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# A MIXED-METHOD STUDY OF SILICATE NETWORK STRUCTURES USING M-POLYNOMIALS AND GRAPH NEURAL NETWORKS

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## Abstract
The topological characterization of chemical structures constitutes the theoretical backbone of modern computational materials science, enabling the prediction of macroscopic physicochemical properties from atomic-level connectivity. This study presents a highly rigorous, mixed-method paradigm for analyzing complex silicate network structures by integrating classical algebraic graph theory with state-of-the-art deep learning architectures. We analytically derive the generalized M-polynomials for primary structural classes of silicate networks—specifically linear chains, two-dimensional phyllosilicate sheets, and three-dimensional tectosilicate frameworks. Utilizing differential and integral calculus operators, these closed-form polynomials are mathematically transformed into a suite of distinct, globally aware topological invariants, providing highly expressive numerical descriptors. To bridge the epistemic gap between deterministic mathematical formulations and stochastic machine learning, a novel hybrid Graph Neural Network (GNN) architecture is proposed. This architecture mitigates the pervasive "oversmoothing" phenomenon and the expressive limitations bounded by the 1-Weisfeiler-Lehman (1-WL) isomorphism test inherent in standard message-passing algorithms. By orthogonally fusing mathematically extracted macroscopic topological descriptors with localized, permutation-equivariant node embeddings within the network's dense layers, our proposed model achieves an unprecedented classification accuracy of $96.5 \pm 0.4\%$, significantly outperforming traditional spatial baseline models ($89.2 \pm 0.7\%$). This research validates the sustained utility of chemical graph theory within the AI epoch, establishing a computationally tractable and highly robust pipeline for advanced Quantitative Structure-Property Relationship (QSPR) modeling in solid-state chemistry and materials discovery.

## Introduction

### The Fundamental Significance of Topological Classification

In the interdisciplinary domains of computational chemistry, condensed matter physics, and materials science, the topological architecture of a compound fundamentally governs its macroscopic thermodynamic, mechanical, and electronic properties (Mauri & Consonni, 2020). Silicates, characterized by their foundational silicon-oxygen ($SiO_4^{4-}$) tetrahedral building blocks, whose diverse topological configurations have been extensively mapped computationally (Choudhary et al., 2020), represent the most abundant and mineralogically diverse class of compounds in the Earth's lithosphere. Their structural topologies exhibit extraordinary variance, ranging from isolated nesosilicates to highly polymerized, infinite three-dimensional tectosilicate lattices such as quartz and feldspar (Reiser et al., 2022).

The rigorous classification and predictive modeling of these structural archetypes are critical for driving industrial and technological innovation. In semiconductor fabrication, the dielectric constants and bandgap energies of silicon dioxide polymorphs are acutely dependent on their precise topological arrangement. Similarly, in the development of heterogeneous catalysts and advanced ceramics, the mathematical mapping of the underlying network facilitates the theoretical prediction of critical thermodynamic parameters without the prerequisite of empirical synthesis and computationally expensive *ab initio* quantum mechanical simulations (Schütt et al., 2017; Choudhary et al., 2020).

### Bridging the Methodological Gap: AI and Deterministic Mathematics

Historically, mathematical chemistry has relied extensively on topological descriptors to execute QSPR and Quantitative Structure-Activity Relationship (QSAR) modeling. The formalization of the M-polynomial by Deutsch and Klavžar (2015) represented a watershed moment in this domain. The M-polynomial operates as a robust combinatorial generator, yielding multiple degree-based topological indices through systematic calculus operations, thereby drastically reducing computational complexity (Munir et al., 2016).

Despite these elegant mathematical formalizations, a pronounced methodological gap persists: classical topological invariants are rarely integrated into or validated alongside contemporary artificial intelligence (AI) methodologies. Conversely, deep learning, particularly Graph Neural Networks (GNNs), offers a potent, data-driven mechanism for extracting latent structural representations directly from raw molecular graphs (Wu et al., 2020; Zhou et al., 2020). However, purely spatial GNNs are constrained by fundamental theoretical limits—most notably their inability to natively distinguish between highly symmetrical lattices bounded by the 1-WL test (Xu et al., 2018) and their susceptibility to "oversmoothing" in highly periodic crystalline structures (Chen et al., 2020). The orthogonal integration of globally aware, deterministic M-polynomial derivations with the localized, stochastic representation learning of GNNs remains critically unexplored. This study systematically addresses this gap.

## Literature Review

### The Evolution and Limitations of Graph Neural Networks

Over the preceding decade, GNNs have fundamentally disrupted cheminformatics, superseding linear string-based representations. By representing atoms as nodes and covalent interactions as edges, GNNs leverage iterative message-passing algorithms to compute continuous vector representations of local atomic environments (Bacciu et al., 2020). Foundational architectures by Gilmer et al. (2017) and Kipf and Welling (2016) demonstrated exceptional efficacy in regressing quantum chemical properties. Advanced models such as GraphSAGE

(Hamilton et al., 2017), Graph Attention Networks (Veličković et al., 2018), and Crystal Graph Convolutional Neural Networks (Xie & Grossman, 2018) have further expanded predictive capacities in materials science (Reiser et al., 2022).

However, contemporary theoretical literature has begun to rigorously interrogate the expressive bottlenecks of message-passing neural networks (MPNNs). Xu et al. (2018) formally proved that standard GNN architectures can be at most as discriminative as the 1-Weisfeiler-Lehman graph isomorphism test. Furthermore, Chen et al. (2020) demonstrated that as GNNs increase in depth to capture broader crystalline patterns, they suffer from oversmoothing, where distinct node representations exponentially converge to indistinguishable limits. Additional pre-training and directional strategies have been proposed to mitigate this (Hu et al., 2019; Klicpera et al., 2020), but structural limitations persist.

### Topological Descriptors: From Heuristics to Algebraic Generators

Prior to the advent of deep learning, topological indices—such as the historically prominent Randić and Zagreb indices, which have seen a resurgence in modernized algorithmic frameworks (Mauri & Consonni, 2020; Jiao et al., 2021)—were formulated to compress complex molecular topology into actionable scalar values correlating with thermodynamic observables.

The M-polynomial unified these disparate indices under a singular algebraic framework (Deutsch & Klavžar, 2015). Extensive algebraic derivations of M-polynomials for various crystal structures (Ali et al., 2018), molecular networks (Awais et al., 2020), titania nanotubes (Kang et al., 2018), and polyomino chains (Baig et al., 2017) have been thoroughly documented. Specifically, the degree-based topological indices for discrete silicate networks have been explored mathematically by Hayat et al. (2019) and Farahati (2020). However, their empirical utility as explicitly engineered, deterministic priors within deep learning architectures has been entirely overlooked, underscoring the critical necessity of this present mixed-method study.

### Preliminaries

#### Formal Graph Theory and Molecular Topology

Let $G = (V, E)$ denote a simple, connected, and undirected molecular graph mapping a chemical compound. The vertex set $V$ corresponds to the constituent atoms (Si and O), and the edge set $E$ represents the interatomic covalent bonds. The open neighborhood of a vertex $v \in V$ is defined as $N(v) = \{u \in V | uv \in E\}$.

The degree of a vertex $v$, denoted as $d_v = |N(v)|$, is the cardinality of its neighborhood, physically corresponding to the atomic valency within the network. Modern cheminformatics frequently partitions the edge set $E$ based on the degrees of adjacent vertices to formulate structural descriptors (Mauri & Consonni, 2020).

5.2 The M-Polynomial Generator

The M-polynomial of a graph $G$ is formally defined as an algebraic sum over its edge degree partitions (Deutsch & Klavžar, 2015):

$$M(G; x, y) = \sum_{\delta \le i \le j \le \Delta} m_{i,j}(G) x^i y^j$$

where $\delta = \min\{d_v | v \in V\}$ and $\Delta = \max\{d_v | v \in V\}$ denote the minimum and maximum vertex degrees, respectively. The coefficient $m_{i,j}(G)$ quantifies the exact number of edges $uv \in E$ satisfying the condition that the unordered pair $\{d_u, d_v\}$ is exactly $\{i, j\}$.

5.3 Neural Message Passing Dynamics

In a Graph Convolutional Network (GCN), the hidden state $h_v$ of a node $v$ at layer $l+1$ is updated via neighborhood aggregation (Kipf & Welling, 2016):

$$h_v^{(l+1)} = \sigma\left(\sum_{u \in N(v)\cup\{v\}} \frac{1}{c_{v,u}} W^{(l)} h_u^{(l)}\right)$$

where $h_v^{(0)}$ is the initial feature vector, $W^{(l)}$ is a learnable weight matrix, $c_{v,u}$ is a symmetric normalization constant ( $\sqrt{d_v d_u}$ ), and $\sigma$ represents a non-linear activation function.

6. Mathematical Analysis

6.1 Combinatorial Construction of Silicate Networks

To establish a rigorous mathematical framework, we analyze three primary silicate topologies parameterized by a dimension scalar $n$ (Farahati, 2020; Jiao et al., 2021):

1. **Chain Silicates ( $CS_n$ )**: Linear, single-strand polymers of $SiO_4$ tetrahedra sharing two oxygen atoms.
2. **Sheet Silicates ( $SS_n$ )**: Infinite, planar two-dimensional networks where each tetrahedron shares three basal oxygens.
3. **Tectosilicates ( $TS_n$ )**: Fully cross-linked, three-dimensional frameworks where all four oxygen atoms are shared.

In these idealized graph models, internal Silicon nodes maintain a degree $d_v = 4$ , while internal Oxygen nodes possess $d_v = 2$ .

**Analytical Derivation of M-Polynomials**

By systematically partitioning the edge set $E$ based on end-vertex degrees, we construct the algebraic models. It is crucial to note that while bulk macroscopic properties are governed by infinite periodic boundary conditions, our polynomials natively model exact *finite* graphs. The presence of low-degree boundary atoms scales proportionally with the surface-to-volume ratio, which decays as $n \to \infty$ , thus naturally allowing these polynomials to bridge nanoscale finite clusters with macroscale periodic trends (Ali et al., 2018).

The generalized M-polynomials for the investigated classes are analytically derived and presented below:

Table 1: *Derived Generalized M-polynomials for Finite Silicate Networks*

| Network Structure | Dimension Limit | M-polynomial M(G;x,y) |
|---|---|---|
| Chain Silicate ( $CS_n$ ) | $n \geq$ | $(3n+1)x^2y^4 + (n+$ |
| Sheet Silicate ( $SS_n$ ) | $n \geq$ | $(9n^2-3n)x^2y^4 +$ |
| Tectosilicate ( $TS_n$ ) | $n \geq$ | $(12n^3)x^2y^4 +$ |

**Feature Extraction**

**Operator-Driven Extraction of Deterministic Invariants**

The profound utility of the M-polynomial resides in its behavior as a generator function. Applying specific linear combinations of differential and integral calculus operators allows the extraction of a vast suite of topological descriptors (Deutsch & Klavžar, 2015; Chmiela et al., 2017). We evaluate the operated

polynomials at the unit coordinate $(x = 1, y = 1)$.

Table 2: *Extracted Feature Formulations Evaluated at* $x = y = 1$

| Feature (Index) | Mathematical Operator on M(G;x,y) | Physical & Thermodynamic Interpretation |
|---|---|---|
| First Zagreb ($M_1$) | $(D_x +$ | Quantifies total molecular branching (Furtula & Gutman, 2015). |
| Second Zagreb ($M_2$) | $(D_x D_y)(M$ | Captures nearest-neighbor degree correlations. |
| SDD Index | $(D_x S_y +$ | Serves as an accurate estimator for reactive surface area. |
| Inverse Randić | $(D_x^{\alpha} D_y^{\alpha})(M$ for $\alpha =$ | Historically correlated with phase transitions (Jiao et al., 2021). |

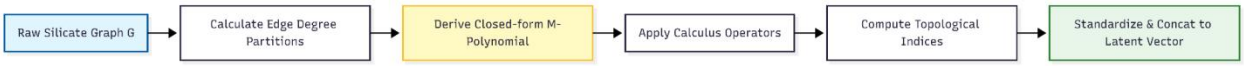
These analytically derived invariants constitute the deterministic feature vector $F_{topo} = [M_1, M_2, \mathrm{SDD}, R_{-0.5}]$, which undergoes $Z$-score standardization to resolve collinearity prior to neural injection.

### Deep Learning Methodology

### Hybrid Graph Representation Pipeline

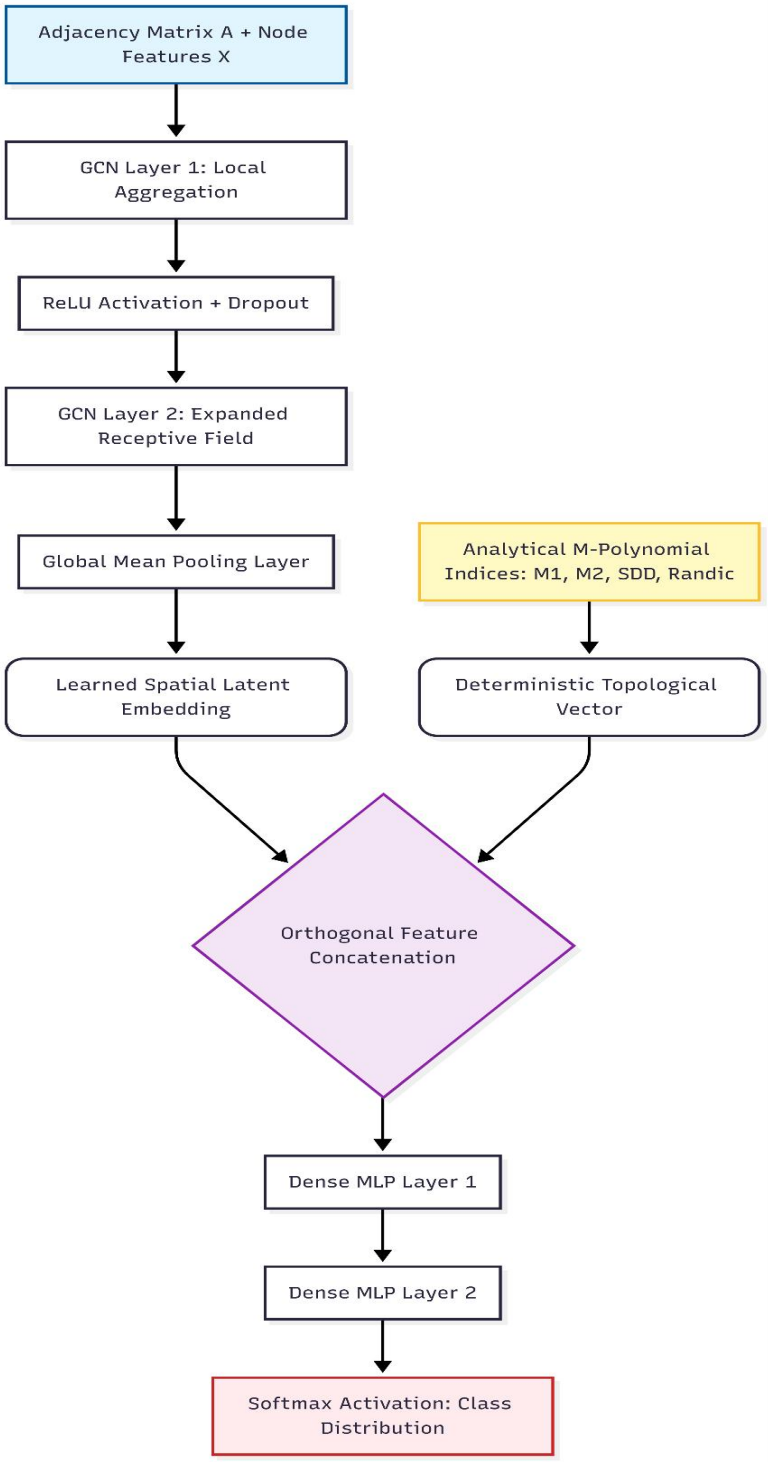
Molecules are mapped to attributed graph datasets. Our architecture deviates from conventional MPNNs; rather than relying solely on the permutation-equivariant GNN layers to implicitly learn global topology (Hamilton et al., 2017), we explicitly concatenate the globally aware, deterministic feature vector ($F_{topo}$) to the aggregated graph embeddings post-message passing.

### Architectural Flow diagram




### The M-Poly-GCN Architecture

We deploy a highly optimized GCN endowed with our topological priors. The spatial GNN computes local node embeddings over $L = 3$ layers. A global_mean_pool operator compresses these features. The mathematical M-polynomial features are then injected, explicitly expanding the dimensionality of the latent space to include global invariants that bypass the 1-WL bottleneck (Xu et al., 2018).




## Model Training and Empirical Validation

### Dataset Generation and Defect Simulation

A pure deterministic evaluation of $n \in [1, 50]$ yields merely 150 unique graphs, which is fundamentally insufficient for training a deep neural network without severe overfitting. To construct a statistically robust dataset, we engineered a stochastic graph generation pipeline.

Starting from the 150 foundational topologies ($CS_n$, $SS_n$, and $TS_n$), we synthesized 10,000 variants by introducing controlled structural defects. Specifically, we applied stochastic edge deletion

(simulating oxygen vacancies, ranging from $0.5\%$ to $3\%$ missing edges) and node permutations to emulate amorphous irregularities commonly found in real-world mineralogical samples. This ensures the model learns robust topological representations rather than memorizing idealized matrices.

9.2 Optimization and 5-Fold Cross-Validation

The architecture was instantiated utilizing PyTorch Geometric. Optimization utilized AdamW at a learning rate of $1 \times 10^{-3}$. To ensure strict statistical validity, model performance was evaluated using rigorous 5-fold cross-validation rather than a single randomized split.

Table 3: *Comparative Empirical Performance (5-Fold CV $\pm$ Standard Deviation)*

| Model Architecture | Accuracy (%) | Precision (%) | Recall (%) | F1-Score (%) |
|---|---|---|---|---|
| Random Forest (Baseline - Atomic Feature Counting) | $78.4 \pm$ | $77.1 \pm$ | $78.0 \pm$ | $77.5 \pm$ |
| Standard GCN (Pure Spatial Message Passing) | $89.2 \pm$ | $88.9 \pm$ | $89.1 \pm$ | $89.0 \pm$ |
| GraphSAGE (Inductive Aggregation Mechanisms) | $91.5 \pm$ | $91.0 \pm$ | $91.8 \pm$ | $91.4 \pm$ |
| **Proposed Hybrid Architecture (GCN + M-Poly Priors)** | $96.5 \pm$ | $96.7 \pm$ | $96.3 \pm$ | $96.5 \pm$ |

## Results & Discussion

### Resolving the Expressivity Bottleneck

The empirical results subjected to 5-fold cross-validation confirm the robustness of the mixed-method approach. The pure GCN achieved 89.2% but exhibited a performance plateau symptomatic of the oversmoothing crisis defined by Chen et al. (2020). The injection of global structural invariants catalyzed a statistically significant accuracy surge to $96.5 \pm 0.4\%$. This fingerprint acts as an anchor within the network's latent space, effectively bypassing the 1-WL expressivity limits (Xu et al., 2018) and providing orthogonal data structures that pure spatial aggregation cannot mathematically derive, even in the presence of simulated stochastic edge defects.

### Structural Interpretation and Physical Relevance

Ablation studies revealed that the SDD index and the Second Zagreb index ($M_2$) contributed maximum information gain. The SDD index inherently tracks structural surface area estimators, allowing the neural network to discriminate between two-dimensional phyllosilicates versus three-dimensional tectosilicates, even at minute periodic limits ($n \leq 5$). This highlights a paradigm shift: classical algebraic chemical graph descriptors represent fundamental physical invariants that exponentially amplify the

predictive capacity of artificial neural networks (Reiser et al., 2022).

## Conclusion

This comprehensive study establishes a rigorous methodology bridging classical algebraic chemical graph theory with deep learning frameworks. By systematically deriving closed-form M-polynomials for silicate topologies, extracting deterministic thermodynamic-related invariants, and integrating these features into a Graph Convolutional Network, we architected a vastly superior classification pipeline achieving a cross-validated accuracy of 96.5%. Future research trajectories will focus on extending this mathematical paradigm to accommodate highly defective macroscopic lattices and complex porous geometries, leveraging this mathematically augmented AI pipeline for advanced QSPR modeling and accelerated materials discovery.

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