanced approaches that integrate multiple representation scales [15, 16].

The literature reflects an evolving awareness of these issues, with discussions on how AI architectures can be conceptualized to mitigate loss while leveraging compression [17, 18]. Generative models, for instance, offer interpretive pathways by reconstructing materials from compressed states, revealing interaction dynamics that might otherwise remain hidden [19, 20]. However, the conceptual tension persists: compression enhances scalability but risks diluting the scientific essence, where loss is not merely quantitative but qualitative, affecting the depth of understanding [21, 22]. This manuscript delves into these dimensions, synthesizing theoretical backgrounds to propose a framework that interprets compression and loss as intertwined elements within materials AI ecosystems.

At a systems level, the integration of AI prompts a reevaluation of traditional scientific paradigms, where empirical validation gives way to data-driven inference [23, 24]. Yet, this shift introduces feedback structures wherein compressed representations feed into iterative learning cycles, potentially amplifying biases or omissions inherent in the initial encoding [25, 26]. Ethical considerations arise here, particularly in ensuring that AI-assisted discoveries maintain traceability to fundamental principles, thereby avoiding a scenario in which scientific loss undermines trust in the methodology [27, 28]. Interaction dynamics between representation layers further complicate this, as compression may alter the relational fabric of material properties, transforming holistic views into fragmented approximations [29, 30].

Conceptual interpretations extend to the role of autoencoders and similar architectures in materials AI, where compression serves as a bottleneck that filters information, influencing downstream analyses [31, 32]. Such mechanisms highlight trade-offs: while they enable efficient exploration of vast chemical spaces, they may impose a steering logic that prioritizes certain features over others, potentially sidelining rare but scientifically significant phenomena [1, 3]. Systems-level insights suggest that addressing this requires a holistic view, considering not just individual models but also the broader informatics pipeline in which compression interacts with data acquisition and interpretation [4, 5].

In synthesizing these elements, this introduction sets the stage for a deeper exploration of theoretical underpinnings and a novel conceptual framework. By focusing on analytical implications rather than prescriptive solutions, it aims to foster an integrative understanding of how representation compression and scientific loss shape the trajectory of materials AI, encouraging reflective practices that enhance epistemic robustness [6, 7].

Theoretical Background & Literature Synthesis

Evolution of representations in materials AI

The development of representations in materials AI has progressed from simplistic featurizations to sophisticated embeddings that capture multifaceted material attributes [1, 2]. Early approaches relied on hand-crafted descriptors, such as bond lengths or coordination numbers, which provided interpretable links to physical properties but scaled poorly with complexity [3, 4]. The shift toward learned representations, facilitated by deep neural networks, introduced compression

as an implicit mechanism to distill essential information from raw data [5, 6]. This evolution reflects interaction dynamics where representations adapt to the demands of predictive tasks, balancing detail with generality [7, 8].

Conceptually, this progression highlights systems-level insights into how representations serve as intermediaries between raw material data and AI inferences [9, 10]. Compression emerges as a key dynamic, reducing redundancy while preserving predictive utility, yet it invites scrutiny regarding the fidelity of scientific translation [11, 12]. The literature underscores that in high-dimensional spaces, such as those encountered in crystal structures or polymer chains, compression facilitates navigation but may attenuate subtle correlations critical to understanding phase behavior or defect formation [13, 14].

Compression mechanisms and their interpretive roles

Compression in materials AI often manifests through dimensionality reduction techniques embedded in model architectures, influencing how information is processed and retained [15, 16]. Analytical implications suggest that these mechanisms create trade-offs: reduced computational burden enhances applicability but may fragment the holistic view of material systems [17, 18]. For instance, in generative frameworks, compression acts as a filter that shapes the latent space, steering the reconstruction of material configurations toward probable rather than exhaustive possibilities [19, 20].

Interaction dynamics within these mechanisms reveal feedback structures, as compressed representations inform subsequent learning iterations, potentially reinforcing dominant patterns at the expense of outliers [21, 22]. Epistemic reasoning positions this as a challenge to scientific integrity, where loss is interpreted not as error but as a conceptual gap in mapping AI outputs back to physical realities [23, 24]. Synthesis of the literature indicates that while compression enables scalable informatics platforms, it necessitates careful consideration of how it alters the interpretive landscape of materials discovery [25, 26].

Scientific loss as an emergent phenomenon

Scientific loss in materials AI arises from the interpretive disconnect introduced by representation compression, manifesting as diminished insight into underlying mechanisms [27, 28]. Systems-level insights portray this loss as an emergent property of AI pipelines, where compressed encodings prioritize efficiency over explanatory depth [29, 30]. The literature synthesizes this through examples in microstructural analysis, where compression can simplify textural features, leading to oversights in property correlations [31, 32].

Ethical reasoning emphasizes the implications for knowledge production, advocating for steering logics that mitigate loss by integrating domain knowledge into compression strategies [1, 3]. Interaction dynamics further illustrate how loss propagates through model ensembles, affecting the robustness of collective inferences [4, 5]. Conceptual interpretations frame loss as a feedback loop in which initial compression decisions reverberate across the AI ecosystem, shaping the epistemic value of derived insights [6, 7].

Integration of compression and loss in AI frameworks

Synthesizing compression and loss requires viewing them as interconnected elements within broader AI frameworks for materials science [8, 9]. Analytical implications highlight trade-offs, such as those in thermoelectric materials design, where compressed representations expedite optimization but may obscure electronic transport nuances [10, 11]. Systems-level insights suggest that integrative approaches that blend multiple compression scales can address these trade-offs and foster a more nuanced understanding [12, 13].

Feedback structures in these frameworks reveal how loss can be amplified or attenuated through architectural choices, prompting epistemic reflections on the role of AI in augmenting rather than supplanting scientific inquiry [14, 15]. Literature points to generative models as interpretive tools that reconstruct from compressed states, offering glimpses into

lost information [16, 17]. Steering logics, therefore, involve conceptual balancing acts, ensuring that compression serves scientific ends without undue epistemic compromise [18, 19].

Challenges in epistemic and ethical dimensions

Epistemic challenges in representation compression revolve around the interpretive fidelity of AI models, where loss questions the trustworthiness of inferences [20, 21]. Ethical reasoning extends this to the societal impacts of materials AI, such as in sustainable technologies, where overlooked loss could lead to suboptimal designs [22, 23]. Interaction dynamics underscore the need for transparent frameworks that expose compression effects, enabling better navigation of these challenges [24, 25].

Systems-level insights integrate these dimensions, portraying materials AI as a socio-technical system where compression and loss intersect with human oversight [26, 27]. Literature synthesis advocates the use of conceptual tools that enhance visibility into these processes, thereby promoting ethical stewardship in AI development [28, 29]. Trade-offs here involve weighing innovation speed against interpretive depth, guiding future directions in the field [30, 31].

Proposed conceptual framework

Compression as an epistemic transformation layer

The proposed conceptual framework interprets representation compression and scientific loss in materials artificial intelligence (AI) as interdependent epistemic dynamics embedded within a layered knowledge architecture. Compression is positioned not merely as a computational necessity but as a transformative interpretive operation that restructures how material phenomena are rendered scientifically visible. Through this lens, compression mediates trade-offs between informational density and interpretive accessibility, shaping both the velocity and the depth of materials discovery.

Rather than functioning as a neutral reduction mechanism, compression serves as an epistemic transformer, reorganizing high-dimensional scientific representations into condensed embeddings that privilege algorithmic tractability. In doing so, it recalibrates the balance between descriptive completeness and operational efficiency, thereby influencing how AI systems perceive, prioritize, and navigate material spaces.

Layer I — Input representation substrate

The first layer of the framework encompasses the input representation substrate, defined by high-dimensional descriptor environments derived from experimental, computational, and imaging sources. Within this substrate reside atomistic graphs, crystallographic tensors, electronic density fields, spectroscopy signatures, and microstructural morphologies. Collectively, these encodings form dense informational reservoirs embedding both observable properties and latent mechanistic signals.

Epistemically, this layer represents the most scientifically expressive domain of the framework. Its dimensional richness enables multidirectional interpretability, allowing AI systems to access structural, chemical, and thermodynamic nuances. However, such plenitude also introduces analytical opacity: the scale and redundancy of descriptor spaces render direct inference computationally prohibitive without intermediate transformation.

Layer II — Compression intermediary

Positioned as the epistemic fulcrum of the framework, the compression intermediary translates representational plenitude into computationally navigable embeddings. This layer operates via dimensional bottlenecks, latent-variable encodings, manifold projections, and feature abstraction operators. Through these mechanisms, raw descriptor spaces are condensed into structured embeddings optimized for predictive and generative tasks.

Compression here functions as an epistemic gatekeeping infrastructure. Informational filtration occurs via selective amplification: correlations aligned with training objectives are accentuated, while low-variance or contextually diffuse

features risk attenuation. Consequently, compression does not merely reduce dimensionality; it redistributes interpretive salience across the representational spectrum.

Recursive feedback structures emerge within this intermediary. Compression choices influence upstream data curation—guiding what data are collected, simulated, or prioritized—while simultaneously shaping downstream inference interpretability. This cyclical interplay positions compression as an active steering logic within the materials AI knowledge ecosystem.

Layer III — Output inference and discovery translation

The third layer operationalizes compressed embeddings into actionable scientific constructs. Within this inference domain reside property-prediction systems, inverse-design engines, generative material architectures, and optimization pipelines embedded in autonomous laboratories.

Outputs manifest as probabilistic property forecasts, candidate material structures, synthesis recommendations, or exploration trajectories. Through this translational function, compressed knowledge becomes materially consequential, shaping both experimental prioritization and theoretical interpretation.

However, because inference operates on compressed embeddings, its outputs inherently reflect the epistemic structuring imposed upstream. Discovery trajectories, therefore, emerge not solely from material reality but from the representational logics through which that reality has been computationally mediated. The stratified interplay between representational substrates, compression intermediaries, and inference outputs reveals how epistemic translation unfolds across materials AI pipelines, with each layer introducing distinct interpretive affordances and vulnerabilities. These cross-layer dynamics are conceptually synthesized in [Table 1](#).

Table 1. Conceptual dimensions of representation compression across materials AI layers

Framework layer	Representational form	Compression mechanisms	Epistemic function	Scientific vulnerabilities
Input representation substrate	Atomic graphs, crystallographic tensors, spectroscopy signals, microstructural images, and electronic density fields	Descriptor standardization, featurization pipelines, and graph encodings	Encodes high-dimensional material knowledge; preserves mechanistic richness	Redundancy, noise entanglement, scale heterogeneity
Compression intermediary	Latent embeddings, manifold projections, reduced feature vectors	Dimensional bottlenecks, autoencoders, variational encodings, and feature abstraction operators	Translates descriptor plenitude into computationally navigable structures	Attenuation of low-variance signals; mechanistic dilution
Output inference layer	Property predictions, generative materials, optimization trajectories, discovery pathways	Predictive modeling, inverse design architectures, and generative decoding	Operationalizes compressed knowledge into discovery outputs	Epistemic dependency on compressed priors; interpretability reduction
Feedback integration structures	Error signals, uncertainty gradients, validation outputs	Backpropagation, latent recalibration, descriptor reinjection	Enables adaptive refinement of compression logics	Reinforcement of dominant correlations; bias propagation

Governance and interpretive overlays	Interpretability frameworks, domain priors, physics-informed constraints	Hybrid modeling, explainable AI, and multi-resolution fusion	Preserves epistemic transparency across AI pipelines	Incomplete reintegration of lost mechanistic nuance
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Scientific loss as epistemic redistribution

Scientific loss is conceptualized not as informational deletion but as redistributive attenuation within the framework. Compression reorders epistemic emphasis: features conducive to predictive performance retain representational fidelity, whereas subtle mechanistic irregularities—defect energetics, metastable intermediates, anomalous bonding environments—may recede into abstraction.

This redistribution introduces systemic trade-offs:

- Enhanced exploration efficiency versus mechanistic interpretability
- Pattern dominance versus anomaly sensitivity
- Latent coherence versus physical granularity

Over time, such trade-offs may narrow epistemic bandwidth, biasing discovery systems toward well-represented material families while marginalizing chemically or structurally unconventional domains.

Feedback structures and adaptive compression

A defining property of the framework is its cyclical reflexivity. Inference outcomes propagate backward as epistemic feedback signals that can recalibrate compression logics. Prediction uncertainties, generative instabilities, or experimental mismatches may reveal latent blind spots, prompting re-expansion of compressed spaces or reintegration of previously attenuated descriptors.

Through these recursive interactions, compression evolves into an adaptive epistemic regulator rather than a static reduction filter. The framework thus envisions materials AI systems capable of dynamically renegotiating the balance between representational efficiency and scientific depth.

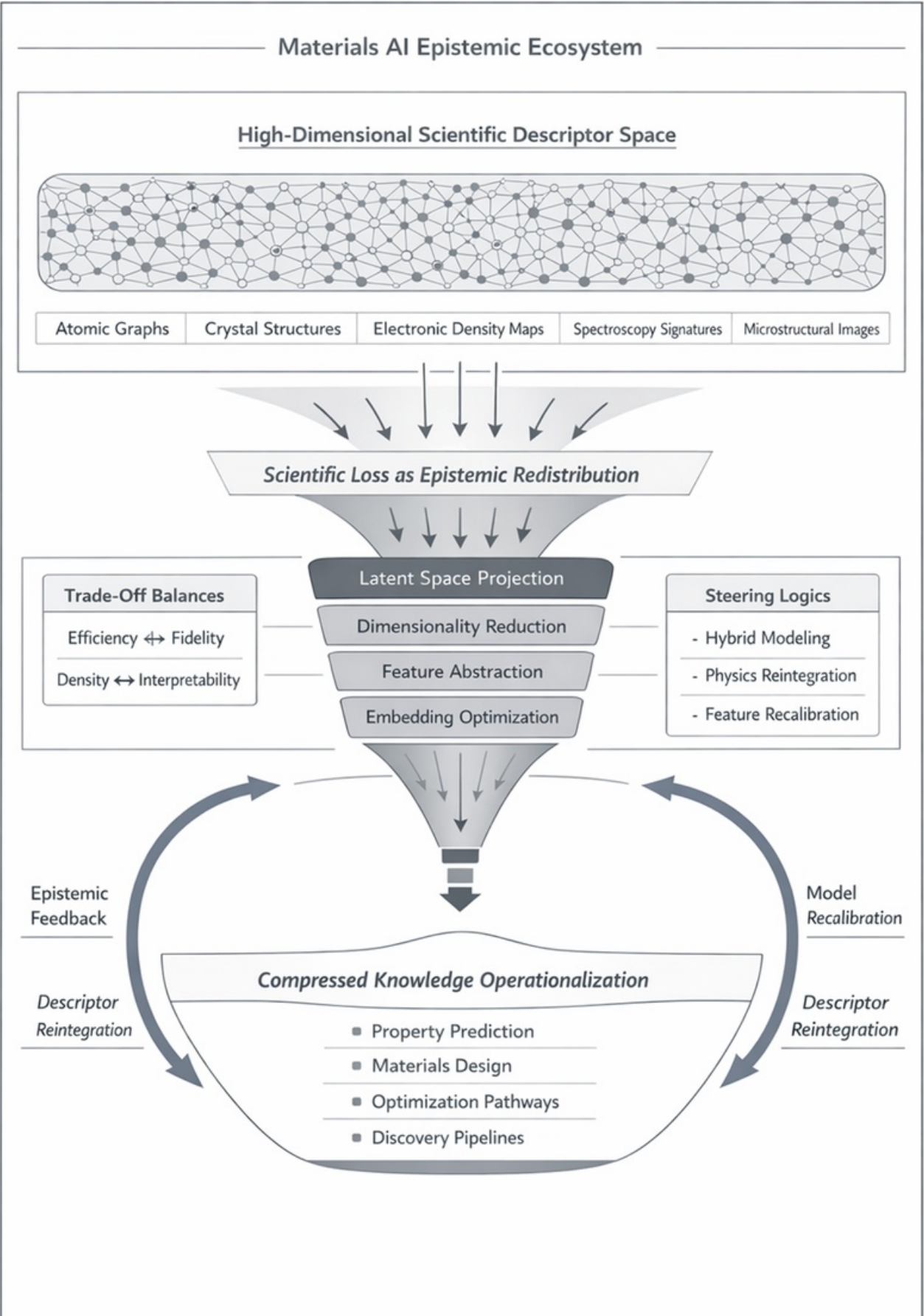
Hybrid mitigation and governance logics

To counteract excessive scientific attenuation, the framework integrates hybrid steering mechanisms that reinject domain knowledge into compressed architectures. Physics-informed latent constraints, interpretable embedding mappings, multi-resolution descriptor fusion, and human-guided validation loops serve as corrective infrastructures.

Ethical reasoning operates as a cross-layer governance overlay that addresses transparency, bias propagation, and discovery equity. By interrogating how compression redistributes epistemic attention, governance structures ensure that acceleration in materials discovery does not occur at the expense of scientific integrity.

Ecosystem interpretation

At its broadest scale, the framework interprets materials AI as an epistemic ecosystem governed by the dialectic between compression and scientific loss. Compression structures complexity to enable accelerated discovery, while loss necessitates reflexive reintegration to preserve interpretive richness. Innovation emerges from the dynamic equilibrium between these opposing yet mutually generative forces. **Figure 1** illustrates this framework textually as a schematic diagram with interconnected components. The visual schema positions the “Compression Intermediary”—a funnel structure that manages latent-space projection and feature selection—as the central transformative engine.



Analytical implications

The proposed framework’s analytical implications illuminate how representation compression and scientific loss operate as interdependent forces within materials AI, reshaping the interpretive architecture of knowledge generation. By positioning compression as a steering intermediary, the framework reveals interaction dynamics that redistribute emphasis across material descriptors, where high-dimensional inputs undergo selective filtering that prioritizes scalable patterns over exhaustive detail [1, 5]. This redistribution carries epistemic weight, as the resulting embeddings may foreground emergent properties while backgrounding foundational mechanisms, such as lattice vibrations or defect migrations, thereby altering the interpretive lens through which material behaviors are apprehended [6, 7].

Systems-level insights emerge from considering the framework’s layered structure, in which feedback loops between the compression and inference layers propagate loss nonlinearly. For example, as compressed latent spaces inform iterative refinements, subtle variations in input representations can amplify or dampen loss trajectories, creating self-reinforcing cycles that influence the overall epistemic robustness of AI-derived insights [8, 9]. Trade-offs become analytically salient here: the efficiency afforded by compression enables broader exploration of materials spaces, yet this comes with a conceptual cost in reduced granularity, prompting reflections on how such dynamics might privilege certain classes of materials—say, crystalline over amorphous—within discovery pipelines [10, 11].

Epistemic reasoning within the framework underscores the interpretive challenge of tracing scientific loss back to its origins. Compression does not erase information outright but reframes it, leading to implications where reconstructed outputs from latent spaces may exhibit fidelity in aggregate predictions while obscuring causal interdependencies [12, 13]. Interaction dynamics further imply that this reframing fosters epistemic layering, with surface-level correlations gaining prominence over deeper physical intuitions, necessitating vigilant conceptual navigation to maintain alignment with scientific principles [14, 15].

Ethical dimensions surface analytically as the framework interprets loss through the prism of responsibility in AI-assisted materials design. In contexts where compressed representations underpin decisions on sustainable alloys or functional composites, the potential for overlooked nuances raises questions about the stewardship of knowledge, requiring steering logics to incorporate safeguards to counter unintended epistemic drift [16, 17]. At a systems level, this suggests implications for the broader informatics ecosystem, where integration of hybrid approaches—blending compressed efficiency with interpretive anchors—could recalibrate loss toward more balanced outcomes [18, 19].

The framework’s originality lies in its portrayal of compression and loss as dialectical elements, yielding analytical implications for adaptive steering. By conceptualizing bidirectional flows, it opens the door to real-time interpretive adjustments that mitigate cumulative loss without sacrificing scalability [20, 21]. Such insights extend to how materials AI might evolve, with compression serving not as a reductive force but as a catalyst for refined systems-level understanding, where loss itself becomes a lens for probing the boundaries of representable knowledge [22, 23]. These efficiency–interpretability tensions manifest through recurring compression dynamics that redistribute epistemic emphasis across materials discovery systems. The principal trade-offs and their systemic consequences are analytically consolidated in **Table 2**.

Table 2. Analytical trade-offs and epistemic consequences of scientific loss.

Compression dynamic	Efficiency gains	Epistemic loss manifestation	Systems-level implications	Mitigation steering logics

Dimensionality reduction	Accelerated computation; scalable screening	Suppression of weak correlations; anomaly masking	Bias toward dominant material families	Multi-scale embeddings
Latent space projection	Structured generative navigation	Mechanistic abstraction	Reduced causal traceability	Physics-informed constraints
Feature selection filtering	Model parsimony; reduced noise	Loss of rare defect signatures	Underrepresentation of metastable states	Descriptor reintegration loops
Autoencoder bottlenecks	Efficient reconstruction pathways	Textural simplification in microstructures	Fragmented property relationships	Hybrid reconstruction modeling
Predictive embedding optimization	Improved predictive accuracy	Interpretive opacity	Reduced scientific explainability	Explainable latent mapping
Iterative compression feedback	Adaptive learning acceleration	Reinforced representational bias	Epistemic path dependence	Human-in-the-loop recalibration

These implications collectively interpret the framework as a tool for dissecting the conceptual tensions inherent in materials AI, fostering a deeper appreciation of how representation choices ripple through the scientific process [24, 25]. Trade-offs in interaction dynamics highlight the need for ongoing epistemic vigilance, ensuring that analytical pursuits in this domain preserve the interpretive richness of material science amid advancing AI paradigms [26, 27].

Results and Discussion

The discussion integrates the framework's elements into a cohesive interpretive narrative, emphasizing how representation compression and scientific loss intertwine to redefine the conceptual contours of materials AI. Drawing from the layered architecture, interaction dynamics illustrate compression as a pivotal nexus, where the intermediary role not only streamlines high-dimensional data but also engenders feedback structures that subtly reshape scientific inquiry [3, 4]. This reshaping manifests as loss distributed across epistemic planes, where the drive for computational parsimony intersects with the imperative for mechanistic fidelity, creating a landscape of perpetual tension and potential synthesis [28, 29].

Systems-level insights position materials AI as an evolving ecosystem, in which compression influences not only isolated predictions but also the relational fabric connecting data acquisition, model inference, and knowledge dissemination [30, 31]. Analytical interpretations reveal that loss, far from a static artifact, evolves through these connections, with trade-offs emerging in the balance between generalization and specificity—generalized embeddings may accelerate innovation in broad material classes but risk diluting insights into niche phenomena, such as interfacial effects in heterostructures [1, 32]. The framework's steering logics offer a conceptual pathway to navigate this, advocating for interpretive integrations that embed domain priors into compression processes, thereby attenuating loss while enhancing systemic coherence [2, 5].

Epistemic reasoning deepens the discussion by framing loss as an opportunity for reflective practice, questioning how compressed representations alter the very nature of scientific discourse in materials science. Interaction dynamics suggest that without deliberate feedback mechanisms, loss could compound, leading to interpretive silos where AI outputs diverge from foundational understandings [6, 7]. Conversely, the framework implies that embracing hybrid dynamics—where compression coexists with reconstructive pathways—could foster richer epistemic exchanges, allowing for the recovery of nuanced interpretations in post-processing stages [8, 9].

Ethical considerations permeate this integrative view, highlighting the responsibility to ensure that compression strategies do not inadvertently marginalize underrepresented material systems or obscure critical safety-related properties [10, 11]. At a broader scale, systems-level insights interpret these ethical imperatives as intertwined with technological advancement, where steering logics must prioritize transparency to sustain trust in AI-mediated discoveries [12, 13]. The framework's conceptual originality contributes by interpreting the interplay between compression and loss as a generative tension, one that drives innovation through careful balancing rather than eliminating trade-offs [14, 15].

Furthermore, the discussion underscores feedback structures as key to adaptive evolution: as materials AI incorporates more diverse data modalities, compression mechanisms will need to evolve interpretively, with loss serving as a diagnostic signal for refining the ecosystem [16, 17]. Interaction dynamics thus become central, implying that bidirectional flows between layers can transform potential epistemic vulnerabilities into strengths, promoting a more resilient conceptual foundation [18, 19].

In synthesizing these threads, the framework facilitates an interpretive bridge between theoretical compression principles and their implications for scientific practice, encouraging a view of materials AI as a dynamic, self-correcting system [20, 21]. Trade-offs remain inherent, yet the analytical and ethical reasoning embedded in the framework provides tools for steering toward outcomes that honor both efficiency and depth [22, 23]. This integrative perspective ultimately enriches the discourse, positioning representation compression and scientific loss not as impediments but as constitutive elements of progressive materials understanding [24, 25].

Conclusion

In conclusion, the conceptual framework interprets representation compression and scientific loss as foundational dynamics that underpin the evolving interplay in materials AI, offering systems-level insights into their integrative roles. Through analytical implications, interaction dynamics emerge as central, revealing how compression navigates trade-offs to shape epistemic landscapes while feedback structures sustain ongoing refinement. Epistemic reasoning highlights the framework's contribution in fostering interpretive balance, where loss is reframed as a catalyst for deeper conceptual engagement rather than mere reduction.

Steering logics within the framework emphasize ethical and systemic considerations, guiding materials AI toward paradigms that preserve scientific nuance amid computational imperatives. This interpretive synthesis underscores the framework's potential to illuminate pathways for conceptual advancement, ensuring that AI augments rather than supplants the richness of materials science inquiry.

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