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From Fullerenes to 2D Structures: A Unified Design Principle for Boron Nanostructures

Dr. Nevill Gonzalez Szwacki from the Faculty of Physics at the University of Warsaw has developed a groundbreaking model that explains the diversity of boron nanostructures—from hollow molecular clusters to ultrathin 2D layers. His research, published in the prestigious "2D Materials", shows that the key to the stability and electronic properties of these structures lies in the atomic coordination, the number of neighboring atoms. This discovery not only makes it possible to understand existing boron nanostructures, but also to predict and design new materials with desirable properties.

Boron, a chemical element next to carbon in the periodic table, is known for its unique ability to form complex bond networks. Unlike carbon, which typically bonds with two or three neighboring atoms, boron can share electrons among several atoms. This leads to a wide variety of nanostructures. These include boron fullerenes, which are hollow, cage-like molecules, and borophenes, ultra-thin metallic sheets of boron atoms arranged in triangular and hexagonal patterns.

Dr. Nevill Gonzalez Szwacki has developed a breakthrough model explaining the variety of boron nanostructures. The analysis presented in the article combines more than a dozen known boron nanostructures, including the experimentally observed B_{40} and B_{80} fullerenes. Using first-principles quantum-mechanical calculations, the study shows that the structural, energetic, and electronic properties of these systems can be predicted by looking at the proportions of atoms with four, five, or six bonds. The results reveal clear links between finite and extended boron structures. The B_{40} cage corresponds to the χ_3 borophene layer, while B_{65}, B_{80}, and B_{92} connect with the β_{12}, α, and *bt* borophene sheets, respectively. These structural links suggest that new boron cages could be created by using known two-dimensional boron templates.

This coordination-based approach not only brings together previously separate structural families but also explains general trends: higher atomic coordination usually leads to greater stability of boron nanostructures, while their electronic properties depend more on geometry and how the orbitals are arranged. For instance, some cages like B_{40} have large electronic gaps because of their compact and symmetrical shapes, while highly coordinated structures may be metallic or have smaller gaps. Therefore, the number of atomic connections serves as a unifying and predictive factor rather than a direct measure of electronic properties. "The concept presented here serves as a guide for designing new boron nanostructures with specific magnetic, electronic, or mechanical features. It may also support future

experiments using cluster-beam or surface-growth techniques," emphasizes Dr. Nevill Gonzalez Szwacki.

The publication by the University of Warsaw researcher demonstrates that boron remains an exceptionally versatile platform for creating tunable nanoscale materials, bridging the molecular and two-dimensional worlds.

Faculty of Physics at the University of Warsaw

Physics and astronomy at the University of Warsaw appeared in 1816 as part of the then Faculty of Philosophy. In 1825, the Astronomical Observatory was established. Currently, the Faculty of Physics at the University of Warsaw consists of the following institutes: Experimental Physics, Theoretical Physics, Geophysics, the Department of Mathematical Methods in Physics. The research covers almost all areas of modern physics on scales from quantum to cosmological. The Faculty's research and teaching staff consists of over 250 academic teachers. About 1350 students and over 150 doctoral students study at the Faculty of Physics UW. The University of Warsaw is among the 200 best universities in the world, educating in the field of physics according to Shanghai's Global Ranking of Academic Subjects.

SCIENTIFIC PUBLICATION:

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GRAPHIC MATERIALS:

FUW251208b_fot01
https://www.fuw.edu.pl/tl_files/press/images/2025/FUW251208b_fot01.png
Structural correspondence between boron fullerenes and 2D borophenes. The B_{40} cage relates to the χ_3 borophene layer, while B_{65} matches the β_{12} layer.

FUW251208b_fot02
https://www.fuw.edu.pl/tl_files/press/images/2025/FUW251208b_fot02.png
Energetic stability of boron fullerenes as a function of size and atomic coordination. Clusters B_{40}, B_{65}, and B_{80} bridge the world of finite structures and single layers of boron.

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