Unifying Topological Description, Symmetry Detection, and Structure Generation for Two-Dimensional Carbon Allotropes

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Abstract

The exploration of two-dimensional carbon allotropes beyond graphene has generated significant interest in materials science, yet systematic enumeration and characterization of these structures remain challenging [1]. We introduce the *embedding tensor Φ*, a rank-3 integer tensor that provides a unique, coordinate-free representation of any three-connected two-dimensional carbon lattice[2]. Unlike traditional adjacency matrices, which cannot distinguish between topologically distinct structures with identical connectivity, the embedding tensor unifies vertices, edges, and polygonal faces into a single mathematical framework, enabling exact identification of structural isomorphism.

The tensor formalism obeys summation rules derived from Euler characteristics and can be cast into a flag graph representation. This enables tolerance-free identification of wallpaper symmetries through purely algebraic operations, avoiding the numerical precision issues inherent in coordinate-based symmetry detection methods. Building on this framework, we developed an iterative add-dimer search algorithm that generates all structures with N_F faces from crystals with $N_F - 1$ faces. The algorithm automatically discards duplicates via tensor isomorphism checking and identifies non-primitive cells through symmetry analysis. By exploiting symmetry to restrict dimer insertion to symmetry-unique positions, we transform an otherwise exponential combinatorial search into a tractable approach, successfully enumerating structures up to $N_F = 7$, yielding 1,823 unique primitive cells without triangles and 12,450 total structures including triangular rings.

Once candidate topologies are enumerated, approximate real-space coordinates and lattice vectors can be reconstructed analytically from Φ and sparse crossing matrices using a non-iterative least-squares approach. This provides initial geometries suitable for subsequent electronic structure or vibrational calculations. The method delivers an end-to-end pipeline from exhaustive symmetry-aware enumeration to metadata tagging and coordinate generation, requiring only integer arithmetic and avoiding floating-point tolerances until the final coordinate reconstruction step.

This work establishes a rigorous mathematical foundation for high-throughput computational exploration of two-dimensional materials, with immediate applications to carbon allotropes and potential extensions to other planar networks including boron nitride and boron-carbon-nitrogen compounds.

References

[1] A. Macmillan, E.C. Girao, V. Meunier, Carbon 203 (2023) 611.
[2] L. Macmillan, E.C. Girao, V. Meunier, Npj Computational Materials 12 (2026) 65.