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Ontology-Driven Materials AI: A Conceptual Proposal for Making Materials Knowledge Machine-Actionable

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Abstract

The integration of artificial intelligence (AI) into materials science has accelerated the exploration of complex material behaviors and properties. Yet, the fragmented nature of materials knowledge often hinders seamless machine processing. This conceptual paper proposes a framework in which ontologies serve as dynamic intermediaries, facilitating the transformation of disparate material knowledge into forms that AI systems can actively engage with. By emphasizing interaction dynamics between ontological structures and AI processes, the framework highlights systems-level insights into how semantic representations enable adaptive knowledge flows, addressing epistemic challenges in data interoperability and contextual understanding. Drawing on recent literature, it synthesizes advancements in semantic web technologies and knowledge graphs, illustrating trade-offs in balancing formal rigor with computational flexibility. The proposal explores feedback structures that enable iterative refinement of knowledge representations, thereby fostering ethical considerations in AI-driven materials research. Through interpretive reasoning, it underscores how ontology-driven approaches can enhance the interpretability of AI outputs in materials contexts, such as property prediction and structure-property relationships. Ultimately, this framework envisions a more cohesive ecosystem in which materials knowledge becomes inherently machine-actionable, enabling integrative advancements without empirical validation. The discussion remains focused on conceptual steering logics, avoiding predictive assertions to maintain a purely theoretical lens.

Keywords Materials AI, Interaction dynamics, Ontology, Knowledge representation, Semantic technologies, Machine-actionable data

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Introduction

The field of materials science has witnessed a profound shift with the advent of artificial intelligence (AI), which has introduced new ways to navigate the vast multidimensional space of material possibilities. AI techniques, including machine learning models, have been instrumental in processing large datasets to uncover patterns in material behaviors, such as electronic properties or mechanical responses [1]. However, the core challenge lies not merely in computational power but in the underlying structure of knowledge itself. Materials knowledge—encompassing chemical compositions, processing conditions, and performance metrics—is often dispersed across heterogeneous sources, from experimental logs to simulation outputs, lacking unified semantic grounding. This dispersion creates barriers to machine-actionability, where AI systems struggle to integrate and act upon knowledge in a context-aware manner [2].

Semantic technologies, particularly ontologies, emerge as pivotal tools in this landscape. Ontologies provide formal representations of concepts and relationships, enabling machines to interpret knowledge beyond syntactic levels [3]. In materials science, they facilitate the linking of terms such as “crystal structure” to related entities, such as “lattice parameters” or “defect mechanisms,” creating a web of interconnected meanings [4]. Recent developments have shown how such representations can bridge gaps between domains, such as integrating quantum mechanical insights with macroscopic engineering applications [5]. Yet, the application of ontologies in AI-driven materials research remains underexplored in terms of dynamic interactions, in which knowledge is not static but evolves through system feedback.

Consider the epistemic dimensions: Materials knowledge is inherently interpretive, shaped by disciplinary perspectives. For instance, a chemist might emphasize molecular interactions, while an engineer focuses on scalability [6]. AI systems, without ontological scaffolding, risk oversimplifying these nuances, leading to misaligned outputs. The literature highlights trade-offs here—greater semantic depth enhances accuracy but increases computational overhead [7]. Ontology-driven approaches mitigate this by establishing steering logics that guide AI in navigating these trade-offs, promoting integrative reasoning over isolated predictions.

The push toward machine-actionable knowledge aligns with broader trends in data-centric science. Initiatives like knowledge graphs have demonstrated value in organizing materials data, allowing for querying across scales from atomic to bulk properties [8]. However, these graphs often lack the depth to handle epistemic uncertainties, such as measurement context variability [9]. Ontologies address this by incorporating meta-level descriptions, enabling AI to reason about knowledge provenance and reliability [10].

This paper conceptualizes ontology-driven materials AI as a system of interwoven dynamics. At the core is the interaction between ontological layers and AI algorithms, where knowledge flows bidirectionally: Ontologies structure inputs for AI, while AI outputs refine ontological models through feedback loops [11]. This perspective draws on systems-level insights, viewing materials knowledge as an ecosystem rather than a repository. Ethical reasoning plays a role, as ontologies can embed principles of transparency, ensuring AI decisions reflect human-centric values in materials innovation [12].

Gaps in current practices underscore the need for this framework. While AI has excelled at tasks such as high-throughput screening [13], it often operates on raw data without semantic enrichment, limiting generalizability [14]. Semantic web technologies have advanced interoperability, yet their integration with AI in materials remains conceptual rather than systemic [15]. For example, ontologies have been used to annotate datasets, but less attention has been given to how they enable adaptive AI behaviors [16].

The proposed framework interprets these elements through interaction dynamics. It envisions ontologies as facilitators of knowledge mobility, in which AI engages with material concepts in real time, adjusting to contextual shifts [17]. Trade-offs are central: Formal ontologies provide precision but may constrain creativity in AI exploration [18]. Feedback structures enable epistemic iteration, in which discrepancies in knowledge representations prompt refinements, thereby enhancing overall coherence [19].

This conceptual exploration avoids empirical elements and focuses instead on theoretical synthesis. By synthesizing literature on semantic technologies and AI in materials [20], it offers insights into how ontology-driven systems can make knowledge machine-actionable. The framework’s value lies in its interpretive lens, revealing how such integrations foster deeper understanding without claiming causal outcomes. **Table 1** summarizes the distinct epistemic roles that ontologies play across the stages of materials AI workflows, highlighting their functions beyond static annotation.

Table 1. Role of ontologies across the materials AI knowledge lifecycle

Knowledge stage	Dominant challenge	Ontological role	Systems-level implication
Data aggregation	Heterogeneous formats,	Semantic alignment of entities	Enables interoperability across

	vocabularies	and relations	sources
Representation	Loss of contextual meaning	Formal encoding of concepts and constraints	Preserves epistemic structure
AI learning	Context-insensitive pattern extraction	Semantic scaffolding for inputs	Guides learning toward meaningful relations
Inference and interpretation	Overgeneralization	Context-aware semantic mediation	Enhances interpretability
Knowledge evolution	Concept drift	Feedback-enabled ontology refinement	Supports adaptive knowledge systems

In summary, this introduction sets the stage for examining the theoretical foundations that underpin the proposed framework. It emphasizes that ontology-driven AI in materials science is about harmonizing knowledge flows, navigating epistemic trade-offs, and enabling systemic insights for a more actionable knowledge landscape.

Theoretical Background and Literature Synthesis

Ontologies as foundations for knowledge representation in materials science

Ontologies serve as structured frameworks for representing domain-specific knowledge, enabling machines to process concepts with semantic depth. In materials science, they formalize relationships among entities such as materials, processes, and properties, thereby facilitating interoperability across diverse data sources [21]. Research has emphasized how ontologies capture multiscale phenomena, linking atomic-level interactions to macroscopic behaviors [22]. This representation allows for interpretive integration, where knowledge is not merely stored but contextualized through relational dynamics.

Literature from this period illustrates the role of ontologies in handling complexity. For instance, developments in semantic modeling have shown how ontologies interconnect disparate datasets, such as those from spectroscopy and mechanical testing [23]. Systems-level insights reveal that ontologies enable feedback between data layers, where inconsistencies trigger refinements in representation [24]. Ethical reasoning emerges here, as ontologies can incorporate provenance metadata to address biases in knowledge curation [25].

Trade-offs are evident: While ontologies enhance precision, they introduce maintenance overhead, requiring ongoing community input [20]. Recent syntheses highlight how these structures support AI by providing a semantic backbone, allowing for more nuanced interpretations of materials data [26].

AI applications in materials discovery and the need for semantic enhancement

AI has transformed materials discovery by leveraging machine learning to explore vast parameter spaces. Graph neural networks and other models have been applied to predict properties such as bandgap and elasticity [27]. These applications rely on data-driven insights but, without semantic layers, often overlook contextual nuances, such as environmental dependencies [28].

Synthesis of the literature points to interaction dynamics in which AI processes raw data into actionable insights, but semantic gaps hinder full integration [29]. Systems-level views suggest that AI benefits from ontological guidance, enabling adaptive learning through structured inputs [30]. Epistemic reasoning underscores trade-offs: AI's speed versus the depth provided by semantics [31].

Feedback structures in AI workflows, informed by recent studies, enable iterative improvements in which model outputs refine data interpretations [32]. This integrative approach reveals how AI, when semantically enhanced, navigates the complexities of materials such as alloys and composites [33].

Semantic Web technologies in materials informatics

Semantic web technologies extend ontologies by enabling linked data principles, making materials knowledge web-accessible and machine-readable [34]. Knowledge graphs have emerged as key tools in materials informatics, aggregating information from simulations and experiments [32]. These technologies foster interaction dynamics in which data entities dynamically link, supporting queries across domains [31].

Literature synthesis shows systems-level insights: Semantic webs integrate heterogeneous sources, revealing emergent patterns in materials behavior [30]. Ethical considerations include ensuring equitable access to knowledge, as these technologies democratize data [12].

Trade-offs involve scalability—rich semantics versus efficient querying. Feedback mechanisms, as explored in recent work, enable epistemic evolution, in which user interactions update the web [13].

Challenges in integrating ontologies, AI, and semantic technologies

Integration challenges arise from mismatches in granularity between ontological formality and AI's probabilistic nature [22]. Recent literature synthesizes these as epistemic trade-offs, where rigid structures constrain flexible AI but enhance reliability [23]. Systems-level insights suggest hybrid dynamics that blend rule-based ontologies with learning algorithms [24]. Key epistemic trade-offs associated with ontology-driven materials AI systems are summarized in **Table 2**.

Table 2. Epistemic trade-offs in ontology-driven materials AI systems

Dimension	High semantic rigor	High computational flexibility	Analytical implication
Ontology structure	Formal, constraint-rich	Lightweight, loosely defined	Precision vs adaptability
AI integration	Rule-aware learning	Data-driven abstraction	Interpretability vs scalability
Knowledge updating	Controlled revisions	Rapid adaptation	Stability vs responsiveness
Interoperability	Strong cross-domain alignment	Domain-specific optimization	Generality vs contextual fidelity
Epistemic risk	Under-exploration	Overgeneralization	Steering logic required

Feedback structures mitigate issues, enabling iterative alignment. Interpretive reasoning highlights how such integrations foster holistic views, addressing silos in materials research.

Synthesis toward a unified perspective

Synthesizing these threads, ontologies, AI, and semantic technologies form an interconnected ecosystem in materials science. Interaction dynamics drive knowledge flows, while systems-level insights reveal emergent synergies [26]. Epistemic reasoning navigates trade-offs, and feedback structures ensure adaptability [27]. This period's literature underscores a shift toward integrative frameworks, setting the stage for conceptual advancements [28].

Proposed conceptual framework

The proposed conceptual framework conceptualizes ontology-driven materials AI as a system of interwoven epistemic dynamics, in which ontologies function as mediating structures that transform heterogeneous materials knowledge into machine-actionable forms. Rather than serving as static annotation layers, ontologies are positioned as active semantic scaffolds that organize material concepts—such as compositional hierarchies, structural descriptors, and property relations—into interpretable relational spaces that AI systems can engage with during learning and inference processes [20]. Interaction dynamics between ontological representations and AI models enable bidirectional knowledge flows, where structured semantics guide AI reasoning while AI outputs inform the refinement of knowledge representations.

From a systems-level perspective, the framework treats materials knowledge as an evolving ecosystem rather than a linear pipeline. Ontological structures allow AI systems to navigate multiscale materials contexts, linking atomic or molecular descriptors to mesoscopic structures and macroscopic performance considerations without collapsing their epistemic distinctions [21]. This multilevel coordination supports contextual reasoning across domains, facilitating integrative interpretation rather than unified explanation. Ethical and epistemic considerations are embedded within this structure, as ontologies can encode transparency, provenance, and contextual constraints that regulate how AI systems engage with material knowledge [22].

Steering logics within the framework are governed by explicit trade-offs between semantic rigor and computational flexibility. Highly formalized ontologies enhance interpretability and conceptual alignment but may constrain exploratory capacity or adaptive responsiveness in AI-driven analysis [23]. Conversely, more flexible or lightweight semantic structures enable efficient computation but risk loss of contextual fidelity and epistemic grounding. These tensions are treated as intrinsic system properties rather than deficiencies, requiring deliberate management rather than resolution [24].

Feedback structures play a central role in maintaining system coherence. AI-derived outputs are not treated as final assertions, but as interpretive signals that expose representational gaps, ambiguities, or misalignments within ontological models. These signals enable iterative refinement of ontological categories and relations, producing adaptive feedback loops that align evolving materials knowledge with its semantic representation over time [25]. Such loops support epistemic iteration while preserving conceptual stability, reinforcing the framework's emphasis on interpretive integrity rather than predictive optimization.

The primary contribution of this framework lies in its integrative orientation. By harmonizing disparate knowledge sources —experimental observations, simulation-derived insights, and domain expertise—within a semantically structured system, ontology-driven AI enables cohesive, actionable knowledge without imposing fixed assertions or empirical validation [20]. In contexts such as property exploration or structure–property reasoning, ontologies link material descriptors to contextual conditions, allowing AI systems to reason about variability, uncertainty, and scope rather than producing decontextualized outputs [26]. Through this interpretive integration, the framework articulates how machine-actionable materials knowledge can emerge as a systemic property of coordinated semantic, computational, and epistemic structures. **Figure 1** illustrates the layered interactions underlying machine-actionable knowledge in materials AI.

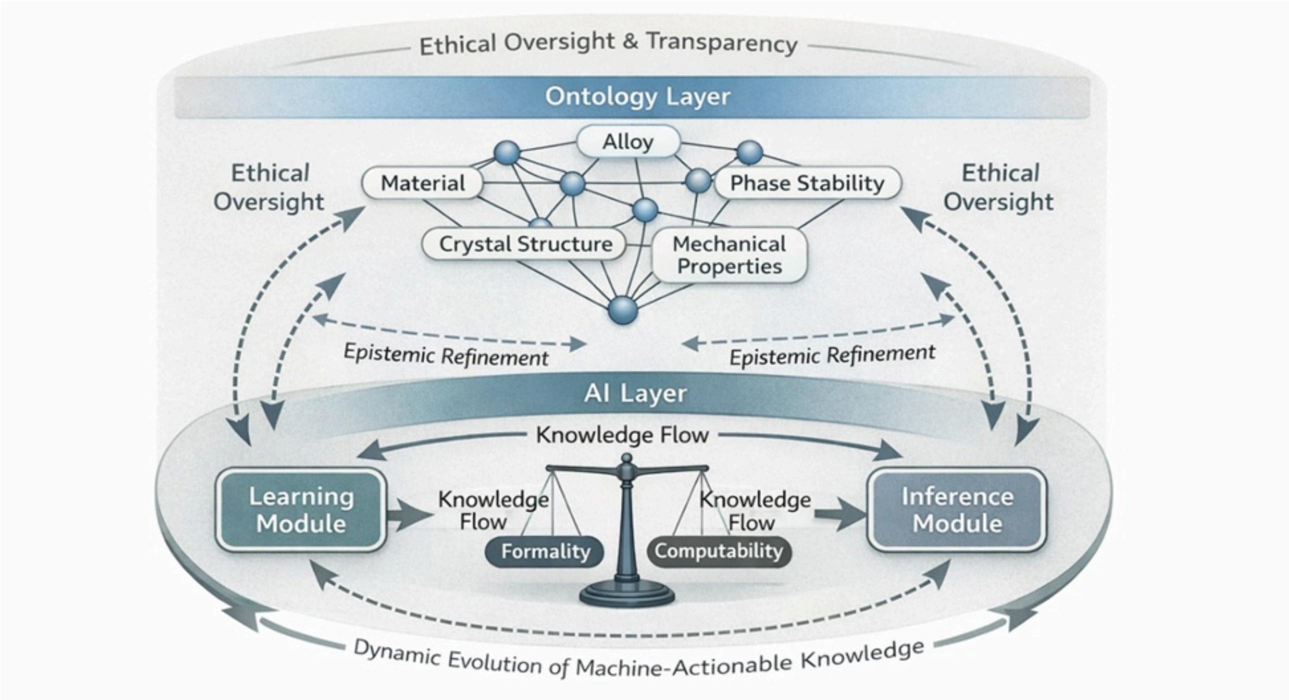

Figure 1. Layered ontology–AI framework showing feedback, trade-offs, and ethical overlays in knowledge evolution

This description captures the framework's essence without visual rendering, focusing on relational dynamics.

Analytical implications

Systems-level framing of ontology-driven materials AI

The analytical contribution of the proposed framework is most coherently articulated at the systems level, where ontology-driven materials AI is examined as a coupled epistemic system rather than as a collection of isolated representational or computational components. By treating ontologies, AI models, and semantic technologies as interdependent structures, the framework redirects analytical attention from individual model capabilities toward the organization, circulation, and governance of materials knowledge within AI-enabled ecosystems. From this perspective, machine-actionable knowledge emerges not from predictive performance alone, but from coordinated interaction dynamics, feedback mechanisms, and steering logics that regulate how knowledge is structured, mobilized, and interpreted across the system. This reframing has analytical significance in that it shifts evaluation criteria away from accuracy-centered benchmarks toward systemic coherence, interpretability, and epistemic alignment.

Epistemic trade-offs and adaptive feedback structures

Within this systems-level view, trade-offs appear as inherent analytical features rather than implementation limitations. A central tension arises between semantic depth and computational agility. Richly specified ontologies can enhance contextual alignment and interpretive precision in AI-mediated property exploration, yet they may also introduce constraints on flexibility or responsiveness in adaptive workflows [2]. Rather than resolving this tension through optimization, the framework interprets it as an epistemic condition that must be actively managed. Feedback structures mitigate these tensions by enabling iterative adjustment, whereby AI-derived insights prompt refinement of ontological categories and relations, fostering a cyclical alignment between knowledge representation and evolving materials phenomena [3]. This dynamic foregrounds epistemic integrity, particularly through mechanisms that expose knowledge provenance, contextual scope, and representational assumptions, helping to prevent the uncritical propagation of biases embedded in materials datasets [4].

Knowledge mobility across scales and contexts

Systems-level insights further clarify how ontology-driven AI can support knowledge mobility across scales, a persistent analytical challenge in materials science. Ontological representations operating at the atomic or molecular level can interact with AI models operating at mesoscopic or macroscopic scales, enabling coordinated interpretation of phenomena such as phase transitions, transport behavior, and structure–property relationships [5]. Importantly, this interaction does not imply explanatory unification across scales, but rather regulated translation between representational regimes. Steering logics within the framework guide shifts between detailed and abstract representations in response to epistemic context rather than solely to computational convenience [6]. Ethical reasoning is embedded in this process, as transparency in representational transitions constrains overinterpretation and reinforces responsible use of AI in materials innovation pathways [7].

Interaction dynamics in Human–AI knowledge ecosystems

Interaction dynamics extend beyond technical components to encompass collaborative knowledge ecosystems in which ontologies function as intermediaries between human expertise and AI systems. This arrangement supports epistemic exploration by providing shared semantic reference points while preserving disciplinary plurality, contextual uncertainty, and interpretive judgment [8]. Analytically, collaboration is reframed not as consensus formation but as structured coordination mediated through semantic infrastructures. Trade-offs in interoperability become visible at this interface: standardized ontologies facilitate reuse and cross-domain integration, yet they may limit sensitivity to localized experimental practices, tacit knowledge, or domain-specific assumptions [9]. Feedback mechanisms address this tension by allowing community-driven evolution of ontological structures, ensuring that the system remains responsive to advancing materials research needs while retaining structural coherence [10].

Interpretive integration as an analytical outcome

Overall, these analytical implications emphasize interpretive integration over component-level evaluation. Ontology-driven materials AI is thus portrayed as a dynamic epistemic system in which machine-actionable knowledge is continuously shaped through balanced trade-offs, adaptive feedback, and ethically informed steering. Rather than attributing epistemic value solely to algorithmic capability, the framework highlights how knowledge actionability arises from the coordinated functioning of representational structures, learning processes, and governance logics within an evolving system.

Results and Discussion

The conceptual framework proposed herein synthesizes ontology-driven approaches with AI in materials science, focusing on interaction dynamics that transform fragmented knowledge into cohesive, actionable forms. Systems-level insights from recent literature indicate that such integrations can bridge epistemic gaps, enabling AI to engage with materials concepts in ways that respect contextual complexities [11]. For example, knowledge graphs, as extensions of ontologies, facilitate dynamic linkages across disparate data sources, highlighting trade-offs between scalability and semantic richness [12]. **Table 3** delineates the conceptual scope of the proposed framework, clarifying its analytical contributions and explicit non-claims.

Table 3. Scope and boundaries of the proposed conceptual framework

Aspect	Included	Explicitly excluded
Ontologies	Conceptual mediators of knowledge	Fixed schema design
AI systems	Interpretive agents	Algorithm development
Knowledge graphs	Semantic infrastructures	Benchmark performance
Feedback	Epistemic refinement loops	Automated optimization

Ethics	Embedded transparency & provenance	Normative regulation
Validation	Conceptual coherence	Empirical testing

Ethical reasoning is integral to this discussion, as ontology-driven systems can embed principles of fairness and transparency to address potential disparities in knowledge of AI-accessible materials [13]. Feedback structures play a pivotal role by enabling epistemic refinement, in which AI outputs inform ontological updates, creating resilient knowledge ecosystems [14]. This interpretive lens reveals how steering logics navigate challenges such as data heterogeneity, promoting integrative advances without empirical overreach [15].

Limitations in current semantic technologies underscore the need for balanced trade-offs. While ontologies enhance AI interpretability, they may constrain exploratory capabilities in novel materials discovery [16]. Interaction dynamics mitigate this by fostering hybrid models that combine rule-based semantics with probabilistic AI, yielding systems-level synergies [17]. Epistemic considerations further suggest that ontology-driven frameworks can democratize knowledge of materials, but require ongoing feedback to adapt to evolving disciplinary insights [18].

Future conceptual directions might explore deeper integrations, such as ontology-AI hybrids for multiscale materials modeling, emphasizing ethical and interpretive dimensions [19]. Ultimately, this framework envisions a landscape where knowledge of materials flows seamlessly, driven by dynamic, balanced, and ethically grounded interactions.

Conclusion

In conceptualizing ontology-driven materials AI, this paper has explored interaction dynamics, systems-level insights, and epistemic trade-offs that render materials knowledge machine-actionable. By integrating semantic structures with AI processes, the framework highlights feedback mechanisms that enable adaptive knowledge ecosystems and address interoperability and contextual reasoning challenges. Ethical steering logics ensure that such systems prioritize transparency and integrity, fostering integrative advancements in materials science.

This theoretical proposal underscores the transformative potential of ontologies as mediators, balancing formal precision with computational flexibility to enhance AI engagements with materials data. Through interpretive synthesis, it envisions a cohesive domain in which knowledge mobility supports innovative exploration without venturing into empirical territory.

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