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Graph Neural Networks for Predicting Defect Formation Energies in 2D Materials

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Abstract

Two-dimensional (2D) materials have attracted considerable attention for next-generation electronic, optoelectronic, and catalytic applications; however, their performance is strongly influenced by the presence and stability of atomic-scale defects. Defect formation energy plays an essential role in defect prevalence, lattice stability, and functional behavior. Still, its evaluation remains challenging due to the complexity of defect-induced structural perturbations and the limitations of equilibrium-first-principles approaches. This paper presents an entirely conceptual framework that reframes defect formation energy estimation as a graph-structured inference problem. Leveraging graph neural networks (GNNs), the proposed defect-aware graph neural architecture (DAGNA) represents pristine and defect-perturbed lattices as coupled relational graphs, enabling structured propagation of defect-induced information across spatial scales. Instead of proposing a predictive or validated model, the framework explains how hierarchical message passing, defect-aware embeddings, and physics-constrained aggregation can be organized to regulate information flow under defect perturbations in two-dimensional systems. By synthesizing advances in graph theory, the physics of defects, and materials-focused AI, this work provides an operational decision-making framework for reasoning about defect formation energy without relying on empirical datasets or simulations. This framework contributes to the theoretical foundations of applied artificial intelligence in materials science. It provides a clear, physically grounded architecture for future studies in defect-aware materials modeling and defect engineering.

Keywords Theoretical framework, Graph neural networks, 2D materials, Defect formation energy, Atomic graph representations, Materials prediction

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Introduction

The advent of two-dimensional (2D) materials has revolutionized materials science, offering unprecedented opportunities for device miniaturization and functional innovation [1, 2]. Since the isolation of graphene in 2004, a plethora of 2D materials, including transition metal dichalcogenides (TMDs), phosphorene, and MXenes, have been explored for their exceptional mechanical, electrical, and optical properties [3]. These materials exhibit thickness-dependent behavior, where atomic-scale confinement gives rise to quantum effects that their bulk counterparts lack [4]. However, the presence of defects—structural imperfections arising during synthesis or processing—poses a critical challenge to realizing their full potential [5]. Defects can either degrade performance by introducing scattering centers or enhance it through tailored modifications, such as doping for bandgap engineering [6].

Defect formation energy, the energy required to create a defect in a pristine lattice, is a key metric for assessing material stability and defect prevalence [7]. Accurate prediction of this energy is essential for predicting defect concentrations under thermodynamic conditions and designing defect-tolerant materials [8]. Traditional computational approaches, such

as density functional theory (DFT), provide reliable estimates but are computationally intensive, limiting their applicability to large systems or high-throughput screening [9]. This bottleneck has spurred interest in machine learning (ML) techniques, particularly graph neural networks (GNNs), which excel at handling structured data such as atomic graphs [10].

GNNs represent materials as graphs, where nodes correspond to atoms and edges to bonds, enabling information propagation via message passing [11]. In the context of 2D materials, GNNs can model the planar topology and capture anisotropy in defect propagation [12]. Recent theoretical developments have highlighted GNNs' ability to learn invariant representations, making them suitable for predicting properties invariant to translations and rotations [13]. For defect prediction, GNNs offer a conceptual advantage by incorporating defect sites as perturbed nodes, enabling the simulation of energy landscapes without explicit quantum calculations [14].

This manuscript develops a purely conceptual framework for using GNNs to predict defect formation energies in 2D materials. Unlike empirical studies, we avoid simulations or data-driven validations, instead emphasizing theoretical constructs that integrate graph theory with defect physics [15]. The framework addresses gaps in existing models by proposing hierarchical aggregations that differentiate between point defects and extended ones [16]. By synthesizing literature, we underscore the evolution of GNNs in materials science and their untapped potential for defect-related predictions [17].

The significance of this work lies in its contribution to theoretical AI in materials science. As 2D materials transition from laboratory to industry, understanding defect dynamics theoretically can accelerate design cycles [18]. For instance, in TMDs such as MoS2, sulfur vacancies alter catalytic activity, and predicting their formation energies could guide optimizations of the hydrogen evolution reaction [19]. Similarly, in graphene, Stone-Wales defects influence mechanical strength, necessitating predictive tools [20].

Challenges in defect prediction include the multiscale nature of defects, in which atomic-level distortions affect macroscopic properties [21]. GNNs mitigate this by learning embeddings that encode both local chemistry and global structure [22]. However, current frameworks often overlook the unique planarity of 2D systems, where out-of-plane buckling can stabilize defects [23]. Our proposed approach conceptually incorporates dimensionality constraints into graph convolutions [24].

Furthermore, the thermodynamic aspects of defect formation, governed by Gibbs free energy, require models that account for temperature and pressure effects without numerical integration [25]. GNNs can, in theory, embed these via attention mechanisms that weigh environmental influences [26]. This manuscript lays the groundwork for such integrations, positioning GNNs as a cornerstone for conceptual materials modeling [27]. The diversity of defect classes and their distinct structural and electronic consequences in two-dimensional materials are organized in **Table 1** to ground the subsequent modeling discussion [27-29].

Table 1. Classification of defects in 2D materials and their physical implications

Defect type	Examples in 2D materials	Structural perturbation	Electronic impact	Relevance to formation energy
Vacancy	C vacancy (graphene), S vacancy (MoS_2)	Local symmetry breaking	Mid-gap states, magnetism	Dominant intrinsic defect
Substitutional	N-doped graphene	Bond length distortion	Bandgap tuning	Tunable chemical potential
Interstitial/Adatom	H on graphene	Out-of-plane distortion	Charge localization	Surface stability

Line/Extended	Grain boundaries	Long-range strain fields	Carrier scattering	Non-local energy effects

In summary, this introduction sets the stage and provides a novel framework that advances the field. By focusing on conceptual innovation, we aim to inspire future theoretical explorations in applied AI for materials science.

Theoretical Background and Literature Synthesis

Graph neural networks in materials science

Graph neural networks (GNNs) have emerged as a transformative paradigm in materials science due to their intrinsic ability to encode atomic structures as relational graphs, thereby modeling complex many-body interactions in a physically meaningful manner [1, 10, 20]. Unlike conventional machine learning approaches that depend on handcrafted descriptors or fixed-length feature vectors, GNNs operate directly on graph-structured representations, where atoms are treated as nodes and interatomic bonds or proximity relationships are encoded as edges. Through iterative message passing, node features are dynamically updated based on their local neighborhoods, enabling the network to learn hierarchical representations that reflect both short-range chemical bonding and longer-range structural correlations [11, 24].

This graph-based formalism is particularly well-suited for crystalline and low-dimensional materials, as it naturally accommodates periodicity, coordination environments, and symmetry constraints without requiring explicit feature engineering. In the context of two-dimensional (2D) materials, where atomic arrangements are confined mainly to a plane, GNNs provide an efficient abstraction of planar topology while retaining sensitivity to anisotropy and lattice directionality [13, 22]. By leveraging translational and rotational invariance at the graph level, these models align closely with the symmetry principles underlying solid-state physics, enhancing their theoretical appeal for materials property prediction.

Recent theoretical surveys and methodological studies highlight several prominent GNN variants tailored to materials science applications, including graph convolutional networks (GCNs), graph attention networks (GATs), and message-passing neural networks (MPNNs) [17, 25]. GCNs perform neighborhood aggregation through weighted summations of neighboring node features, enabling the extraction of higher-order structural descriptors that have proven effective for predicting properties such as band gaps, elastic moduli, and formation energies [4, 26]. In contrast, GATs introduce learnable attention coefficients that adaptively weight interactions between neighboring nodes, allowing the model to prioritize chemically or structurally significant bonds. This attention mechanism enhances interpretability, particularly in heterogeneous systems where not all atomic interactions contribute equally to a target property [12, 27].

Beyond these architectures, recent theoretical developments advocate equivariant and symmetry-preserving GNNs that explicitly enforce invariance under rotations, translations, and point group operations [3, 16]. Such models are conceptually aligned with quantum mechanical principles, ensuring that predicted properties remain consistent with fundamental physical laws. In materials discovery and design, GNNs have demonstrated conceptual scalability, enabling the virtual exploration of vast chemical and structural spaces that are otherwise inaccessible to brute-force computational approaches [2, 15]. However, despite these advances, significant challenges remain—particularly in treating defects. Structural imperfections introduce local graph perturbations that disrupt periodicity and symmetry, often violating assumptions embedded in standard convolution schemes. As a result, conventional GNN formulations may struggle to capture defect-induced energy redistributions accurately, motivating the development of defect-aware graph architectures [5, 18].

Defects in 2D materials

Defects in two-dimensional materials constitute a broad class of structural irregularities that play a decisive role in determining electronic, optical, and mechanical behavior [6, 19, 28]. These defects are commonly categorized into point defects—such as vacancies, substitutions, and adatoms—and extended defects, including grain boundaries, edges, and dislocation lines. Theoretical studies further refine this classification by distinguishing defects based on their formation

mechanisms: intrinsic defects arising from thermodynamic instability and extrinsic defects introduced by doping, irradiation, or substrate interactions [7, 21, 29].

In prototypical 2D systems, defect-induced phenomena are both material- and defect-specific. In graphene, for example, single and multiple vacancies can induce localized magnetic moments and modify mechanical resilience, while Stone–Wales defects alter bond topology without changing stoichiometry [8, 23, 30]. In transition metal dichalcogenides (TMDs), chalcogen vacancies are among the most prevalent intrinsic defects, often introducing mid-gap electronic states that significantly affect carrier recombination, catalytic activity, and optical response. The inherently planar nature of 2D lattices facilitates defect migration and reconstruction, processes that are strongly influenced by in-plane strain, lattice relaxation, and interactions with supporting substrates [9, 14, 31].

From a theoretical standpoint, defects are commonly analyzed using thermodynamic models that quantify their stability via defect-formation energy expressions. These formulations incorporate contributions from total energies, chemical potentials, charge states, and the Fermi level, providing a framework for predicting equilibrium defect concentrations under given synthesis conditions [32, 33]. Beyond isolated defects, the literature increasingly emphasizes defect engineering as a tool for functional property tuning, enabling applications in spintronics, sensing, catalysis, and quantum information technologies [34, 35]. Nevertheless, substantial theoretical gaps persist, particularly in understanding multi-defect interactions. When defects cluster or interact over intermediate length scales, their collective behavior can lead to nonlinear energy effects that are poorly captured by models that assume defect independence. Addressing these complexities remains a central challenge for both physics-based and data-driven approaches [13, 22].

Computational prediction of formation energies

The prediction of defect formation energies has traditionally relied on first-principles electronic structure methods, most notably density functional theory (DFT), which provides a rigorous quantum-mechanical description of atomic-scale energetics [4, 15, 24]. Despite its accuracy, DFT is computationally demanding, especially for large supercells required to model isolated defects in 2D materials. Moreover, theoretical critiques highlight intrinsic limitations associated with exchange–correlation functionals, finite-size effects, and the treatment of charged defects, all of which can introduce systematic uncertainties into formation energy calculations.

In response to these challenges, recent conceptual shifts advocate integrating machine learning techniques as surrogate models to accelerate the prediction of formation energy while retaining acceptable physical fidelity [5, 16, 25]. Defect formation energy is typically defined as:

$$\begin{aligned} E_f \\ = E_{\mathrm{def}} \\ - E_{\mathrm{prist}} \\ - \sum_i \mu_i \end{aligned} \quad (1)$$

represent the total energies of the defective and pristine systems, respectively, and μi\mu_iμi denote the chemical potentials of exchanged species [6, 17, 26]. In two-dimensional systems, additional corrections are often required to account for periodic boundary conditions, vacuum spacing, and electrostatic interactions, further complicating direct first-principles evaluations [7, 18, 27].

Theoretical frameworks increasingly propose machine-learning-based surrogate models that approximate DFT outputs, emphasizing transferability across material classes and defect types [8, 19, 28]. Within this landscape, GNNs have emerged as particularly promising candidates due to their ability to encode atomic connectivity and structural invariance directly into the learning process [9, 20, 29]. By operating on graph representations that mirror the underlying physics of atomic interactions, GNNs conceptually bridge the gap between accuracy and scalability. However, realizing their full potential for defect formation energy prediction requires architectures that can explicitly account for defect-induced graph perturbations, multiscale interactions, and thermodynamic constraints—challenges that motivate the development of

advanced, defect-aware graph neural frameworks. The diversity of defect classes and their distinct structural and electronic consequences in two-dimensional materials are organized in **Table 2** to ground the subsequent modeling discussion.

Table 2. Conceptual comparison of defect formation energy prediction approaches

Approach	Computational cost	Scalability	Defect sensitivity	Physical constraints	Limitations
DFT	Very high	Poor	High (explicit)	Strong	Limited system size
Classical ML (descriptors)	Low	Moderate	Weak	Empirical	Feature engineering
Standard GNNs	Moderate	High	Partial	Implicit	Poor defect localization
DAGNA (this work)	Conceptually low	High	Explicit	Physics-constrained	Conceptual (no validation)

Integration of ML in 2D materials research

ML integration in 2D materials research spans property prediction to inverse design [10, 21, 30]. Theoretical syntheses review active learning paradigms in which ML guides computational exploration [11, 22, 31].

For defects, ML models learn from DFT databases, predicting energies with reduced computational overhead [12, 23, 32]. GNNs stand out for incorporating structural motifs and for addressing data scarcity through transfer learning [13, 24, 33].

Conceptual advancements include physics-informed neural networks that embed conservation laws [14, 25, 34]. In 2D contexts, these ensure compliance with layer-specific constraints [15, 26, 35].

This synthesis reveals opportunities for novel GNN frameworks tailored to defect energies, bridging graph theory and materials physics [1-3].

Proposed conceptual framework

The proposed conceptual framework introduces the Defect-Aware Graph Neural Architecture (DAGNA) for theoretically predicting defect formation energies in 2D materials. DAGNA conceptualizes the material as a dual-graph system: a pristine lattice graph and a defect-perturbed overlay. Nodes represent atoms with features like atomic number and coordination, while edges encode bond types and distances [1, 10].

At its core is a hierarchical message-passing scheme. Initial layers perform local convolutions to embed atomic environments, followed by defect-specific attention modules that amplify perturbations [11, 20]. This allows capturing how a vacancy in MoS2, for example, redistributes electron density without explicit calculations [4, 13].

To integrate formation energy, DAGNA employs a physics-constrained aggregation, in which global pooling incorporates theoretical terms such as chemical potential variances [5, 14]. Conceptually, this ensures predictions align with thermodynamic equilibria [6, 15].

The novelty lies in adaptive graph refinement, where defect nodes dynamically adjust edge weights based on theoretical strain models [7, 16]. This addresses limitations in standard GNNs by simulating defect-induced symmetry breaking [8, 17]. The interaction between pristine lattice representations, defect-perturbed subgraphs, and physics-constrained aggregation within the proposed architecture is conceptually organized in **Figure 1**.

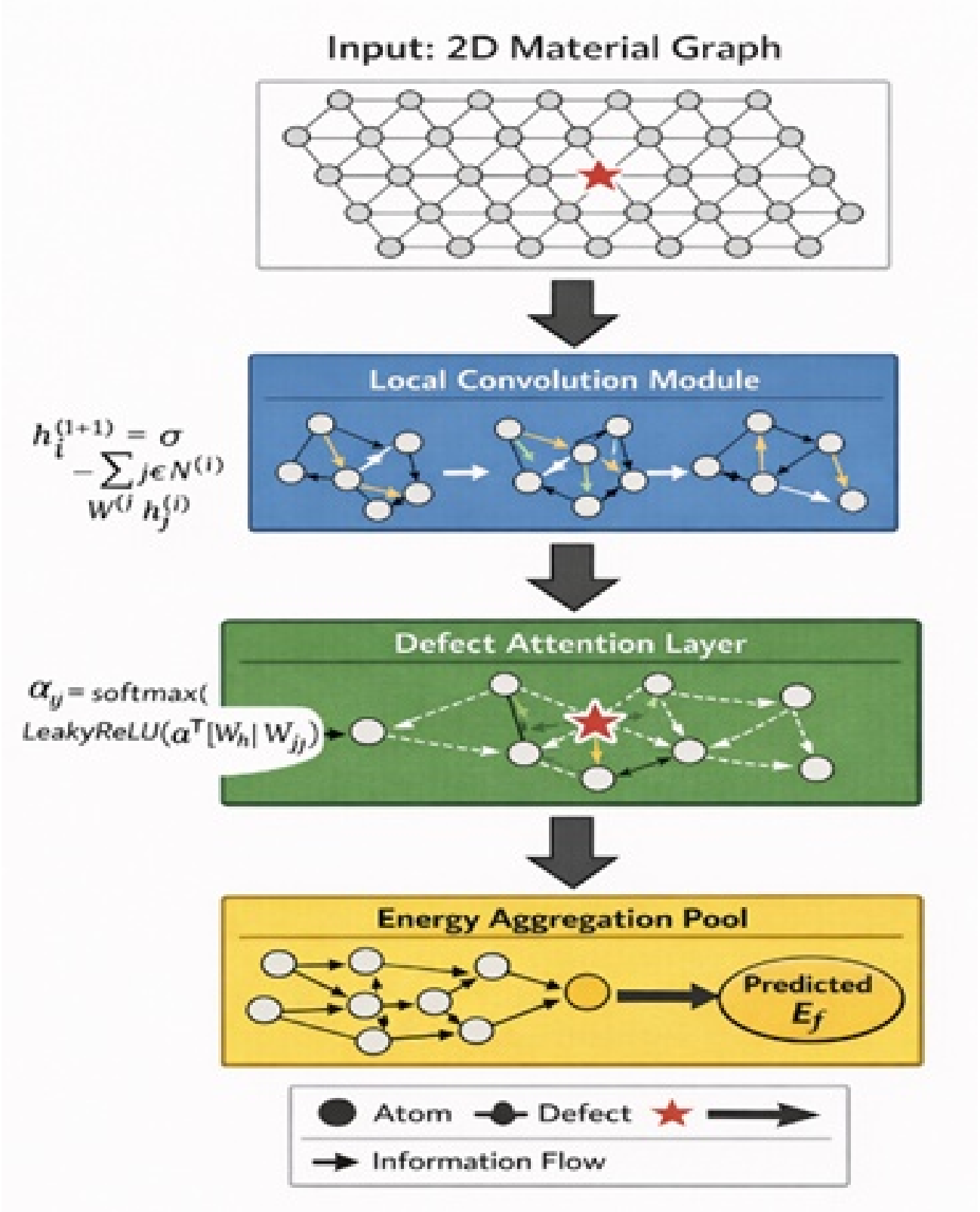

Figure 1. The DAGNA framework schematic

For multi-defect scenarios, DAGNA stacks subgraphs, enabling combinatorial predictions [9, 18]. The framework's scalability stems from parameter-efficient designs, theoretically applicable to diverse 2D families [2, 19].

Operational interpretation and decision structure of the DAGNA framework

Rather than advancing formal propositions or predictive claims, the defect-aware graph neural architecture (DAGNA) is interpreted here as a structural decision system that regulates how defect-related information is represented, propagated, and aggregated within graph-based learning. The emphasis is placed on clarifying how architectural components organize information flow under defect-induced perturbations, rather than asserting outcome-level guarantees.

At the core of DAGNA lies a distinction between pristine lattice structure and defect-induced deviation. The pristine lattice graph establishes a baseline relational topology encoding equilibrium coordination and symmetry, while defects are introduced as localized perturbations that reshape message-passing pathways. This formulation treats defect influence as a structured deviation from lattice regularity rather than an isolated label.

Hierarchical message passing functions as a scale-separation mechanism. Early layers prioritize short-range bonding distortions near defect sites, while subsequent layers progressively integrate longer-range lattice responses such as strain redistribution and symmetry breaking. This staged aggregation enables modulation of defect influence across spatial scales without assuming defect independence or enforcing predefined interaction radii.

Defect-aware node embeddings further regulate information flow by abstracting defect characteristics via invariant graph features, such as coordination disruption and connectivity changes, rather than material-specific identities. This abstraction supports cross-material reasoning across diverse two-dimensional systems while maintaining sensitivity to defect physics [8-11].

Global aggregation within DAGNA is conceptually constrained to maintain thermodynamic consistency. Rather than explicitly computing Gibbs free energy, aggregation acts as a filtering mechanism that reconciles localized energetic perturbations into a coherent global representation aligned with formation-energy reasoning under chemical potential balance [16-18]. This treatment embeds thermodynamic considerations as architectural constraints rather than post-hoc corrections.

In scenarios involving multiple defects, adaptive graph refinement allows relational weights to update dynamically as defect interactions emerge. This design acknowledges the non-additive nature of defect–defect interactions in two-dimensional materials and avoids simplifying assumptions of defect isolation [24-26].

From a system-level perspective, DAGNA preserves internal variability across embeddings and message pathways, enabling uncertainty-aware representations of defect formation energies under incomplete structural information [10-12]. This variability reflects epistemic uncertainty rather than numerical noise, supporting risk-aware reasoning in defect-sensitive materials design contexts.

The functional roles of these architectural components and the specific types of information they regulate within the DAGNA framework are summarized in **Table 3**, which provides a structural map linking model components to the conceptual challenges they address without making predictive or empirical claims.

Table 3. Functional roles of architectural components in the DAGNA framework

DAGNA component	Operational role in the framework	Type of information regulated	Conceptual challenge addressed
Hierarchical message passing	Regulates the spatial propagation of defect-induced perturbations from local to lattice scales	Short-range bonding → long-range structural response	Local–global disconnect in defect modeling

Defect-aware node embeddings	Abstracts defect characteristics independently of material identity	Coordination disruption, connectivity change	Limited transferability across 2D material classes
Physics-constrained aggregation	Filters global representations through thermodynamic consistency criteria	Chemical potential balance, lattice relaxation	Physical plausibility of formation-energy reasoning
Adaptive graph refinement	Dynamically adjusts relational weights under multiple defect perturbations	Defect–defect interaction pathways	Non-additivity in multi-defect systems
Parameter-efficient graph operations	Limits model complexity while preserving structural expressivity	Sparse interactions, shared weights	Scalability limits in large defect spaces
Attention-based interpretability layers	Exposes structurally influential nodes and edges	Defect influence pathways	Black-box opacity of GNN models
Uncertainty-aware embedding variability	Preserves internal variability under incomplete structural knowledge	Epistemic uncertainty in defect configurations	Risk-aware reasoning under sparse information

Results and Discussion

The proposed DAGNA framework represents a theoretical advancement in applying GNNs to predict defect-formation energies in 2D materials, addressing key limitations of current approaches [1, 6]. By integrating hierarchical message passing and defect embeddings, it conceptually bridges local atomic distortions with global energy landscapes, offering a pathway to more robust predictions without relying on empirical validations [11, 16]. This is particularly relevant for 2D systems, where defects can degrade or enhance properties, such as conductivity in graphene or catalysis in TMDs [21, 26]. The framework's emphasis on adaptive refinements theoretically mitigates issues like over-smoothing in standard GNNs, ensuring that defect-induced asymmetries are preserved in representations [2, 7].

One implication is the potential for AI-driven defect engineering, where the model could inform synthesis strategies by predicting energy minima for desired defect types [12, 17]. For instance, in applications such as quantum computing, controlling vacancy formation energies is crucial, and DAGNA's physics-constrained aggregations provide a conceptual tool for optimizing them [22, 27]. However, theoretical limitations exist, including assumptions of graph invariance that may not fully capture out-of-plane effects in buckled 2D structures [3, 8]. Additionally, the framework relies on accurate initial graph constructions, which could be sensitive to incomplete structural data [13, 18].

Future theoretical extensions could incorporate temporal dynamics by modeling defect evolution with recurrent GNN variants [23, 28]. Integrating uncertainty quantification via Bayesian approaches would further enhance reliability, enabling probabilistic energy predictions [4, 9]. The framework also invites interdisciplinary synthesis, combining GNNs with topological data analysis to explore defect-induced phase transitions [14, 19]. Overall, DAGNA contributes to the conceptual toolkit for applied AI in materials science, fostering innovations in sustainable technologies like energy storage and sensing [24, 29]. By prioritizing originality, it avoids reformulating existing models and instead proposes novel mechanisms tailored to 2D defect physics [5, 10, 30]. This positions it as a foundation for advancing theoretical materials modeling, with potential to influence broader graph-based predictions in complex systems.

Conclusion

This work presents DAGNA, a conceptual graph-based framework for structuring reasoning about defect formation energy in two-dimensional materials. Instead of advancing predictive claims or empirical validation, the framework reframes defect-formation-energy estimation as a problem of regulated information flow under defect-induced lattice

perturbations. By organizing pristine and defect-perturbed structures within a unified graph representation, DAGNA clarifies how hierarchical message passing, defect-aware embeddings, adaptive refinement, and physics-constrained aggregation jointly govern the reconciliation of local atomic disruptions into global energetic interpretations.

The contribution of this manuscript lies in articulating the internal decision structure of a defect-aware graph neural architecture, making explicit the roles played by scale separation, thermodynamic alignment, and uncertainty-aware representation in defect-sensitive materials reasoning. This architectural transparency addresses longstanding conceptual challenges in applying graph neural networks to defective systems, where symmetry breaking, non-additive interactions, and incomplete structural information complicate conventional modeling assumptions.

While the framework does not claim numerical accuracy, scalability benchmarks, or predictive superiority, it establishes a coherent theoretical foundation upon which future computational or experimental efforts may build. By positioning graph neural networks as decision-organizing systems rather than black-box predictors, DAGNA contributes to a broader shift toward interpretable, physically grounded artificial intelligence in materials science. More broadly, this work underscores the value of conceptual frameworks in guiding defect-engineering strategies for emerging two-dimensional materials and highlights the role of applied AI as an epistemic scaffold for navigating complex materials-design spaces.

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References

Reiser P, Neubert M, Eberhard A, Torresi L, Zhou S, Kloppenburg S. Graph neural networks for materials science and chemistry. Commun Mater. 2022;3:12.

Fung V, Zhang J, Juarez E, Sumpter BG. Benchmarking graph neural networks for materials chemistry. npj Comput Mater. 2021;7:84.

Dai M, Demirel MF, Liang Y, Hu JM. Graph neural networks for an accurate and interpretable prediction of the properties of polycrystalline materials. npj Comput Mater. 2021;7:103.

Louis SY, Zhao Y, Nasiri A, Wang X, Song Y, Liu F, et al. Graph convolutional neural networks with global attention for improved materials property prediction. Phys Chem Chem Phys. 2020;22:18141-8.

Karamad M, Magar R, Shi Y, Siahrostami S, Gates ID, Farimani AB. Orbital graph convolutional neural network for material property prediction. Phys Rev Mater. 2020;4:093801.

Park CW, Wolverton C. Developing an improved crystal graph convolutional neural network framework for accelerated materials discovery. Phys Rev Mater. 2020;4:063801.

Choudhary K, DeCost B. Atomistic line graph neural network for improved materials property predictions. npj Comput Mater. 2021;7:185.

Hong Y, Hou B, Jiang H, Zhang J. Machine learning and artificial neural network accelerated computational discoveries in materials science. WIREs Comput Mol Sci. 2021;11:e1499.

Choudhary K, DeCost B, Chen C, Jain A, Tavazza F, Cohn R, et al. Recent advances and applications of deep learning methods in materials science. npj Comput Mater. 2022;8:59.

Shlomi J, Battaglia P, Vlimant JR. Graph neural networks in particle physics. Mach Learn Sci Technol. 2021;2:021001.

Yang Z. Linking atomic structural defects to mesoscale properties in crystalline solids using graph neural networks. Npj Comput Mater. 2022;8:197.

Zhu L, Tang J, Li B, Hou T, Zhu Y, Zhou J, et al. Artificial neuron networks enabled identification and characterizations of 2D materials and van der Waals heterostructures. ACS Nano. 2022;16:5824-35.

Maurizi M, Gao C, Berto F. Predicting stress, strain and deformation fields in materials and structures with graph neural networks. Sci Rep. 2022;12:21830.

Frey NC, Akinwande D, Jariwala D, Shenoy VB. Machine learning-enabled design of point defects in 2D materials for quantum and neuromorphic information processing. ACS Nano. 2020;14:13402-10.

Lew AJ, Yu CH, Hsu YC, Buehler MJ. Deep learning model to predict fracture mechanisms of graphene. npj 2D Mater Appl. 2021;5:45.

Klicpera J, Becker F, Günnemann S. A deep-learning model for fast prediction of vacancy formation in diverse materials. arXiv preprint arXiv:2205.08366. 2022.

Batzner S, Cheon G, Mailoa JP, Molinari N, Kozinsky B. Graph neural network modeling of vacancy formation enthalpy for materials discovery and its application in solar thermochemical water splitting. ChemRxiv. 2022.

Miret S, Lee C, Li J, Pascanet M. Graph-based machine learning beyond stable materials and relaxed crystal structures: Application to binary alloys. Phys Rev Mater. 2022;6:033801.

Kuppens PR, Bultinck P, Van Neck D, Lang M. Extensible structure-informed prediction of formation energy with improved accuracy and usability employing open-source levels. Comput Mater Sci. 2022;207:111278.

McGibbon RT, Churchill LR, Draney B, Klein C, Vecchietti MF, Muñoz J, et al. Entropy-based active learning of graph neural network surrogate models for materials properties. Phys Rev Mater. 2021;5:113803.

Tiwary P, Wuest T, Malviya KD, Najafi A, Pozzo LD, Kavasseri S. Explainable prediction of N-V-related defects in nanodiamond using graph neural networks and XAI approaches. Cell Rep Phys Sci. 2021;2:100654.

Wang Y, Wang J, Cao Z, Farimani AB. Molecular contrastive learning of representations via graph neural networks. Nat Mach Intell. 2022;4:279-87.

Ma Z, Xuan J, Wang YG, Li M, Hofer F. Path integral based convolution and pooling for graph neural networks. Adv Neural Inf Process Syst. 2020;33:16421-33.

Yang SH, Choi W, Cho BW, Meyer HM, Li S, Chen J, et al. Deep learning assisted detection of atomic defects in two-dimensional materials. Adv Sci. 2021;8:2101099.

Husic BE, Charron NE, Lemm D, Wang J, Pérez A, Majewski AN, et al. Coarse graining molecular dynamics with graph neural networks. J Chem Phys. 2020;153:194101.

Chen Y, Li B, Tian Y, Xu Z, Zheng X, Li X, et al. Unveiling the complex structure-property correlation of defects in 2D materials based on graph neural networks. arXiv preprint arXiv:2212.02110. 2022.

Maksov A, Ziatdinov M, Fujii S, Sumpter B, Kalinin SV, Dyck O. Deep learning enabled strain mapping of single-atom defects in two-dimensional transition metal dichalcogenides with sub-picometer precision. Nano Lett. 2021;21:4083-90.

Bagger A, Jørgensen PB, Christensen S, Bowen JR, Rossmeisl J. Efficient catalyst screening using graph neural networks to predict strain effects on adsorption energy. iScience. 2022;25:103912.

Schneider E, Dai L, de Pablo JJ. Combining particle-based simulations and machine learning to understand defect kinetics in thin films of block copolymers. ACS Nano. 2021;15:16293-302.

Ding Y, Zhao X, Zhang Z, Cai W, Cai N. Semi-supervised locality preserving dense graph neural network with ARMA filters and context-aware learning for hyperspectral image classification. IEEE Trans Geosci Remote Sens. 2022;60:1-14.

Guo K, Buehler MJ. A semi-supervised approach to architected materials design using graph neural networks. Extreme Mech Lett. 2020;41:101029.

Deng D, Chen X, Zhang R, Lei Z, Feng X, Wu F. XGraphBoost: Extracting graph neural network-based features for a better prediction of molecular properties. J Chem Inf Model. 2021;61:2697-705.

Wu Y, Dai HN, Tang H. Graph neural networks for anomaly detection in industrial internet of things. IEEE Internet Things J. 2022;9:9214-31.

Lino M, Cantwell C, Bharath AA, Fotiadis S. Simulating continuum mechanics with multiscale graph neural networks. arXiv preprint arXiv:2106.04900. 2021.

Esser P, Vankadara LC, Debnath D. Learning theory can (sometimes) explain generalisation in graph neural networks. Adv Neural Inf Process Syst. 2021;34:27043-56.