

# UCLA

## UCLA Previously Published Works

### Title

Quantum-Chemically Informed Representation Learning for Molecular Crystal Property Prediction via Multimodal Graph Neural Networks

### Permalink

<https://escholarship.org/uc/item/5q86s30z>

### Journal

Journal of Chemical Information and Modeling

### ISSN

1549-9596

### Authors

Ihri, Ferdawss

Garcia-Garibay, Miguel A

Alexandrova, Anastassia N

### Publication Date

2026-09-04

### DOI

10.1021/acs.jcim.6c01012

### Copyright Information

This work is made available under the terms of a Creative Commons Attribution License, available at <https://creativecommons.org/licenses/by/4.0/>

Peer reviewed

# Quantum-Chemically Informed Representation Learning for Molecular Crystals Property Prediction *via* Multimodal Graph Neural Networks

Ferdawss Ihiri<sup>1</sup>, Miguel A. Garcia-Garibay<sup>\*1</sup>, and Anastassia N. Alexandrova<sup>\*1,2</sup>

<sup>1</sup>Department of Chemistry and Biochemistry, University of California, Los Angeles, CA, USA

<sup>2</sup>Department of Materials Science and Engineering, University of California, Los Angeles, CA, USA

<sup>\*</sup>Email: alexandrova@ucla.edu, mgarciagaribay@ucla.edu

## Abstract

Machine-learning based modeling of molecular crystals is limited by representations that encode geometric structure while overlooking the electronic features that often govern solid-state behavior. We introduce a multimodal learning framework that integrates crystal graphs with solid-state Quantum Theory of Atoms in Molecules (QTAIM) informed molecular graphs for enhanced predictions of solid-state properties. Our architecture employs modality-specific graph neural network encoders and a bi-directional gated fusion mechanism to capture complementary information between the two representations. When applied to band-gap prediction in organic molecular crystals, the fused model outperforms geometry-only and molecular-only baselines. Analysis of the learned representations reveals that QTAIM descriptors contribute interpretable signals associated with intermolecular interactions and density redistribution within the crystal, highlighting the value of quantum-informed learning for advancing data-driven solid-state modeling.

**KEYWORDS:** Multimodal Learning; Molecular Crystals; QTAIM; Solid-State Property Prediction

## Introduction

A central objective of machine learning (ML) in chemistry and materials science is to learn effective representations of atomic structure that enable accurate structure–property prediction. Representation learning is therefore fundamental to materials modeling, as predictive performance depends critically on how structural and electronic information are encoded.[1] In crystalline solids, ML models must account for periodicity, long-range interactions, and collective electronic effects that arise from the infinite repetition of a unit cell in three dimensions.[2, 3] These challenges are especially pronounced in organic molecular crystals, whose solid-state properties arise from a delicate interplay between intramolecular electronic structure and emergent collective properties mediated by weak intermolecular packing forces.[4] Unlike ionic or covalent inorganic solids dominated by strong extended bonding networks, molecular crystals are governed primarily by van der Waals interactions,  $\pi$ – $\pi$  stacking and hydrogen bonding, among several others (such as halogen bond, chalcogen bond, charge transfer, dipole-dipole and quadrupolar interactions).[5–7] Consequently, their electronic properties are highly sensitive to subtle variations in molecular conformation, packing geometry, and charge redistribution.[4, 8–11] A clear example of this sensitivity is the electronic band gap of molecular crystals, which is technologically central to organic semiconductors,[12] optoelectronic materials,[13, 14] and energy conversion devices,[15]. Even modest changes in crystal packing or density redistribution can strongly impact energetics, transition probabilities and redox behavior.[16, 17] Accurate prediction of electronic properties

in these systems therefore requires representations that capture both local bonding environments and non-local intermolecular effects. As a result, developing representations that more directly incorporate electronic information remains a bottleneck for materials discovery, particularly when high-throughput screening is desired. In this work, we aim at developing an approach that provides high-throughput accurate prediction of electronic properties by taking advantage of multimodal representations that capture both local bonding environments and non-local intermolecular effects using features based on electronic information available from quantum mechanical methods.

Current approaches have demonstrated that graph neural networks (GNNs),[18–20] trained directly on structural data, can learn structure-property relationships for molecules, inorganic solids, and organic crystals.[21–26] Crystal graph models such as CGCNN,[23] ALIGNN,[25], MEGNet[22], and other variants, encode the periodic arrangements of atoms in crystalline systems and have achieved strong performance on tasks involving inorganic materials,[27] and more recently, organic molecular crystals.[28–31]. Still, current approaches rely almost exclusively on geometry-derived representations, implicitly assuming that interatomic distances and connectivity encode all information relevant to the electronic structure. This assumption is frequently violated in molecular crystals since systems with nearly identical geometric motifs can exhibit markedly different electron-density distributions due to subtle polarization effects, variations in hydrogen-bond networks, or packing-induced charge redistribution.[32] Such electronic differences are not recoverable from geometry alone and may underlie persistent challenges in modeling polymorphs and crystals with strong intermolecular electronic coupling.[33]

Several efforts have attempted to enrich crystal graph representations by incorporating higher-order geometric information, such as angular terms or extended neighbor interactions.[25, 34, 35] While these strategies improve the description of local coordination environments, they remain fundamentally geometric proxies. Existing crystal representations are still largely limited to distance-based features, or atom-type embeddings, and even advanced architectures operate without direct access to the electronic degrees of freedom that govern optical and electronic properties of such systems. Consequently, contemporary GNNs are constrained by an inherent representational bias where the model struggles to learn information that is absent from its input. Recent work has begun to account for non-local charge transfer[36] and intermolecular interactions explicitly,[37] highlighting their importance for predicting solid-state properties. Nevertheless, explicit electronic structure information-derived from the quantum mechanics of the system- remains largely absent from graph-based models of molecular crystals, despite successes of quantum-chemically augmented ML strategies when applied to molecular and reaction representations.[38–43] As a result, the connection between crystal geometry and the underlying electronic landscape remains only indirectly captured.

In this work, we address this limitation by introducing a quantum-informed multimodal graph framework that augments crystal-graph representations with a second modality derived from the periodic charge density. Specifically, we construct a quantum-augmented graph that encodes electron density-derived topological descriptors computed in the solid state according to the Atoms in Molecules formalism, and integrate it with a conventional crystal graph through parallel message-passing networks. This approach enables the model to access electronic features, yielding a joint structural–electronic representation tailored for predicting the solid-state properties of solid-state materials.

The Quantum Theory of Atoms in Molecules (QTAIM) provides a principled, transferable way to encode electron-density topology in both molecules and periodic solids.[44–46] QTAIM descriptors quantify features such as electron density at bond critical points, local curvature of the density, Laplacian, energy-density signatures, and other quantities linked to chemical bonding and intermolecular interactions.[47] Prior studies have shown that QTAIM-derived descriptors can significantly improve the performance of machine-learning models for predicting molecular properties and energy barriers.[48–50] In molecular solids, these descriptors are routinely used to rationalize charge redistribution, hydrogen bonding strength, van der Waals contacts and aromaticity.[51–53] Yet they have rarely been used in machine-learning models for solid-state materials, and- to our knowledge- have not been systematically integrated into GNNs architectures for molecular crystals. Here, we introduce a crystal quantum-informed multimodal graph framework that combines (i) a crystal graph encoding the periodic atomic arrangement and (ii) a QTAIM graph encoding electron-density-derived topological descriptors computed in the solid state, **XQTAIM-MM**. The two graphs represent complementary modalities where the crystal graph captures lattice geometry, while the QTAIM graph embeds local

electronic environments and intermolecular electronic coupling. More broadly, the framework establishes a generalizable route toward quantum-aware multimodal learning for molecular crystals and other electronically complex solids.

## Methods

### Training Data

This study uses data extracted from the Organic Materials Database (OMDB-GAP1 dataset)- an open source dataset of organic molecular crystals with computed band gap energies, comprising approximately 12,500 structures.[54] For each crystal, periodic DFT band gaps were obtained from the source calculations, and solid-state QTAIM descriptors were computed via cluster-based QM embedding calculations (see section 2.2 for details). Structures that failed quantum-mechanical processing were excluded to ensure data consistency and reliability. The final dataset for training included 10,472 crystal structures.

### Organic Materials Database (OMDb)

The OMDB-GAP1 dataset provides density-functional-theory (DFT) band gaps for organic molecular crystals alongside their experimentally reported crystal structures. All band gaps correspond to periodic boundary condition DFT calculations performed at the Perdew–Burke–Ernzerhof (PBE)[55] level of theory and are defined as the energy difference between the valence-band maximum and conduction-band minimum, without distinction between direct and indirect gaps (Figure 1).

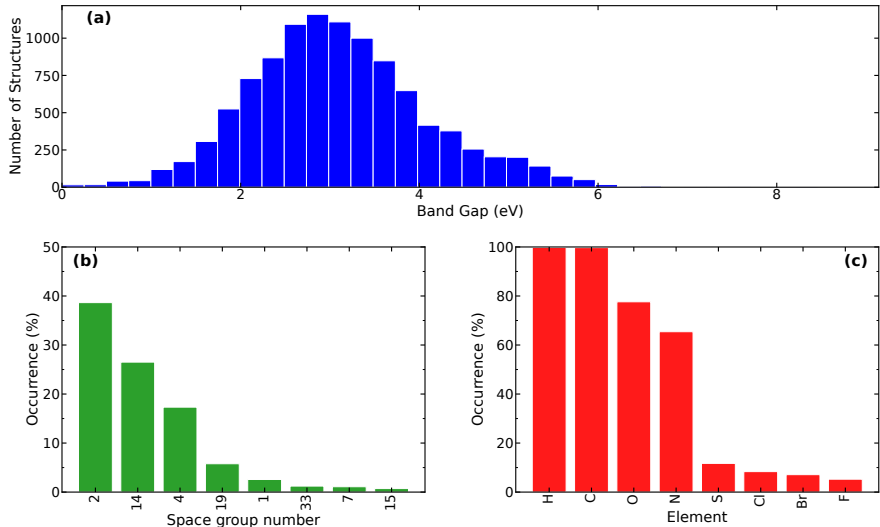


Figure 1: Statistical overview of the OMDB-GAP1 dataset used in this study. (a) Distribution of PBE band gaps (eV); the histogram is approximately unimodal with a pronounced central maximum near 3 eV and a right-skewed tail toward larger gaps. (b) Relative frequencies of the eight most common crystallographic space groups. (c) The most common elements occurring all the structures.

### Quantum Mechanical Calculations and QTAIM analysis

To obtain electronic-structure descriptors representative of the solid-state, we performed quantum-mechanical calculations on finite molecular clusters extracted from experimental crystal structures. This approach builds directly on previous work where embedded cluster QTAIM analysis was shown to capture packing-induced electronic effects relevant to solid-state reactivity. For each crystal, a spherical cluster of 10 Å radius centered on a reference molecule (corresponding to the asymmetric unit, or  $Z'$  molecule) was constructed from the periodic structure (Figure 2).

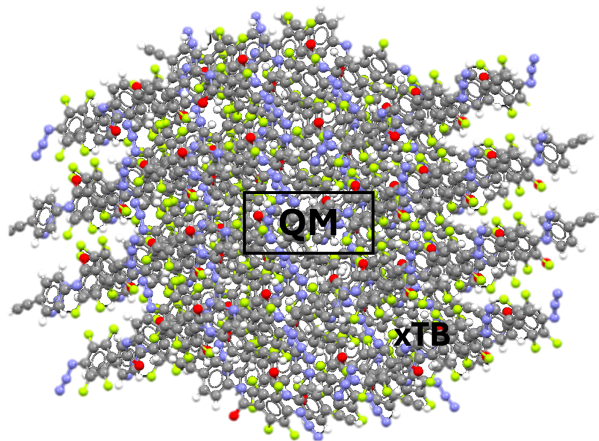


Figure 2: ONIOM subtractive embedding scheme of molecular crystals

Electronic structure calculations were carried out using a hybrid ONIOM[56]-style embedding scheme designed to balance accuracy and computational efficiency. The central molecule was treated at the density functional theory (DFT)[57] level using the same reference PBE functional used to compute the band gaps, in combination with the def2-TZVP basis set,[58] as implemented in ORCA 5.0.4.[59] The surrounding molecules within the cluster were modeled using the semiempirical extended tight-binding (xTB)[60] method for an approximate but efficient description of the electrostatic environment and intermolecular polarization effects imposed by the crystal packing.

Single-point calculations were performed without geometry optimization in order to preserve the experimentally observed crystal geometry. The resulting embedded wavefunctions were subsequently analyzed within the QTAIM framework. Topological analysis of the electron density was carried out using the Multiwfn program,[61] identifying nuclear critical points (NCPs) and bond critical points (BCPs) associated with both intra- and intermolecular interactions.

We note that the use of a molecular cluster embedding instead of periodic DFT is motivated by both practical and methodological considerations. Cluster-based calculations enable access to a broader range of QTAIM descriptors and allow the use of electronic structure methods that are currently not readily available in periodic implementations, particularly those required for future extensions to excited-state and multireference treatments. Additionally, cluster models provide greater flexibility in systematically analyzing local chemical environments and in selecting the level of theory and basis set. To validate the embedded-cluster approach, we performed convergence tests with respect to the ONIOM embedding radius for representative crystals spanning both strongly hydrogen-bonded and weakly dispersion-bound packing motifs, and compared converged embedded-cluster QTAIM descriptors with periodic DFT results. These analyses demonstrate that the QTAIM descriptors associated with the central molecule converge rapidly with embedding radius and closely reproduce the corresponding periodic electronic topology (see Supporting Information, Section S2). Nevertheless, periodic DFT remains a viable alternative framework, and its integration with QTAIM analysis will be explored in future work.

## Overview of the Multimodal Crystal Graph Neural Network Framework

We propose a multimodal learning framework for materials property prediction that integrates two complementary graph-based representations of crystalline systems: (i) periodic crystal structure graphs encoding atomic geometry and lattice periodicity, and (ii) Quantum Theory of Atoms in Molecules (QTAIM) graphs

encoding electron density topology and bonding characteristics derived from first-principles calculations. The proposed architecture employs modality-specific GNN encoders followed by a bi-directional gated fusion mechanism[62] that enables controlled cross-modal information exchange prior to final prediction.

An overview of the architecture is shown in Figure 3.

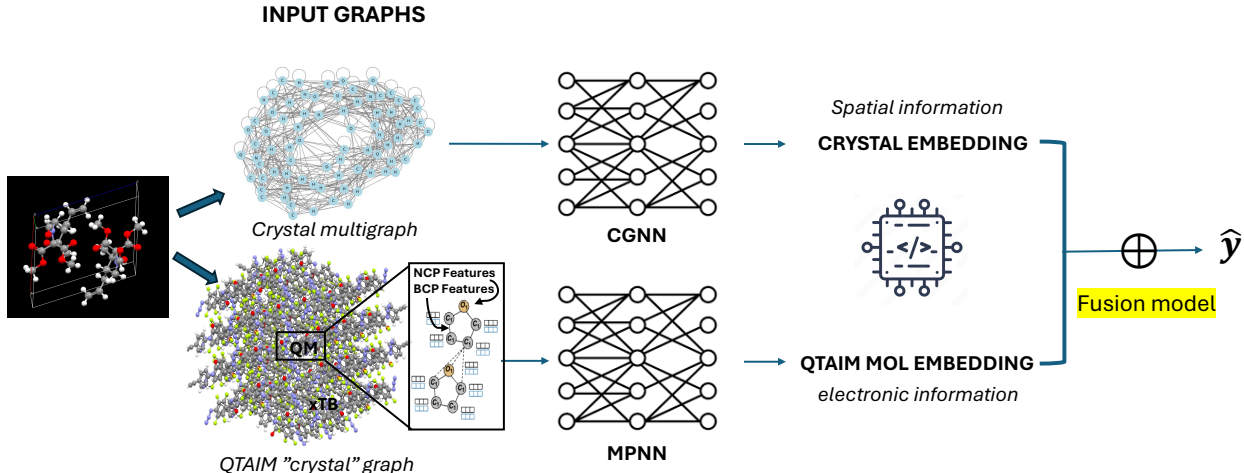


Figure 3: Overview of Multimodal Model for crystal property prediction

## Graph-Based Data Representations

A full description of the graph modalities and their attributes is included in the supporting information.

### Crystal Graphs

Crystal structures were converted into graph representations in which nodes correspond to atoms and edges are defined based on interatomic distances within a specified cutoff, as defined by Xie *et al.*[23]

### QTAIM Graphs

From the QTAIM analysis, a diverse set of electron-density derived descriptors was extracted at both nuclear and bond critical points (Table S1). These descriptors include local measures of electron density accumulation, curvature, and energy density, which collectively characterize the nature and strength of intra- and intermolecular interactions in the crystal. Unlike geometry-based features that depend solely on atomic positions and connectivity, QTAIM descriptors explicitly reflect how electron density is redistributed by crystal packing, polarization, and intermolecular coupling. The extracted quantities were assembled into molecular graph representations, where nodes and edges are augmented with electron-density-derived attributes, and subsequently used as input features for the QTAIM branch of the multimodal learning framework.

## Modality-Specific Encoders

### Crystal Encoder: GATGNN

The crystal modality is encoded using a Graph Attention Network with Global Attention (GATGNN).[63] This architecture augments node features with edge-aware multi-head attention and incorporates a composition-sensitive global pooling mechanism.

**Augmented Graph Attention (AGAT).** Node updates jointly incorporate atomic and bond features via

$$\mathbf{h}_i^{(\ell+1)} = \sigma \left( \sum_{j \in \mathcal{N}(i)} \alpha_{ij}^{(\ell)} \mathbf{W}^{(\ell)} \left[ \mathbf{h}_j^{(\ell)} \parallel \mathbf{e}_{ij} \right] \right),$$

where attention coefficients are computed as

$$\alpha_{ij}^{(\ell)} = \text{softmax}_j \left( \sigma \left( \mathbf{a}^\top \left[ \mathbf{W} \mathbf{h}_i^{(\ell)} \parallel \mathbf{W} \mathbf{h}_j^{(\ell)} \right] \right) \right).$$

**Global Attention Pooling.** Crystal-level embeddings are obtained via

$$\mathbf{z}^{(c)} = \sum_{i \in \mathcal{V}^{(c)}} \beta_i \mathbf{h}_i^{(L)}, \quad \beta_i = \text{softmax} \left( \text{MLP} \left[ \mathbf{h}_i^{(L)} \parallel \mathbf{g}^{(c)} \right] \right).$$

### QTAIM Encoder: FiLM-SchNet

To effectively integrate electron-density derived information into geometric message-passing architectures while preserving chemical interpretability, we encode the QTAIM modality using a feature-wise linear modulation (FiLM) mechanism.[64] Specifically, we leverage the mainstream SchNet[24] model as encoder whose core architecture is well suited for this integration given its design to process 3D molecular graphs using continuous-filter convolutions that operate on interatomic distances, allowing messages to be conditioned smoothly on spatial relationships. The proposed FiLM-conditioned SchNet (FiLM-SchNet) incorporates QTAIM descriptors directly into the message-passing mechanism, rather than appending them as post-hoc global features.[65] Prior multimodal GNN studies typically incorporate expert-crafted descriptors by concatenating them with the learned molecular embedding at the readout stage;[66] however, this late fusion strategy restricts descriptors to act only as global corrections and prevents them from influencing local atomic interactions. In contrast, our approach injects QTAIM edge descriptors into the continuous filter network via FiLM, allowing electronic-structure information to modulate the radial basis features that govern message passing (Figure 4). As a result, interaction strengths become explicitly conditioned on the local electronic environment, with QTAIM descriptors encoding bond character, charge redistribution, and density topology beyond simply geometric proximity. Moreover, the learned FiLM scaling and shifting parameters ( $\gamma$  and  $\beta$ ) provide a direct mechanism for interpreting the relative influence of individual electronic descriptors on the learned interactions, enhancing model explainability.

**Gaussian Distance Expansion.**

$$\phi_k(d_{ij}) = \exp \left[ -\gamma_k (d_{ij} - \mu_k)^2 \right], \quad k = 1, \dots, K.$$

**FiLM Conditioning.**

$$\tilde{\phi}(d_{ij}) = \phi(d_{ij}) \odot (1 + \gamma(\mathbf{e}_{ij}^{(q)})) + \beta(\mathbf{e}_{ij}^{(q)}).$$

$$\text{FiLM}(x|c) = \gamma(c) \odot x + \beta(c)$$

**Continuous-Filter Convolutions.**

$$\mathbf{m}_{ij} = \mathbf{h}_j^{(\ell)} \odot \mathbf{W} \tilde{\phi}(d_{ij}), \quad \mathbf{h}_i^{(\ell+1)} = \mathbf{h}_i^{(\ell)} + \sum_{j \in \mathcal{N}(i)} \mathbf{m}_{ij}.$$

### Bi-Directional Gated Fusion

To integrate geometric and electronic representations while preserving their complementary information, we employ a bi-directional gated fusion mechanism.[62] In contrast to static fusion schemes such as concatenation, this approach allows each modality to selectively modulate the contribution of the other through learned gating functions.

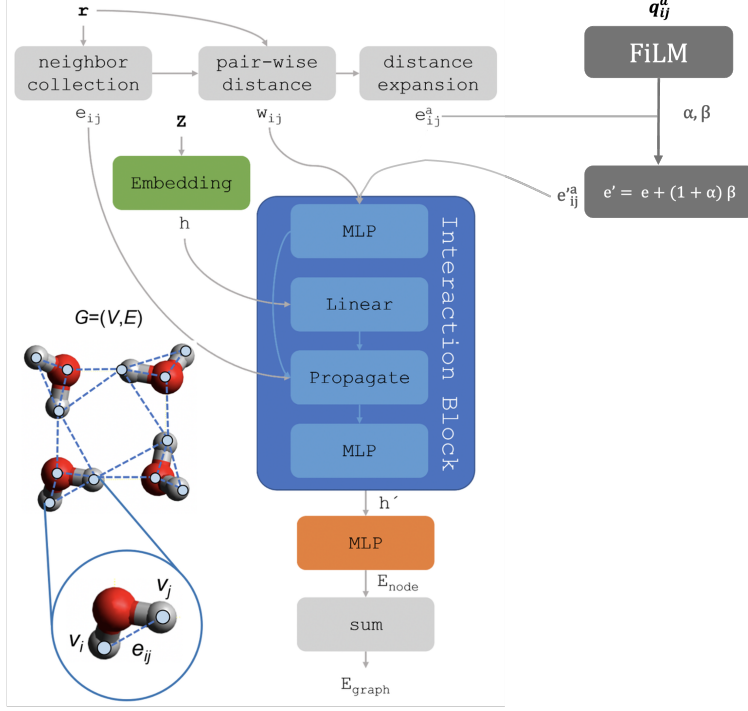


Figure 4: FiLM-Schnet Architecture  
Adapted from DOI:10.48550/arXiv.2211.13853

#### Crystal-Gated QTAIM Pathway.

$$\mathbf{g}^{c \rightarrow q} = \sigma(\mathbf{W}_c \mathbf{z}^{(c)}), \quad \mathbf{f}^{c \rightarrow q} = \mathbf{W}_{\text{out}} \left( \mathbf{g}^{c \rightarrow q} \odot \mathbf{W}_q \mathbf{z}^{(q)} \right).$$

#### QTAIM-Gated Crystal Pathway.

$$\mathbf{g}^{q \rightarrow c} = \sigma(\mathbf{W}'_q \mathbf{z}^{(q)}), \quad \mathbf{f}^{q \rightarrow c} = \mathbf{W}'_{\text{out}} \left( \mathbf{g}^{q \rightarrow c} \odot \mathbf{W}'_c \mathbf{z}^{(c)} \right).$$

#### Fusion and Prediction.

$$\mathbf{f}_{\text{combined}} = \tanh([\mathbf{f}^{c \rightarrow q} \parallel \mathbf{f}^{q \rightarrow c}]), \quad \hat{y} = \text{MLP}_{\text{fusion}}(\mathbf{f}_{\text{combined}}).$$

### Multimodal Training

Beyond the multimodal design that leverages different modality encoders as described above, a key feature of the model is the use of disentangled gradient learning (DGL),[67] which decouples optimization of modality-specific encoders from the fusion module. This prevents gradient interference between structural and electron-density representations, allowing each modality to learn stable, physically meaningful features while still benefiting from cross-modal interactions during fusion. Detailed descriptions of the DGL procedure is included in the supporting information.

**XQTAIM-MM architecture.** A schematic of the proposed XQTAIM-MM architecture with DGL training is shown in Figure 5. Within the disentangled gradient scheme, gradients from the fusion module are not propagated back into the modality-specific encoders, and conversely, encoder-specific losses do not update the fusion block. This gradient truncation prevents cross-modal interference and single-modality dominance effects, ensuring that each encoder learns modality-consistent representations while the fusion module operates on fixed latent embeddings. As a result, cross-modal interactions are learned at the representation level without destabilizing the underlying feature extractors.

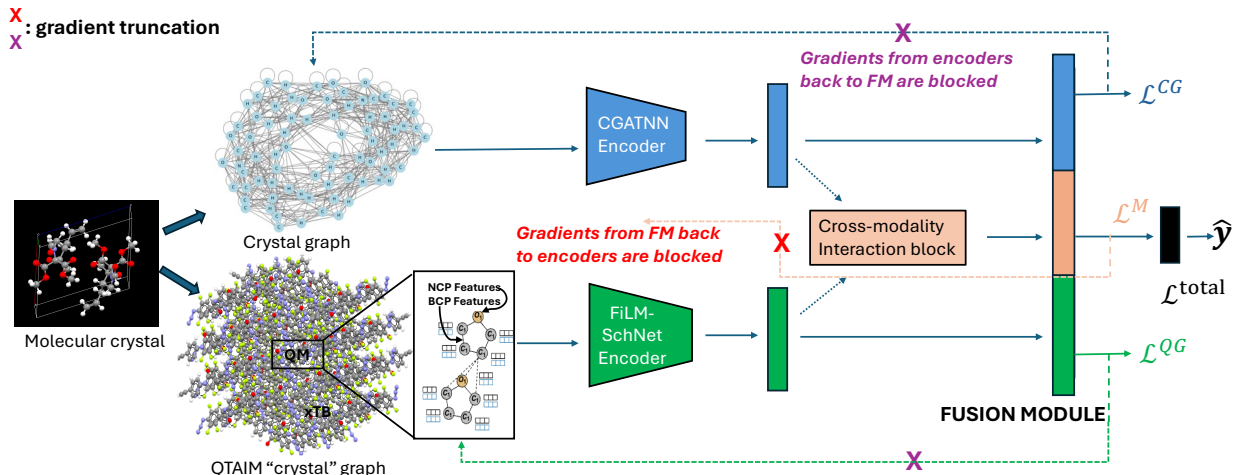


Figure 5: XQTAIM-MM architecture comprising modality-specific encoders, latent projection, a gated cross-modal interaction block, and a fusion module for property prediction. During training, gradients are selectively truncated (as shown with the X marks): encoder-specific losses do not update the fusion module, and fusion gradients are not backpropagated to the encoders.

All machine learning training and inference experiments were conducted on the Bridges-2 supercomputing cluster at the Pittsburgh Supercomputing Center using NVIDIA H100 (90 GB) GPUs.

## Results and Discussion

We first evaluate the predictive performance of established crystal graph neural networks (CGNNs), which serve as strong geometry-only based baseline models for band-gap prediction in organic molecular crystals. Model performance is assessed on held-out test sets using mean-absolute-error (MAE), root-mean-square error (RMSE), and coefficient of determination ( $R^2$ ). For all models, hyperparameters were independently optimized for each representation to ensure a fair comparison.

Table 1 summarizes the performance of representative crystal GNN architectures, including CGCNN, SchNet, GATGNN, MEGNet and ALIGNN, alongside the proposed multimodal XQTAIM-MM model on the OMDb dataset. Consistent with prior studies, geometry-only crystal GNNs achieve strong predictive accuracy, with ALIGNN and MEGNet outperforming earlier architectures. However, incorporating QTAIM-derived electronic descriptors through multimodal fusion yields a systematic improvement over all unimodal baselines. The XQTAIM-MM model achieves the lowest prediction error, with an MAE of 0.23 eV and an RMSE of 0.32 eV (Figure 6) This performance gain indicates that electron-density information provides task-relevant signals that are not recoverable from atomic positions and connectivity alone, even when higher-order geometric features are included such as ALIGNN’s line graph angular information.

Table 1: Test-set performance of crystal graph neural networks and the proposed multimodal XQTAIM-MM model on the OMDb dataset. Reported values are averaged over three random seeds; numbers in parentheses indicate the corresponding standard deviations.

| Model     | MAE                  | RMSE                 | $R^2$                |
|-----------|----------------------|----------------------|----------------------|
| CGCNN     | 0.2728 (0.010)       | 0.3831 (0.010)       | 0.8542 (0.010)       |
| SchNet    | 0.2680 (0.015)       | 0.3817 (0.021)       | 0.855 (0.015)        |
| GATGNN    | 0.263 (0.023)        | 0.376 (0.023)        | 0.860 (0.025)        |
| MEGNet    | 0.239 (0.006)        | 0.332 (0.007)        | 0.884 (0.005)        |
| ALIGNN    | 0.234 (0.003)        | -                    | 0.893 (0.002)        |
| XQTAIM-MM | <b>0.235 (0.008)</b> | <b>0.321 (0.014)</b> | <b>0.903 (0.004)</b> |

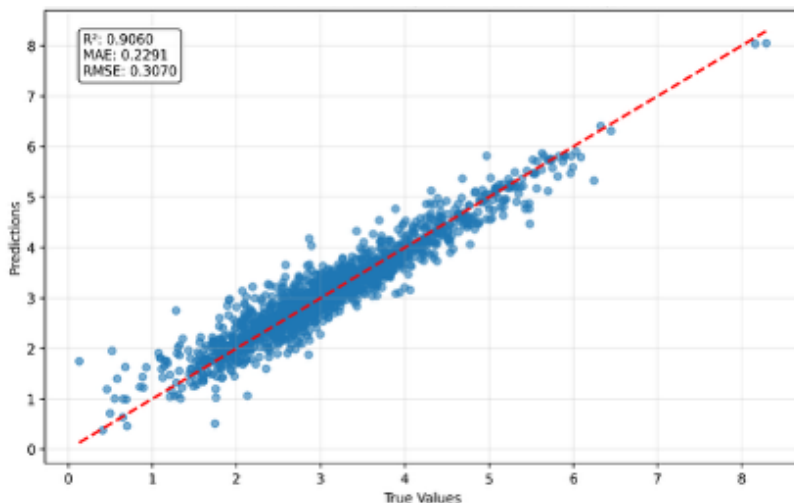


Figure 6: Parity plot comparing predicted vs DFT band gaps for XQTAIM-MM

We further examine the dependence of predictive performance on training set size (Figure 7). Geometry-only unimodal crystal graph models exhibit a strong reliance on data availability, with accuracy degrading rapidly in low-data regimes. In contrast, models incorporating QTAIM molecular graphs maintain substantially better performance when trained on limited data.

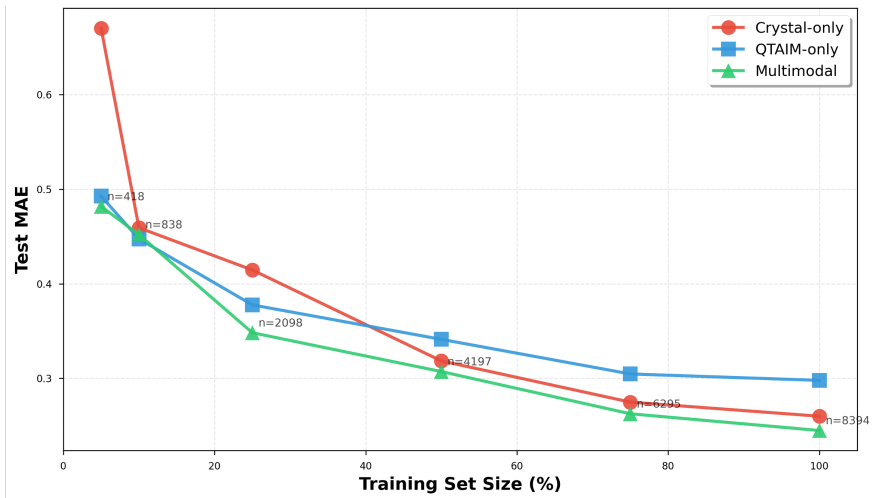


Figure 7: Data-set size sensitivity analysis plot for different molecular crystal graph representation and their respective unimodal model vs XQTAIM-MM. All models were trained using the same data split seed for 100 epochs.

### Generalizability

More importantly, we show that this improvement persists under out-of-domain evaluation and is particularly pronounced for polymorphic systems and polycyclic aromatic hydrocarbons (PAHs). PAHs are prototypical organic semiconductors whose band gaps depend sensitively on molecular conjugation length, topology, and functionalization, as well as on crystal packing effects such as  $\pi$ - $\pi$  stacking and polymorphism.[68, 69]

We use the PAH101 dataset,[70] which comprises crystalline PAHs with various electronic and excited state properties computed at the PBE-DFT and GW+BSE levels of theory, respectively (Figure 8).

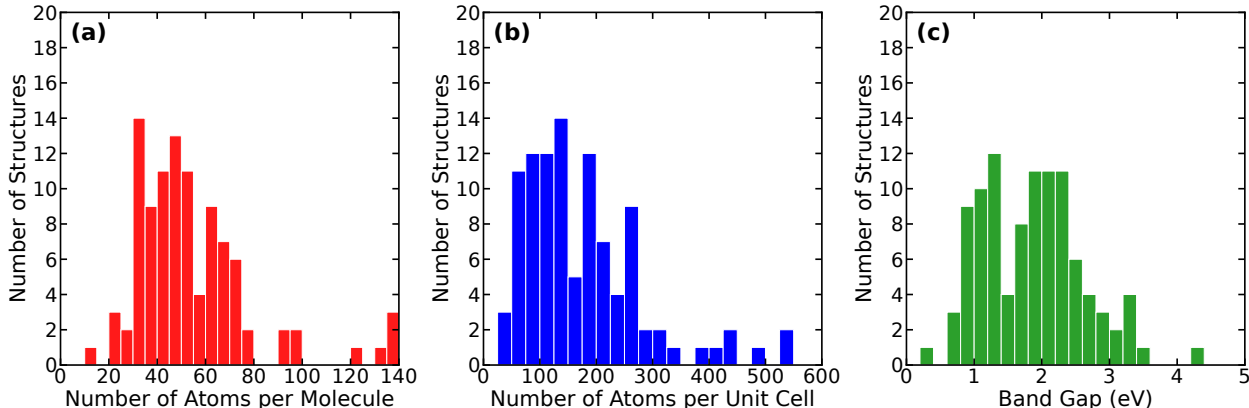


Figure 8: Statistical distributions for the PAH101 dataset. Histograms of (a) the number of atoms per molecule, (b) the number of atoms per crystal unit cell, and (c) the electronic band gap across the dataset.

For our evaluation, we perform zero-shot transfer learning, and test the performance of models trained exclusively on the OMDb dataset without any fine-tuning on the target domain. This evaluation is particularly informative given the nature of the OMDb dataset, which is chemically diverse and structurally heterogeneous but does not explicitly target PAHs as a focused material family or include polymorphs. Since PAHs’ electronic properties are governed by subtle electronic-structure effects, including  $\pi$ -electron delocalization and intermolecular  $\pi$ - $\pi$  interactions, a physically-informed model is expected to generalize more reliably across this chemically coherent data system. As shown in Figure 9, geometry-only crystal graph models exhibit substantial performance degradation under zero-shot transfer, with MAEs ranging from 0.40 to 0.50 eV. In contrast, the proposed XQTAIM-MM model achieves a markedly lower MAE of 0.36 eV (Figure 10), corresponding to a relative improvement of approximately 10–20%. This result demonstrates that incorporating electron-density derived descriptors leads to representations that are not only more accurate in-distribution but also substantially more transferable across chemically distinct regimes. Furthermore, to probe transferability, we evaluate zero-shot performance on polymorphs of ROY (red-orange-yellow), a benchmark molecular crystal known for its rich polymorphism driven by subtle conformational and packing differences.[71] Predicting properties across ROY polymorphs is challenging due to their sensitivity to small structural changes, making this test a stringent assessment of whether our quantum-enriched multi-modal model is truly capturing transferable physics. Consistent with prior results, our model outperforms geometry-only crystal graph baselines with an MAE of 0.124 eV compared to 0.4977 for eV CGCNN (Figure S11-12).

### Physical interpretation

Beyond predictive accuracy, the proposed architecture allows for physical explainability through its explicit integration of electron-density descriptors into the message-passing process. In the FiLM-SchNet encoder, QTAIM edge descriptors modulate the continuous-filter network via learned scaling and shifting parameters ( $\gamma$  and  $\beta$ ), whose magnitudes can be directly inspected to infer how specific electronic features influence interatomic interactions. We observe that the model places the highest importance on descriptors that characterize electron localization, the deviation of the electron density from a non-interacting reference state, and the specific nature of the bond. Specifically, the promolecular density difference ( $\Delta g_{\text{promolecular}}$ ), the electron localization function (ELF), the average local ionization energy, and the  $\eta$  index of bond character induce the largest modulation amplitudes in the radial basis filters (Figure 11). The high importance of the  $\eta$  index ( $\eta = |\lambda_1|/\lambda_3$ ) is particularly notable, as it allows the network to explicitly differentiate between shared-shell covalent interactions ( $\eta > 1$ ) and closed-shell interactions ( $\eta < 1$ ). This suggests that the network strongly conditions learned interaction strengths on regions where electrons are highly localized, or where it must distinguish between strong intramolecular bonds and weaker intermolecular contacts. By contrast, basic density and gradient magnitudes (such as the electron density  $\rho$ , its gradient norm, and ellipticity) exhibit the lowest FiLM weights. This pattern indicates that the model relies less on the raw magnitude or sim-

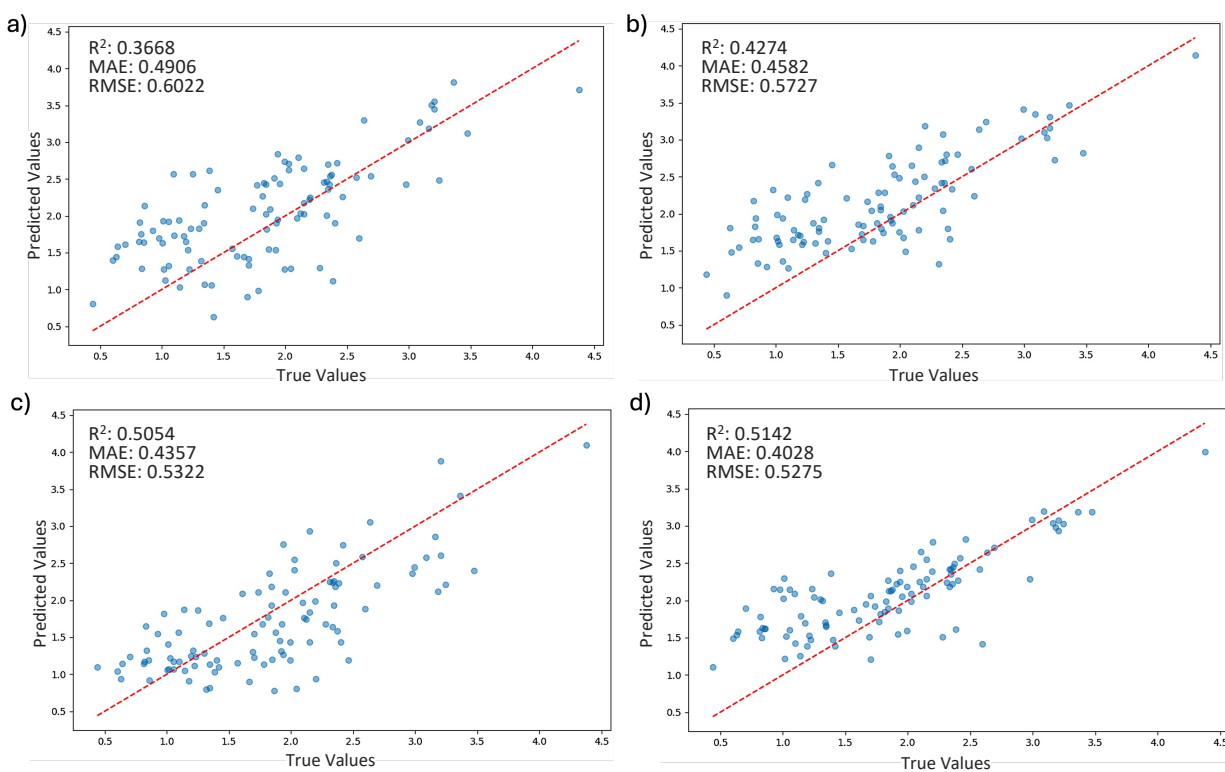


Figure 9: Parity plots of zero-shot transfer learning pre-trained models a) CGCNN b) GATGNN c) SchNet d) MegNet.

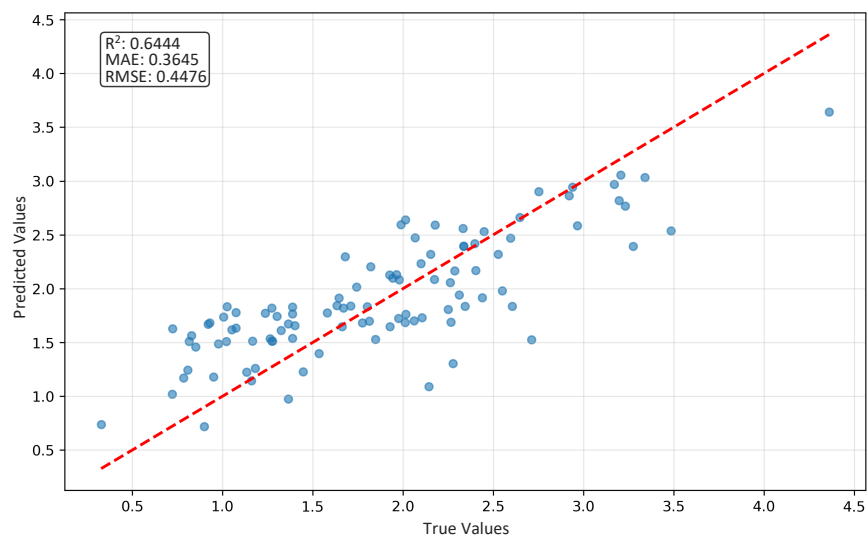


Figure 10: Parity plot of zero-shot transfer learning on PAH101 dataset using XQTAIM-MM OMDb pre-trained model.

ple anisotropy of the density, and more on complex, derived quantities that capture bonding heterogeneity,  $\pi$ -electron delocalization, and subtle charge redistribution effects. These effects are especially relevant for PAH crystals, where band gaps are known to be sensitive to local bonding environments and intermolecular electronic coupling mediated by  $\pi$ - $\pi$  interactions and packing-induced polarization.

It is worth noting that while these FiLM weights provide insight into the model’s internal representations, the exact ranking of feature importance may exhibit some variability depending on model initialization, hyperparameter configuration, descriptor correlations, and the underlying distribution of interaction motifs within the dataset. In particular, descriptors associated with specific interaction types may become more or less influential depending on their prevalence in the training data (see Supporting Information, Section S8). Nevertheless, this analysis demonstrates a concrete pathway for extracting physical insights from the integration of quantum-chemical features into graph neural networks.

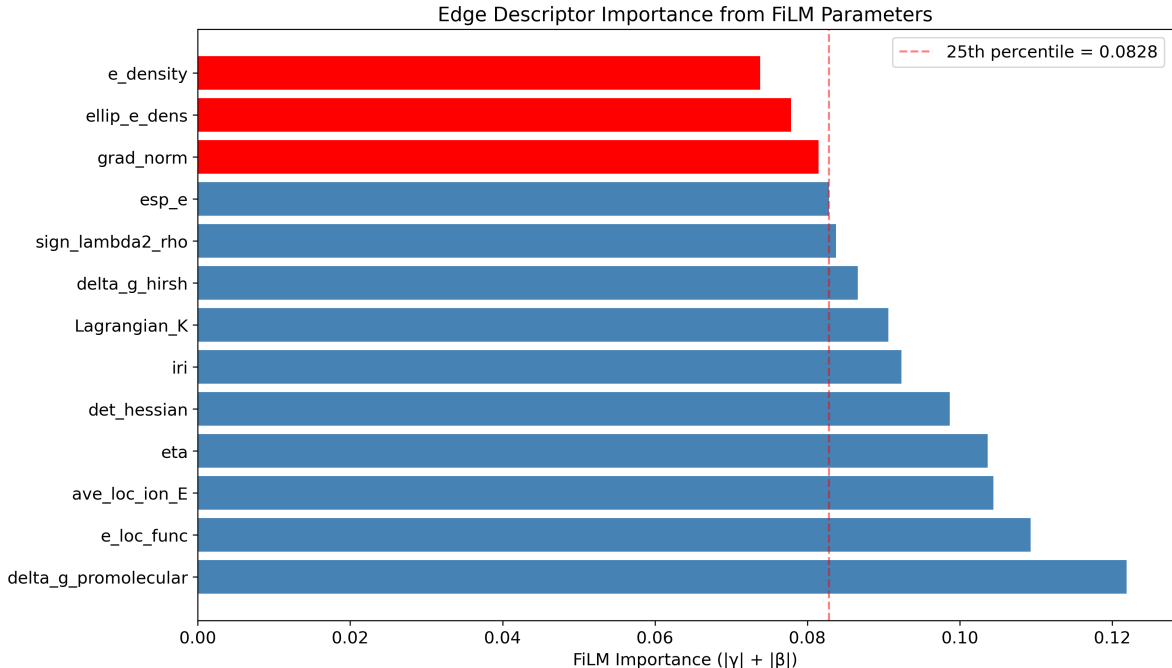


Figure 11: FiLM layer weights

## Conclusion

We presented a multimodal graph learning framework that combines crystal-structure graphs with QTAIM-derived electron-density graphs for band-gap prediction in organic molecular crystals. The proposed XQTAIM-MM model integrates an attention-based crystal graph encoder and a QTAIM FiLM-conditioned SchNet encoder through bi-directional gated fusion and a disentangled gradient training strategy. Across the OMDb dataset, this approach consistently improves prediction accuracy relative to established crystal graph models. More importantly, our contribution remains notably under zero-shot transfer to polycyclic aromatic hydrocarbons and polymorphs, which confirms that the learned representations capture electronic effects that are not well described by simply geometric connectivity descriptors.

Analysis of the FiLM module and learned representations shows that QTAIM descriptors influence the model at the level of local interactions. These observations are consistent with the role of charge redistribution, bonding topology, and intermolecular interactions in influencing the electronic properties of organic semi-conductors.

Finally, the present framework has several limitations. The FiLM-SchNet encoder conditions geometric filters on electronic descriptors but does not impose explicit physical constraints, such as energetic consistency

or density conservation, which may limit its applicability to force-field learning or molecular dynamics. Future work will explore physics-informed loss functions, multi-task training with electronic and energetic targets, and alternative message-passing schemes. More broadly, this study demonstrates that incorporating electron-density topology into graph-based models improves both predictive performance and transferability for molecular crystals properties.

## Acknowledgements

We thank the US National Science Foundation for support of this work through grants CHE-2453395 and DMR-2203519 (M.A.G.-G), CHE-2400314 (A.N.A), and Graduate Research Fellowship Program DGE-2444110 (F.I.). We also acknowledge the UCLA-IDRE cluster Hoffman2, and PSC cluster Bridges2 through the NSF-ACCESS grant, for computational resources.

## Data and Software Availability

The datasets, best model hyperparameters, and code supporting the findings of this study are publicly available on GitHub at: <https://github.com/ferd-ih/XQTAIM-MM/>.

## Supporting Information

Additional details regarding the models, data structures, and training procedures are provided in the supplementary information, which is available free of charge at <http://pubs.acs.org>.

## References

- (1) Staker, J.; Marques, G.; Dakka, J. In *Machine Learning in Chemistry*, Cartwright, H. M., Ed.; The Royal Society of Chemistry: 2020, pp 372–397, DOI: 10.1039/9781839160233-00372.
- (2) Faber, F.; Lindmaa, A.; Von Lilienfeld, O. A.; Armiento, R. Crystal structure representations for machine learning models of formation energies. *Int. J. Quantum Chem.* **2015**, *115*, 16, 1094–1101, DOI: 10.1002/qua.24917.
- (3) Gong, S.; Yan, K.; Xie, T.; Shao-Horn, Y.; Gomez-Bombarelli, R.; Ji, S.; Grossman, J. C. Examining graph neural networks for crystal structures: Limitations and opportunities for capturing periodicity. *Sci. Adv.* **2023**, *9*, 45, eadi3245, DOI: 10.1126/sciadv.adi3245.
- (4) Ryno, S. M.; Risko, C.; Brédas, J.-L. Impact of Molecular Packing on Electronic Polarization in Organic Crystals: The Case of Pentacene vs TIPS-Pentacene. *J. Am. Chem. Soc.* **2014**, *136*, 17, 6421–6427, DOI: 10.1021/ja501725s.
- (5) Silinsh, E. A., *Organic Molecular Crystals: Their Electronic States*; Springer Berlin, Heidelberg: 1980; 392 pp., DOI: 10.1007/978-3-642-81464-8.
- (6) Samoc, M.; Williams, J.; Williams, D. Molecular organic crystals: A survey of their purification, growth and characterization. *Prog. Cryst. Growth Charact. Mater* **1981**, *4*, 1, 149–172.
- (7) Sherrill, C. D. Energy Component Analysis of Interactions. *Acc. Chem. Res.* **2013**, *46*, 4, 1020–1028, DOI: 10.1021/ar3001124.
- (8) Hohenstein, E. G.; Duan, J.; Sherrill, C. D. Origin of the Surprising Enhancement of Electrostatic Energies by Electron-Donating Substituents in Substituted Sandwich Benzene Dimers. *J. Am. Chem. Soc.* **2011**, *133*, 34, 13244–13247, DOI: 10.1021/ja204294q.
- (9) Rossi, M.; Gasparotto, P.; Ceriotti, M. Anharmonic and Quantum Fluctuations in Molecular Crystals: A First-Principles Study of the Stability of Paracetamol. *Phys. Rev. Lett.* **2016**, *117*, 11, 115702, DOI: 10.1103/PhysRevLett.117.115702.
- (10) Reilly, A. M.; Tkatchenko, A. Role of Dispersion Interactions in the Polymorphism and Entropic Stabilization of the Aspirin Crystal. *Phys. Rev. Lett.* **2014**, *113*, 5, 055701, DOI: 10.1103/PhysRevLett.113.055701.
- (11) Marom, N.; DiStasio, R. A.; Atalla, V.; Levchenko, S.; Reilly, A. M.; Chelikowsky, J. R.; Leiserowitz, L.; Tkatchenko, A. Many-Body Dispersion Interactions in Molecular Crystal Polymorphism. *Angew. Chem. Int. Ed.* **2013**, *52*, 26, 6629–6632, DOI: 10.1002/anie.201301938.
- (12) Qian, Y.; Zhang, X.; Xie, L.; Qi, D.; Chandran, B. K.; Chen, X.; Huang, W. Stretchable Organic Semiconductor Devices. *Adv. Mater.* **2016**, *28*, 42, 9243–9265, DOI: 10.1002/adma.201601278.
- (13) Ostroverkhova, O. Organic Optoelectronic Materials: Mechanisms and Applications. *Chem. Rev.* **2016**, *116*, 22, 13279–13412, DOI: 10.1021/acs.chemrev.6b00127.
- (14) Wei, C.; Li, L.; Zheng, Y.; Wang, L.; Ma, J.; Xu, M.; Lin, J.; Xie, L.; Naumov, P.; Ding, X.; Feng, Q.; Huang, W. Flexible molecular crystals for optoelectronic applications. *Chem. Soc. Rev.* **2024**, *53*, 8, 3687–3713, DOI: 10.1039/D3CS00116D.
- (15) Zhu, J.; Wu, W.; Qi, H.; Yao, Y.; Yu, H.; Huang, X.; Wang, N.; Wang, T.; Hao, H. Dynamic organic crystals as exceptionally efficient artificial natural light-harvesting actuators. *Chem. Sci.* **2024**, *15*, 44, 18617–18626, DOI: 10.1039/D4SC05684A.
- (16) Guo, J.; Shi, C.; Zhen, Y.; Hu, W. Rational Control of Packing Arrangements in Organic Semiconducting Materials toward High-Performance Optoelectronics. *Acc. Mater. Res.* **2024**, *5*, 8, 907–919, DOI: 10.1021/accountsmr.4c00054.
- (17) Ueno, N. Tuning organic band structures with Coulomb interactions. *Science* **2016**, *352*, 6292, 1395–1396, DOI: 10.1126/science.aaf8937.
- (18) Guo, Z.; Guo, K.; Nan, B.; Tian, Y.; Iyer, R. G.; Ma, Y.; Wiest, O.; Zhang, X.; Wang, W.; Zhang, C.; Chawla, N. V. Graph-based Molecular Representation Learning. *arXiv:2207.04869*.

- (19) Zhao, B.; Xu, W.; Guan, J.; Zhou, S. Molecular property prediction based on graph structure learning. *Bioinformatics* **2024**, *40*, 5, btac304, DOI: 10.1093/bioinformatics/btac304.
- (20) Atz, K.; Grisoni, F.; Schneider, G. Geometric Deep Learning on Molecular Representations, 2021, DOI: 10.48550/arXiv.2107.12375.
- (21) Reiser, P.; Neubert, M.; Eberhard, A.; Torresi, L.; Zhou, C.; Shao, C.; Metni, H.; Van Hoesel, C.; Schopmans, H.; Sommer, T.; Friederich, P. Graph neural networks for materials science and chemistry. *Commun. Mater.* **2022**, *3*, 1, 93, DOI: 10.1038/s43246-022-00315-6.
- (22) Chen, C.; Ye, W.; Zuo, Y.; Zheng, C.; Ong, S. P. Graph Networks as a Universal Machine Learning Framework for Molecules and Crystals. *Chem. Mater.* **2019**, *31*, 9, 3564–3572, DOI: 10.1021/acs.chemmater.9b01294.
- (23) Xie, T.; Grossman, J. C. Crystal Graph Convolutional Neural Networks for an Accurate and Interpretable Prediction of Material Properties. *Phys. Rev. Lett.* **2018**, *120*, 14, 145301, DOI: 10.1103/PhysRevLett.120.145301.
- (24) Schütt, K. T.; Sauceda, H. E.; Kindermans, P.-J.; Tkatchenko, A.; Müller, K.-R. SchNet – A deep learning architecture for molecules and materials. *J. Chem. Phys.* **2018**, *148*, 24, 241722, DOI: 10.1063/1.5019779.
- (25) Choudhary, K.; DeCost, B. Atomistic Line Graph Neural Network for improved materials property predictions. *npj Comput. Mater.* **2021**, *7*, 1, 185, DOI: 10.1038/s41524-021-00650-1.
- (26) Yan, K.; Liu, Y.; Lin, Y.; Ji, S. Periodic Graph Transformers for Crystal Material Property Prediction. *NeurIPS 2022* **2022**, *1096*, 15066–15080.
- (27) Fung, V.; Zhang, J.; Juarez, E.; Sumpter, B. G. Benchmarking graph neural networks for materials chemistry. *npj Comput. Mater.* **2021**, *7*, 1, 84, DOI: 10.1038/s41524-021-00554-0.
- (28) Taniguchi, T.; Hosokawa, M.; Asahi, T. Graph Comparison of Molecular Crystals in Band Gap Prediction Using Neural Networks. *ACS Omega* **2023**, *8*, 42, 39481–39489, DOI: 10.1021/acsomega.3c05224.
- (29) Nguyen, P.; Loveland, D.; Kim, J. T.; Karande, P.; Hiszpanski, A. M.; Han, T. Y.-J. Predicting Energetics Materials’ Crystalline Density from Chemical Structure by Machine Learning. *J. Chem. Inf. Model.* **2021**, *61*, 5, 2147–2158, DOI: 10.1021/acs.jcim.0c01318.
- (30) O’Connor, D.; Buitrago, P. A. In *Practice and Experience in Advanced Research Computing 2024: Human Powered Computing*, PEARC ’24: Practice and Experience in Advanced Research Computing, ACM: Providence RI USA, 2024, pp 1–4, DOI: 10.1145/3626203.3670584.
- (31) Feng, M.; Zhao, C.; Day, G. M.; Evangelopoulos, X.; Cooper, A. I. A universal foundation model for transfer learning in molecular crystals. *Chem. Sci.* **2025**, *16*, 28, 12844–12859, DOI: 10.1039/D5SC00677E.
- (32) Pulido, A. et al. Functional materials discovery using energy–structure–function maps. *Nature* **2017**, *543*, 7647, 657–664, DOI: 10.1038/nature21419.
- (33) Cruz-Cabeza, A. J.; Reutzel-Edens, S. M.; Bernstein, J. Facts and fictions about polymorphism. *Chem. Soc. Rev.* **2015**, *44*, 23, 8619–8635, DOI: 10.1039/C5CS00227C.
- (34) Cheng, J.; Zhang, C.; Dong, L. A geometric-information-enhanced crystal graph network for predicting properties of materials. *Commun. Mater.* **2021**, *2*, 1, 92, DOI: 10.1038/s43246-021-00194-3.
- (35) Caruso, A.; Venturin, J.; Giambagli, L.; Rolando, E.; El-Machachi, Z.; Noé, F.; Clementi, C. Extending the range of graph neural networks with global encodings. *Nat. Commun.* **2026**, *17*, 1, 1855, DOI: 10.1038/s41467-026-69715-3.
- (36) Ko, T. W.; Finkler, J. A.; Goedecker, S.; Behler, J. A fourth-generation high-dimensional neural network potential with accurate electrostatics including non-local charge transfer. *Nat. Commun.* **2021**, *12*, 1, 398, DOI: 10.1038/s41467-020-20427-2.
- (37) Niu, X.; Zhang, Q.; Dang, Y.; Hu, W.; Sun, Y. MolPackL: Quantification and Interpretation of Intermolecular Interactions Driven by Molecular Packing. *J. Am. Chem. Soc.* **2024**, *146*, 34, 24075–24084, DOI: 10.1021/jacs.4c08132.

- (38) Stuyver, T.; Coley, C. W. Quantum chemistry-augmented neural networks for reactivity prediction: Performance, generalizability, and explainability. *J. Chem. Phys.* **2022**, *156*, 8, 084104, DOI: 10.1063/5.0079574.
- (39) Guan, Y.; Coley, C. W.; Wu, H.; Ranasinghe, D.; Heid, E.; Struble, T. J.; Pattanaik, L.; Green, W. H.; Jensen, K. F. Regio-selectivity prediction with a machine-learned reaction representation and on-the-fly quantum mechanical descriptors. *Chem. Sci.* **2021**, *12*, 6, 2198–2208, DOI: 10.1039/D0SC04823B.
- (40) Biswas, S.; Chung, Y.; Ramirez, J.; Wu, H.; Green, W. H. Predicting Critical Properties and Acentric Factors of Fluids Using Multitask Machine Learning. *J. Chem. Inf. Model.* **2023**, *63*, 15, 4574–4588, DOI: 10.1021/acs.jcim.3c00546.
- (41) Abarbanel, O. D.; Hutchison, G. R. QupKake: Integrating Machine Learning and Quantum Chemistry for Micro-p  $K_a$  Predictions. *J. Chem. Theory Comput.* **2024**, *20*, 15, 6946–6956, DOI: 10.1021/acs.jctc.4c00328.
- (42) Shimakawa, H.; Kumada, A.; Sato, M. Extrapolative prediction of small-data molecular property using quantum mechanics-assisted machine learning. *npj Comput. Mater.* **2024**, *10*, 1, 11, DOI: 10.1038/s41524-023-01194-2.
- (43) Li, S.-C.; Wu, H.; Menon, A.; Spiekermann, K. A.; Li, Y.-P.; Green, W. H. When Do Quantum Mechanical Descriptors Help Graph Neural Networks to Predict Chemical Properties? *J. Am. Chem. Soc.* **2024**, *146*, 33, 23103–23120, DOI: 10.1021/jacs.4c04670.
- (44) Bader, R. F. W. Atoms in molecules. *Acc. Chem. Res.* **1985**, *18*, 1, 9–15, DOI: 10.1021/ar00109a003.
- (45) Bader, R. F. W. Quantum topology of molecular charge distributions. III. The mechanics of an atom in a molecule. *J. Chem. Phys.* **1980**, *73*, 6, 2871–2883, DOI: 10.1063/1.440457.
- (46) Gatti, C. In *The Quantum Theory of Atoms in Molecules*, Matta, C. F., Boyd, R. J., Eds., 1st ed.; Wiley: 2007, pp 163–206, DOI: 10.1002/9783527610709.ch7.
- (47) Bader, R. F. W. A quantum theory of molecular structure and its applications. *Chem. Rev.* **1991**, *91*, 5, 893–928, DOI: 10.1021/cr00005a013.
- (48) Vargas, S.; Gee, W.; Alexandrova, A. High-throughput quantum theory of atoms in molecules (QTAIM) for geometric deep learning of molecular and reaction properties. *Digit. Discov.* **2024**, *3*, 5, 987–998, DOI: 10.1039/D4DD00057A.
- (49) Vargas, S.; Hennefarth, M. R.; Liu, Z.; Alexandrova, A. N. Machine Learning to Predict Diels–Alder Reaction Barriers from the Reactant State Electron Density. *J. Chem. Theory Comput.* **2021**, *17*, 10, 6203–6213, DOI: 10.1021/acs.jctc.1c00623.
- (50) Gee, W.; Doyle, A.; Vargas, S.; Alexandrova, A. N. Multi-level QTAIM-enriched graph neural networks for resolving properties of transition metal complexes. *Digit. Discov.* **2025**, *4*, 11, 3378–3388, DOI: 10.1039/D5DD00220F.
- (51) Menéndez Crespo, D.; Wagner, F. R.; Francisco, E.; Martín Pendás, Á.; Grin, Y.; Kohout, M. Interacting Quantum Atoms Method for Crystalline Solids. *J. Phys. Chem. A* **2021**, *125*, 40, 9011–9025, DOI: 10.1021/acs.jpca.1c06574.
- (52) Seidler, T.; Krawczuk, A.; Champagne, B.; Stadnicka, K. QTAIM-Based Scheme for Describing the Linear and Nonlinear Optical Susceptibilities of Molecular Crystals Composed of Molecules with Complex Shapes. *J. Phys. Chem. C* **2016**, *120*, 8, 4481–4494, DOI: 10.1021/acs.jpcc.5b10026.
- (53) Vener, M. V.; Manaev, A. V.; Egorova, A. N.; Tsirelson, V. G. QTAIM Study of Strong H-Bonds with the OH...A Fragment (A = O, N) in Three-Dimensional Periodical Crystals. *J. Phys. Chem. A* **2007**, *111*, 6, 1155–1162, DOI: 10.1021/jp067057d.
- (54) Olsthoorn, B.; Geilhufe, R. M.; Borysov, S. S.; Balatsky, A. V. Band Gap Prediction for Large Organic Crystal Structures with Machine Learning. *Adv. Quantum Tech.* **2019**, *2*, 7, 1900023, DOI: 10.1002/qute.201900023.
- (55) Perdew, J. P.; Burke, K.; Ernzerhof, M. Generalized Gradient Approximation Made Simple. *Phys. Rev. Lett.* **1996**, *77*, 18, 3865–3868, DOI: 10.1103/PhysRevLett.77.3865.

- (56) Chung, L. W.; Sameera, W. M. C.; Ramozzi, R.; Page, A. J.; Hatanaka, M.; Petrova, G. P.; Harris, T. V.; Li, X.; Ke, Z.; Liu, F.; Li, H.-B.; Ding, L.; Morokuma, K. The ONIOM Method and Its Applications. *Chem. Rev.* **2015**, *115*, 12, 5678–5796, DOI: 10.1021/cr5004419.
- (57) Tsuneda, T., *Density Functional Theory in Quantum Chemistry*; Springer Japan: Tokyo, 2014, DOI: 10.1007/978-4-431-54825-6.
- (58) Weigend, F.; Ahlrichs, R. Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys.* **2005**, *7*, 18, 3297, DOI: 10.1039/b508541a.
- (59) Neese, F. The ORCA program system. *WIREs Comput. Mol. Sci.* **2012**, *2*, 1, 73–78, DOI: 10.1002/wcms.81.
- (60) Bannwarth, C.; Ehlert, S.; Grimme, S. GFN2-xTB—An Accurate and Broadly Parametrized Self-Consistent Tight-Binding Quantum Chemical Method with Multipole Electrostatics and Density-Dependent Dispersion Contributions. *J. Chem. Theory Comput.* **2019**, *15*, 3, 1652–1671, DOI: 10.1021/acs.jctc.8b01176.
- (61) Lu, T.; Chen, F. Multiwfn: A multifunctional wavefunction analyzer. *J. Comput. Chem.* **2012**, *33*, 5, 580–592, DOI: 10.1002/jcc.22885.
- (62) Kiela, D.; Grave, E.; Joulin, A.; Mikolov, T. Efficient Large-Scale Multi-Modal Classification. *AAAI* **2018**, *32*, 1, DOI: 10.1609/aaai.v32i1.11945.
- (63) Louis, S.-Y.; Zhao, Y.; Nasiri, A.; Wang, X.; Song, Y.; Liu, F.; Hu, J. Graph convolutional neural networks with global attention for improved materials property prediction. *Phys. Chem. Chem. Phys.* **2020**, *22*, 32, 18141–18148, DOI: 10.1039/D0CP01474E.
- (64) Perez, E.; Strub, F.; Vries, H. d.; Dumoulin, V.; Courville, A. FiLM: Visual Reasoning with a General Conditioning Layer, 2017, DOI: 10.48550/arXiv.1709.07871.
- (65) Koishekenov, Y.; Bekkers, E. J. An exploration of conditioning methods in graph neural networks. *ICLR* **2023**.
- (66) Liu, Y. (; Moretti, R.; Wang, Y.; Dong, H.; Yan, B.; Bodenheimer, B.; Derr, T.; Meiler, J. Advancements in Ligand-Based Virtual Screening through the Synergistic Integration of Graph Neural Networks and Expert-Crafted Descriptors. **2025**, *65*, 10, 4898–4905, DOI: 10.1021/acs.jcim.5c00822.
- (67) Wei, S.; Luo, C.; Luo, Y. Boosting Multimodal Learning via Disentangled Gradient Learning, 2025, DOI: 10.48550/arXiv.2507.10213.
- (68) Schatschneider, B.; Monaco, S.; Liang, J.-J.; Tkatchenko, A. High-Throughput Investigation of the Geometry and Electronic Structures of Gas-Phase and Crystalline Polycyclic Aromatic Hydrocarbons. *J. Phys. Chem. C* **2014**, *118*, 34, 19964–19974, DOI: 10.1021/jp5064462.
- (69) Nguyen, L. H.; Truong, T. N. Quantitative Structure–Property Relationships for the Electronic Properties of Polycyclic Aromatic Hydrocarbons. *ACS Omega* **2018**, *3*, 8, 8913–8922, DOI: 10.1021/acsomega.8b00870.
- (70) Gao, S.; Liu, X.; Luo, Y.; Wang, X.; Zhao, K.; Chang, V.; Schatschneider, B.; Marom, N. PAH101: A GW+BSE Dataset of 101 Polycyclic Aromatic Hydrocarbon (PAH) Molecular Crystals. *Sci. Data* **2025**, *12*, 1, 679, DOI: 10.1038/s41597-025-04959-0.
- (71) Yu, L. Polymorphism in Molecular Solids: An Extraordinary System of Red, Orange, and Yellow Crystals. *Acc. Chem. Res.* **2010**, *43*, 9, 1257–1266, DOI: 10.1021/ar100040r.

