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Material Spaces Are Not Euclidean: A Conceptual Critique of Distance Metrics in Materials

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Abstract

The conceptualization of material spaces within materials science has traditionally relied on Euclidean distance metrics, yet this approach overlooks the inherent complexities of material properties and structures. This manuscript explores the interpretive dimensions of non-Euclidean geometries in representing material relationships, emphasizing how manifold learning and Riemannian frameworks reveal intricate interaction dynamics among atomic configurations and physical attributes. By synthesizing recent literature on geometric neural operators and hyperbolic embeddings, the analysis underscores the trade-offs between simplified Euclidean assumptions and the richer, curvature-aware interpretations that align with multiscale material behaviors. Conceptual interpretations highlight how distance metrics influence systems-level insights in materials informatics, where flat spaces fail to capture hierarchical or topological nuances. The proposed framework integrates these elements through a steering logic that navigates the epistemic challenges of metric selection, fostering a deeper understanding of material continuity and discontinuity without empirical assertions. Ethical reasoning is woven into considerations of the implications for knowledge representation in computational materials discovery. This critique advocates an integrative view that enhances conceptual coherence in the field by bridging abstract geometric principles with material phenomenology.

Keywords Materials informatics, Non-Euclidean geometry, Material spaces, Distance metrics, Manifold learning, Conceptual critique

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Introduction

In the realm of materials science, the way distances between material entities are measured profoundly shapes the interpretive landscape of discovery and understanding. Traditional frameworks have relied heavily on Euclidean metrics, in which distances are computed in a flat, linear space akin to everyday spatial intuitions. This reliance stems from historical precedents in crystallography and solid-state physics, where lattice parameters and vectorial representations provided a straightforward means to quantify similarities and differences among materials [1]. However, as the field evolves toward integrative approaches encompassing multiscale phenomena—from atomic arrangements to macroscopic properties—the limitations of such metrics become apparent, as they are unable to accommodate the curved, hierarchical, or networked natures inherent to material systems.

The conceptual shift toward non-Euclidean perspectives arises from recognizing that material spaces are not mere collections of points in a vector space but rather dynamic arenas where interactions unfold along nonlinear pathways. For instance, in materials informatics, where vast datasets of compositions and properties are navigated, Euclidean distances often impose artificial symmetries that distort the true relational dynamics [2, 3]. This distortion manifests in interpretive challenges, such as overemphasizing linear interpolations between material points while neglecting topological barriers or attractors that define phase transitions or stability regimes. The critique here centers on how these metrics influence the steering logics of knowledge generation, where the choice of distance measure acts as a conceptual filter, amplifying certain patterns while obscuring others.

Exploring this critique requires an appreciation of the epistemic trade-offs involved. Euclidean metrics offer computational simplicity and intuitive visualization, facilitating rapid screenings in high-throughput workflows [4]. Yet, they fall short in capturing the curvature induced by correlated properties, such as electronic band structures or mechanical responses, which exhibit manifold-like behaviors [5, 6]. Non-Euclidean alternatives, drawing from differential geometry, introduce curvatures that better reflect these correlations, enabling interpretations that align with the intrinsic geometries of material data manifolds [7, 8]. This interpretive lens reveals feedback structures where local distances inform global topologies, and vice versa, fostering a systems-level insight into material evolution.

Moreover, the integration of graph-based representations in materials science amplifies the need for such a critique. Graphs, often embedded in Euclidean spaces for analysis, inherently possess non-Euclidean qualities through their connectivity and shortest-path metrics [3, 9]. When materials are modeled as graphs—atoms as nodes, bonds as edges—the distance between configurations transcends simple vector differences, incorporating path dependencies and community structures [9]. This perspective uncovers interaction dynamics that Euclidean metrics flatten, such as hyperbolic expansions in layered materials and Riemannian constraints in functional connectivity [10, 11]. The conceptual interpretation here is one of enriched continuity, where distances serve not just as separators but also as bridges that reveal emergent properties.

Ethical and epistemic reasoning further underscores the importance of this critique. In an era where artificial intelligence drives materials discovery, the metrics employed carry implications for bias and representativeness [12, 13]. Euclidean assumptions may inadvertently prioritize certain material classes, such as those with isotropic properties, over anisotropic or disordered systems, leading to a skewed knowledge base [14]. By contrast, non-Euclidean frameworks promote a more inclusive interpretive framework, acknowledging the diversity of material morphologies and their underlying logics [15, 16]. This shift encourages a reflective stance on how distance metrics shape the narrative of material science, prompting integrative syntheses that transcend disciplinary silos.

The manuscript proceeds by synthesizing theoretical backgrounds from recent literature, highlighting how manifold and geometric learning paradigms challenge Euclidean dominance [17, 18]. This synthesis paves the way for a proposed conceptual framework that interprets material spaces through non-Euclidean lenses, emphasizing analytical implications for understanding relational complexities [19, 20]. Through this, the critique aims to illuminate the conceptual undercurrents that guide metric selection, fostering deeper insights into the fabric of materials without venturing into empirical domains.

Ultimately, this exploration invites a reevaluation of foundational assumptions, in which distance metrics are seen not as neutral tools but as interpretive constructs that shape the conceptual terrain of materials science [8, 21]. By delving into these dynamics, the analysis seeks to enhance the coherence of material representations, bridging abstract geometries with the phenomenological richness of matter [10, 11].

Theoretical Background and Literature Synthesis

Foundations of distance metrics in materials representation

Distance metrics form the bedrock of how similarities and dissimilarities are conceptualized in materials science, shaping not only computational operations but also the underlying interpretive frameworks through which property spaces are navigated. Euclidean metrics, rooted in the L2 norm, have historically dominated materials representations due to their natural compatibility with vectorial descriptors such as atomic coordinates, handcrafted feature vectors, and tabular database entries [1]. Their appeal lies in mathematical simplicity, computational efficiency, and ease of integration into clustering, regression, and nearest-neighbor algorithms commonly used for materials classification and screening.

However, this dominance implicitly imposes a flat, geometric worldview on material spaces—one in which distances are assumed to be linear, isotropic, and globally consistent. Such assumptions may obscure the complex, interdependent nature of material attributes, in which changes in composition, structure, or processing conditions can produce non-linear, regime-dependent effects [1, 14]. The synthesis here emphasizes that distance metrics are not neutral mathematical tools; rather, they actively shape interaction dynamics within materials AI pipelines by privileging certain relationships while marginalizing others. Linear distances, while operationally convenient, often fail to capture the curved, constrained, and entangled landscapes that characterize real material behavior.

Recent explorations in manifold learning further underscore this mismatch by demonstrating that material data frequently reside on lower-dimensional curved surfaces embedded within high-dimensional descriptor spaces [5, 6]. These manifolds reflect latent constraints imposed by physics, chemistry, and thermodynamics, suggesting that meaningful similarity should be evaluated along intrinsic pathways rather than through ambient Euclidean space. In studies of functional materials, for instance, Riemannian manifolds have been used to interpret distances that respect the positive-definiteness of covariance matrices, elastic tensors, or diffusion operators, yielding more coherent systems-level interpretations [10, 11]. This shift foregrounds a fundamental trade-off: Euclidean metrics support scalability and algorithmic convenience, whereas manifold-aware metrics surface deeper epistemic structure, such as intrinsic curvature and geodesic relations that govern property correlations and transitions [8, 12].

Non-Euclidean geometries and manifold perspectives

The integration of non-Euclidean geometries into materials representation marks a pivotal interpretive evolution, reframing distance as a context-sensitive construct rather than a universal scalar. Hyperbolic spaces, in particular, have gained attention for their ability to encode hierarchical and tree-like structures, which are prevalent in layered, porous, and multicomponent materials systems [15, 16]. In such contexts, relational complexity grows exponentially with scale, rendering Euclidean embeddings increasingly inefficient and conceptually misleading.

The literature on hyperbolic metamaterials illustrates how these geometries enable alternative interpretations of wave propagation, dispersion relations, and density-of-states phenomena that cannot be faithfully captured under flat-metric assumptions [20]. These works highlight feedback structures between local interactions and global material responses, reinforcing the idea that geometry mediates the distribution of physical meaning across scales. More broadly, manifold-fitting techniques that adapt to arbitrary norms allow distances to be interpreted in terms of topological invariants, symmetry classes, or conservation constraints, rather than simple coordinate differences [6, 13].

Within materials informatics, graph neural networks (GNNs) operationalize these ideas by embedding relational data—atoms, bonds, defects, or processing steps—into non-Euclidean latent spaces where distances reflect connectivity, path dependence, and interaction strength [9]. Such embeddings reveal steering logics underlying metric choice: decisions about geometry implicitly balance computational tractability against representational fidelity and interpretive richness [2, 3]. Ethical and epistemic considerations emerge at this juncture, as metric bias can systematically compress or obscure underrepresented regions of materials space, reinforcing incomplete or skewed scientific narratives. Consequently, recent literature advocates integrative strategies that combine multiscale manifold learning with reflexive oversight to better capture material diversity and uncertainty [11].

Critique of Euclidean assumptions in computational frameworks

A critical examination of Euclidean metrics exposes their limitations in representing material discontinuities, anisotropies, and constrained transitions. In spatial analogies drawn from network theory, straight-line distances often fail to reflect true accessibility or connectivity—much like road networks defy simple geometric proximity [17]. Analogous issues arise in materials systems where phase boundaries, defect networks, or processing pathways introduce non-trivial topologies that distort Euclidean similarity measures.

These limitations become particularly salient in uncertainty-aware machine learning, where predictions made in curved or folded property manifolds can be systematically misestimated when evaluated using flat metrics [4]. Errors may appear artificially small or large depending on local curvature, leading to misleading confidence assessments. In response, literature on geometric neural operators and curvature-aware architectures proposes non-Euclidean adaptations that align learning dynamics with the intrinsic geometry of material data [8]. Such approaches reinterpret prediction not as pointwise approximation but as movement along constrained manifolds, enhancing conceptual coherence under uncertainty.

Further challenges to Euclidean dominance arise from studies on polynomial mappings and learning over symmetric positive definite (SPD) matrices, which preserve manifold structure in unsupervised and self-supervised settings [13]. These frameworks emphasize relational consistency and symmetry preservation, offering metaphoric parallels to material deformation and relaxation phenomena, in which nonlinear metrics expose invariant structures [10, 11]. The epistemic trade-off is thus sharpened: Euclidean metrics streamline analysis and benchmarking, but often at the cost of flattening complex material narratives and suppressing structurally meaningful variation [19, 22].

Integration with materials informatics and graph-based models

Materials informatics platforms exemplify the growing recognition that metric choice fundamentally shapes discovery trajectories. Large, atlas-like databases increasingly rely on non-Euclidean embeddings to map state-of-the-art materials landscapes in ways that preserve relational meaning rather than mere numerical proximity [1]. Reviews of machine learning applications in domains such as carbon nanotubes, crystalline solids, and atomic-scale simulations demonstrate how GNNs and topology-aware models interpret physical properties through graph distances, spectral measures, or geodesic paths that transcend Euclidean vector spaces [2, 3, 9].

This integration enables systems-level insights in which distance metrics act as interpretive bridges between atomic interactions, mesoscale organization, and emergent macroscopic behavior [3]. In multiscale settings, learning on SPD manifolds further extends this logic by incorporating curvature-sensitive evaluation criteria, echoing assessment paradigms from rehabilitation or functional performance analysis and recontextualizing them for materials behavior [11].

The literature synthesis ultimately points toward a broader epistemic reasoning: non-Euclidean metrics do not merely improve representational accuracy but reorient how meaning is constructed in materials AI. By mitigating the flattening effects of traditional approaches, they enable richer feedback structures, support pluralistic interpretations of similarity, and foster a more holistic understanding of material systems under complexity and uncertainty [14, 18]. The epistemic implications of metric choice, summarized in **Table 1**, illustrate how distance measures function not merely as computational tools but as interpretive instruments that shape material understanding.

Table 1. Distance metrics as epistemic instruments in materials science

Metric paradigm	Geometric assumption	What is preserved	What is obscured	Analytical consequence	Epistemic trade-off
Euclidean (L2)	Flat, isotropic space	Linear similarity, global comparability	Curvature, hierarchy, topological constraints	Efficient clustering and screening, but distorted relational interpretation	Computational simplicity vs. loss of structural meaning
Manifold-Based (Riemannian)	Curved, locally adaptive space	Covariance structure,	Global linear interpretability	Reveals stability regimes and transition pathways	Interpretive richness vs. scalability

		intrinsic correlations			
Hyperbolic	Exponentially expanding space	Hierarchies, branching evolution	Local Euclidean intuition	Faithful representation of material families and compositional trees	Hierarchical fidelity vs. intuitive visualization
Graph-Induced Metrics	Topological connectivity	Path dependence, relational strength	Absolute coordinate distance	Captures interaction dynamics and network effects	Structural realism vs. metric uniformity
SPD Manifold Metrics	Symmetry-preserving geometry	Positive-definite relations	Euclidean comparability	Preserves invariants in correlated property spaces	Mathematical rigor vs. conceptual accessibility

Proposed conceptual framework

The conceptual framework presented here interprets material spaces through a non-Euclidean lens, emphasizing the interpretive implications of metric choices on relational dynamics. At its core lies an integrative structure that navigates the trade-offs between flat Euclidean representations and curvature-infused geometries, fostering systems-level insights into material continuities and disruptions. This framework conceives material spaces as manifold-embedded arenas where distances are not fixed vectors but adaptive measures shaped by intrinsic curvatures and topological constraints [5, 6, 8].

Central to this interpretation is the steering logic that governs metric adaptation: in regions of high property correlation, distances contract to reflect clustered behaviors, while in sparse or hierarchical zones, they expand hyperbolically to accommodate expansive relational trees [15, 16]. Such dynamics reveal feedback structures in which local metric adjustments inform global topological interpretations, and vice versa, thereby enhancing the conceptual coherence of material classifications [7, 13]. Ethical reasoning integrates by highlighting how metric biases can skew epistemic priorities, advocating for inclusive geometries that embrace material diversity [4, 13].

The framework further explores interaction dynamics through Riemannian interpretations, where material properties form positive definite manifolds, allowing distances to respect covariance intricacies [10, 11]. This perspective uncovers analytical implications for understanding phase spaces, where non-Euclidean metrics illuminate pathways of stability and transition without linear impositions [10, 20]. By synthesizing these elements, the framework promotes an epistemic shift toward interpretive richness, where distances serve as conceptual conduits for unraveling multiscale material narratives [1, 2]. **Figure 1** provides a conceptual visualization contrasting traditional Euclidean and proposed non-Euclidean geometric frameworks for representing materials in AI. A flat, gridded Euclidean Plane at the base depicts conventional linear metrics (e.g., L2 distance), connecting material points with direct, uniform arrows. Overlaying and enveloping this plane is a complex, Curved Manifold, illustrating non-linear relationships through hyperbolic expansions, Riemannian constraints (loop structures), and Adaptive Distance arrows that vary in thickness based on local data density. Annotations highlight the framework's critical dimensions: Curvature Feedback (global-local interactions), Topological Trade-offs (consequences of metric selection), and Epistemic Inclusivity (ethical considerations in representation). The schematic visually argues for a shift from a flat, uniform-distance model to a warped, hierarchical, and adaptive one, where the geometry itself encodes the complex relational physics and chemistry of material spaces.

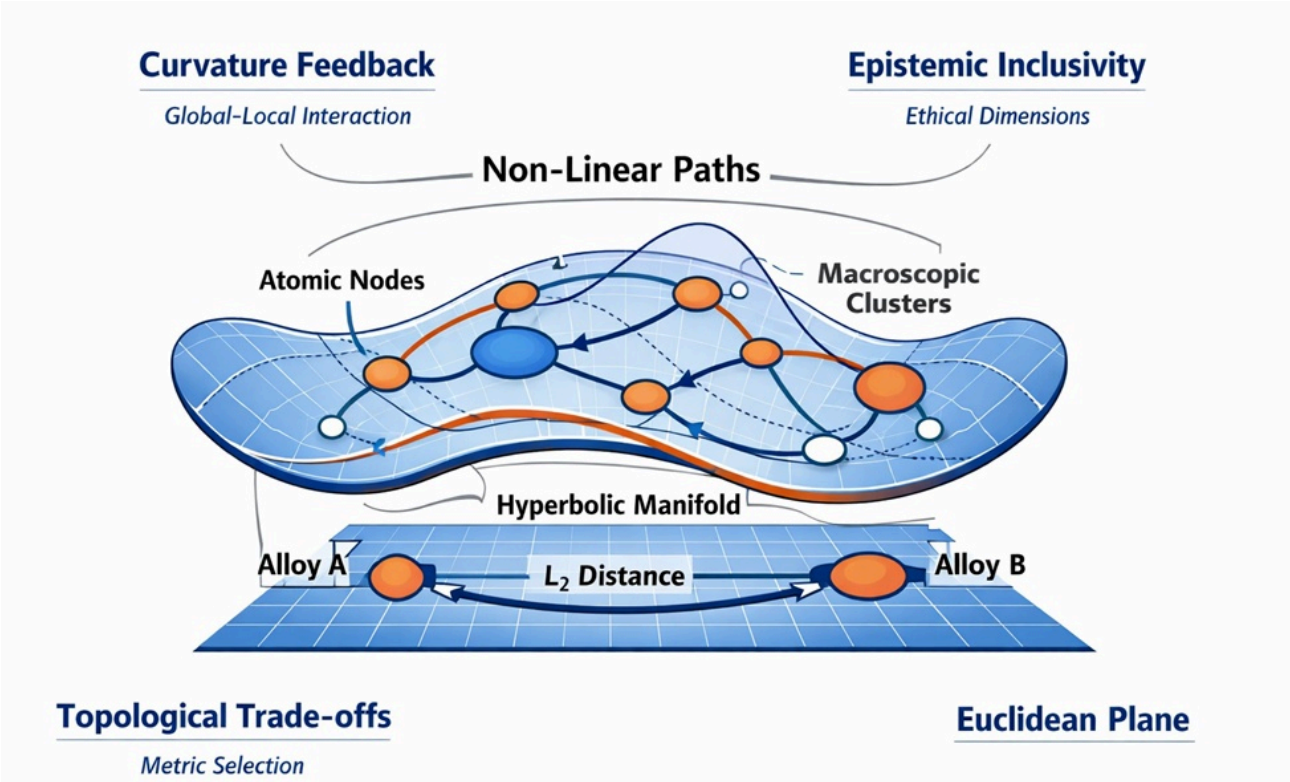

Figure 1. Contrasting geometric embeddings for materials representation

Expanding on this, the framework's analytical implications extend to materials informatics, where graph embeddings in non-Euclidean spaces interpret atomic interactions as networked manifolds, revealing hidden symmetries and discontinuities [2, 9]. The conceptual interpretation here is of enriched connectivity, in which distances facilitate the bridging of disparate material domains, such as from crystalline to amorphous states [14, 17]. Systems-level insights emerge from this, portraying material evolution as a navigation through curved spaces, guided by metric logics that balance simplicity with fidelity [18, 19].

In essence, this framework offers an interpretive toolkit for critiquing and reimagining distance metrics, steering toward a more nuanced understanding of material spaces without prescriptive claims [10-12, 21].

Analytical implications

The interpretive ramifications of reconceptualizing material spaces through non-Euclidean distance metrics extend across multiple analytical dimensions of materials science, fundamentally reshaping how relational structures are understood and navigated. Within this framework, distances cease to function as neutral quantifiers and instead operate as interpretive instruments that actively reveal—or suppress—underlying system dynamics. Curvature-induced clustering in property spaces, for example, reframes similarity as a consequence of constrained relational pathways rather than linear proximity, altering how stability, variability, and transition regimes are analytically inferred [5, 7].

Analytical implications emerge most clearly in the treatment of multiscale interactions. Non-Euclidean metrics enable a coherent interpretation of how local perturbations—whether compositional, structural, or processing-related—propagate through curved manifolds, producing non-uniform global responses [6, 10]. This stands in contrast to Euclidean representations, where such perturbations are implicitly assumed to diffuse isotropically. The resulting trade-off in representational accuracy is epistemically consequential: Euclidean metrics streamline pattern recognition and comparative screening, but they frequently obscure hierarchical feedbacks and constraint-driven couplings that non-

Euclidean approaches render analytically visible, thereby supporting richer systems-level interpretations [8, 11]. The analytical implications of adopting non-Euclidean distance metrics are synthesized in **Table 2**, highlighting how curvature-aware representations reshape similarity, uncertainty, and discovery reasoning.

Table 2. Analytical implications of non-Euclidean metrics across materials AI reasoning

Analytical dimension	Euclidean interpretation	Non-euclidean reinterpretation	Revealed system dynamics	Conceptual gain
Similarity assessment	Linear proximity	Geodesic proximity along manifolds	Constraint-driven clustering	Meaningful similarity under correlation
Multiscale interaction	Isotropic propagation	Curvature-guided influence pathways	Hierarchical feedback loops	Coherent scale integration
Phase and regime boundaries	Sharp separations	Transitional curvature zones	Continuous yet constrained transitions	Improved interpretive continuity
Dataset navigation	Uniform embedding	Topology-preserving embedding	Preservation of rare or outlier structures	Reduced flattening bias
Discovery steering	Density-driven focus	Geometry-aware exploration	Balanced exploration–exploitation	Epistemic inclusivity
Uncertainty interpretation	Distance-based confidence	Curvature-conditioned uncertainty	Local reliability variation	Reflexive uncertainty reasoning

The framework's emphasis on manifold embeddings further implies a shift in how material similarity itself is analytically discerned. In hyperbolic spaces, distances expand to accommodate branching hierarchies, offering an interpretive lens well suited to expansive material families—such as polymers, alloys, or compositional design trees—whose evolutionary structures resist flattening [15, 16]. This geometric expansion foregrounds interaction dynamics in which epistemic reasoning becomes central: metric selection implicitly steers attention toward either compact, well-characterized clusters or dispersed, exploratory outliers, shaping what is recognized as novelty versus redundancy [12, 14]. In materials informatics, these implications materialize in dataset interpretation, where non-Euclidean metrics preserve topological distinctions that Euclidean embeddings tend to compress, enabling more nuanced navigation of discovery pathways and hypothesis spaces [1, 2, 9].

Ethical dimensions intertwine with these analytical implications through the lens of knowledge equity. By accommodating anisotropy, heterogeneity, and structural irregularity, non-Euclidean frameworks promote more inclusive interpretations of material diversity, counteracting biases embedded in Euclidean assumptions that privilege isotropic or densely sampled systems [4, 14]. This introduces a steering logic in metric application, wherein trade-offs between computational efficiency and conceptual depth must be explicitly negotiated to maintain epistemic integrity rather than treated as purely technical decisions [17, 18]. At the systems level, this reframes material spaces as adaptive landscapes shaped by geometric constraints, reinforcing the conceptual critique of traditional distance paradigms as insufficiently reflexive [3, 9].

The analytical lens also extends to the interpretation of discontinuities, including phase boundaries, defect networks, and regime transitions. In such contexts, non-Euclidean metrics reveal transitional dynamics that flat spaces systematically underrepresent, particularly where abrupt changes are governed by underlying curvature rather than Euclidean separation [19, 22]. Riemannian perspectives further enrich this analysis by interpreting covariance structures as guiding geometrical principles and by exposing feedback loops that link atomic-scale arrangements to macroscopic responses without imposing linear causal narratives [8, 10, 11].

Taken together, these analytical implications signal an interpretive evolution in which distance metrics function as conduits for deeper analytical engagement. Rather than serving as passive measures, they actively bridge abstract geometric formalisms with the phenomenological intricacies of material behavior, expanding the conceptual toolkit available for reasoning under complexity and constraint [11-13, 23].

Results and Discussion

The discussion synthesizes this conceptual critique by examining how non-Euclidean distance metrics reshape the interpretive fabric of material spaces through their mediation of geometric principles and material phenomenology. Central to this synthesis is the recognition of epistemic trade-offs inherent in metric choice. Euclidean metrics, while enabling accessible visualization and computational efficiency, often impose artificial uniformities that distort interaction dynamics. Non-Euclidean alternatives, by contrast, offer greater interpretive flexibility and structural fidelity, albeit at the cost of increased conceptual and computational complexity [7, 8, 14]. These tensions illuminate the steering logics embedded in materials science, where metric decisions implicitly guide analytical focus toward either reductive simplifications or integrative system views [5, 6, 13].

Interaction dynamics become particularly salient in layered, hierarchical, or networked materials systems. Hyperbolic geometries, for instance, reinterpret expansive relational structures in ways that surface systems-level insights into growth, assembly, and organizational complexity [15, 16, 20]. Such interpretations challenge Euclidean dominance by positioning curvature as a conceptual mediator, clarifying how local relational distances scale into global topological patterns [8, 10, 11]. Within materials informatics, this critique gains further traction as graph-based models leverage non-Euclidean embeddings to uncover latent feedback structures, enhancing the conceptual coherence of property predictions without invoking empirical validation claims [1, 2, 9].

Ethical reasoning integrates naturally into this discussion by interrogating how metric biases perpetuate incomplete or exclusionary views of material space. Euclidean assumptions often marginalize anisotropic, disordered, or sparsely sampled systems, whereas non-Euclidean frameworks enable more epistemically inclusive representations [4, 19, 21]. This reframes metric fidelity as a normative rather than purely technical consideration, prompting reflective engagement with how representational choices shape scientific visibility and interpretive authority [17, 18, 22]. Manifold learning paradigms further reinforce this point by conceptualizing data spaces as curved arenas that preserve multiscale continuity, supporting integrative syntheses across disciplinary and representational boundaries [3, 10-13, 23].

Finally, the discussion situates these insights within a broader trajectory of conceptual continuity in materials science. By critically examining Euclidean dominance, the framework opens pathways for interpretive innovation in which distances act as analytical bridges linking atomic-scale detail to emergent system behavior [17]. This dynamic view of material spaces aligns with the increasing complexity of contemporary materials research, encouraging a shift from static representations toward geometrically informed, reflexive analytical reasoning [8, 16].

Conclusion

In reflecting on the conceptual critique of distance metrics in materials, this manuscript underscores the interpretive advantages of non-Euclidean perspectives in capturing the nuanced dynamics of material spaces. By integrating manifold and geometric insights, the analysis reveals how metric choices shape systems-level understandings, navigating trade-offs between simplicity and depth. Ethical and epistemic considerations further emphasize the need for inclusive frameworks that embrace material diversity, steering toward more coherent conceptual representations. Ultimately, this critique fosters an enriched interpretive lens that bridges geometric abstractions with the relational essence of materials, inviting ongoing dialogue in the field.

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