Boron Fullerenes: Systematic Computational Search

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Recent experimental realizations of the boron fullerene B_{80} [1] came nearly a decade after its theoretical prediction [2]. Following the earlier confirmation of the B_{40} fullerene [3], it has become clear that boron, much like carbon, can form a rich variety of stable cage architectures. However, the electron-deficient nature of boron introduces complex 3-center 2-electron (3c-2e) bonding patterns, making the systematic discovery of boron fullerenes both a unique materials challenge and an ideal candidate for graph-based structural exploration.

In this work, we present the design and ongoing development of an automated computational framework for the systematic search and screening of viable boron fullerene candidates. Our generative pipeline builds upon crystal structure prediction concepts combined with topological graph descriptors. Initial candidate geometries are generated via Goldberg-Coxeter transformations of base Platonic solids (primarily the icosahedron), parameterized by the Caspar-Klug T-number to establish baseline lattice topology and size scaling. To obtain characteristic boron coordination environments (predominantly 5- and 6-coordinated sites), sub-graphs are generated by removing vertex orbits while strictly preserving targeted point-group symmetries to keep the search space computationally tractable (as illustrated in Fig. 1).

To bypass expensive first-principles calculations during high-throughput screening, candidate quality is evaluated via a two-tier surrogate model: a physics-based 3-body tight-binding (TB) Hamiltonian optimized for multicenter boron bonding, and a graph neural network / graph convolutional network (GNN/GCN) [4] enriched with 3-body topological descriptors, trained on TB-derived binding energies per atom. This integrated framework aims to rapidly identify promising low-energy boron fullerenes for subsequent high-level DFT validation.

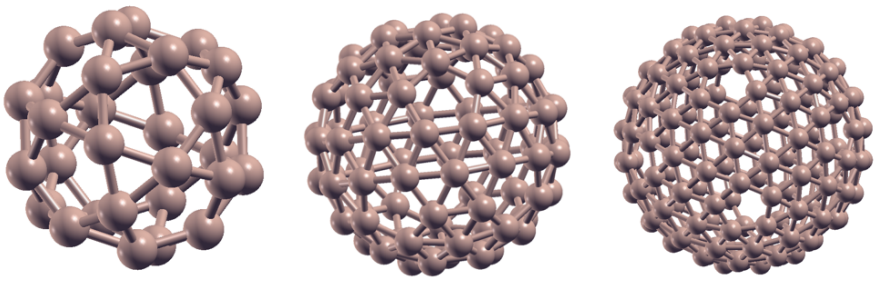

Figure 1: B_{30}, B_{80}, and B_{150} fullerene structures obtained via Goldberg-Coxeter $GC_{h,0}$ expansions ($h = 2, 3, 4$) of an icosahedron followed by the removal of 12 vertices.

References

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