New semiconducting borophene paves the way for the lightest high-performance transistor

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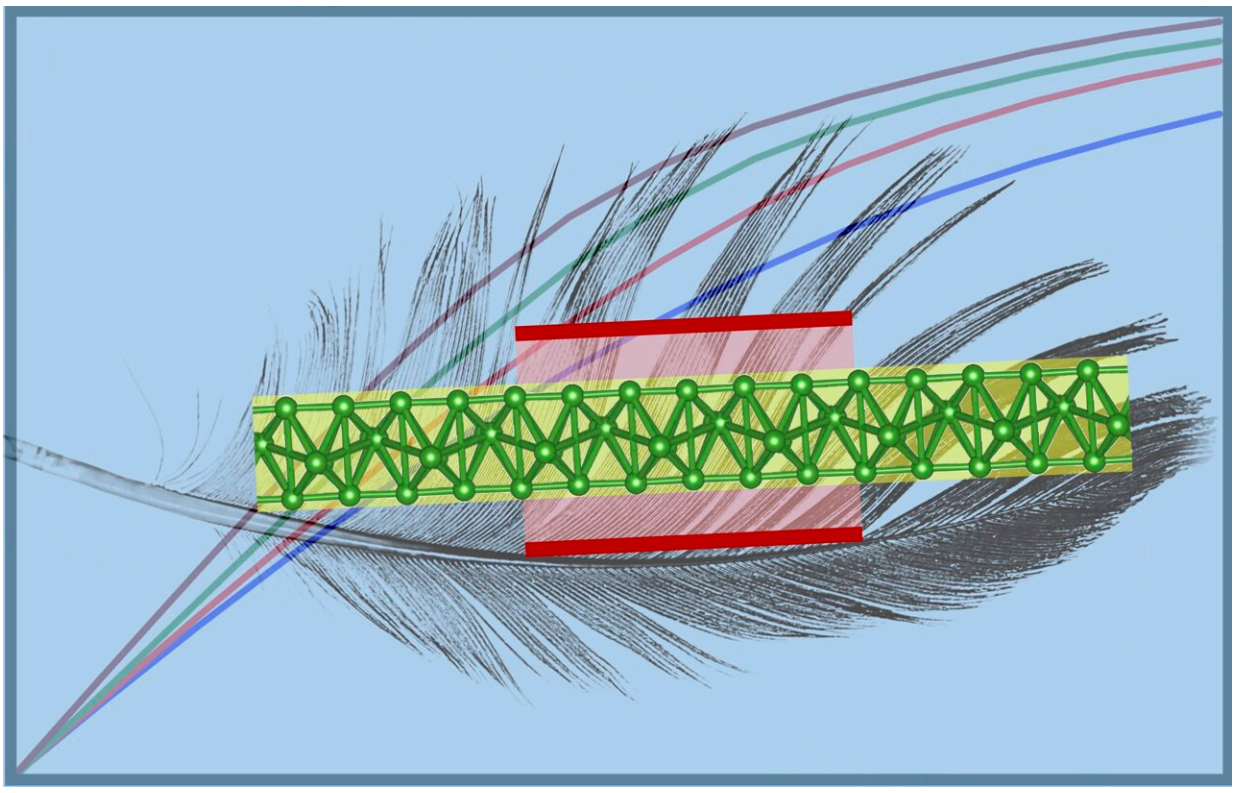

Credit: Santanu Mahapatra

In the year 1808, French chemists Joseph-Louis Gay-Lussac and Louis-Jacques Thenard, and independently, English chemist Humphry Davy, discovered the fifth element of the periodic table—boron. In crystalline

form, boron primarily possesses three polymorphs, i.e., three distinct unit cell configurations: α-rhombohedral, β-rhombohedral, and β-tetragonal, among 16 possible bulk allotropes.

The unique properties of this element have resulted in its use in numerous applications, including chemistry, materials science, life sciences, energy research and electronics. Moreover, based on studies conducted over the past decade, boron has significant potential for use in pharmaceutical drug design as it plays an essential role in bone growth and maintenance, wound healing, prevention of vitamin-D deficiency and other processes.

In the periodic table of elements, boron lies to the left of carbon, which causes boron to have similar valence orbitals but a shorter covalent radius. In contrast to carbon, which favors a 2D (two-dimensional) layered structure (aka graphite) in its bulk form, the bulk allotropes of boron are composed of B_{12} icosahedral cages. As a result, it was challenging to experimentally realize a 2D atomic network of boron, also known as borophene, until 2015.

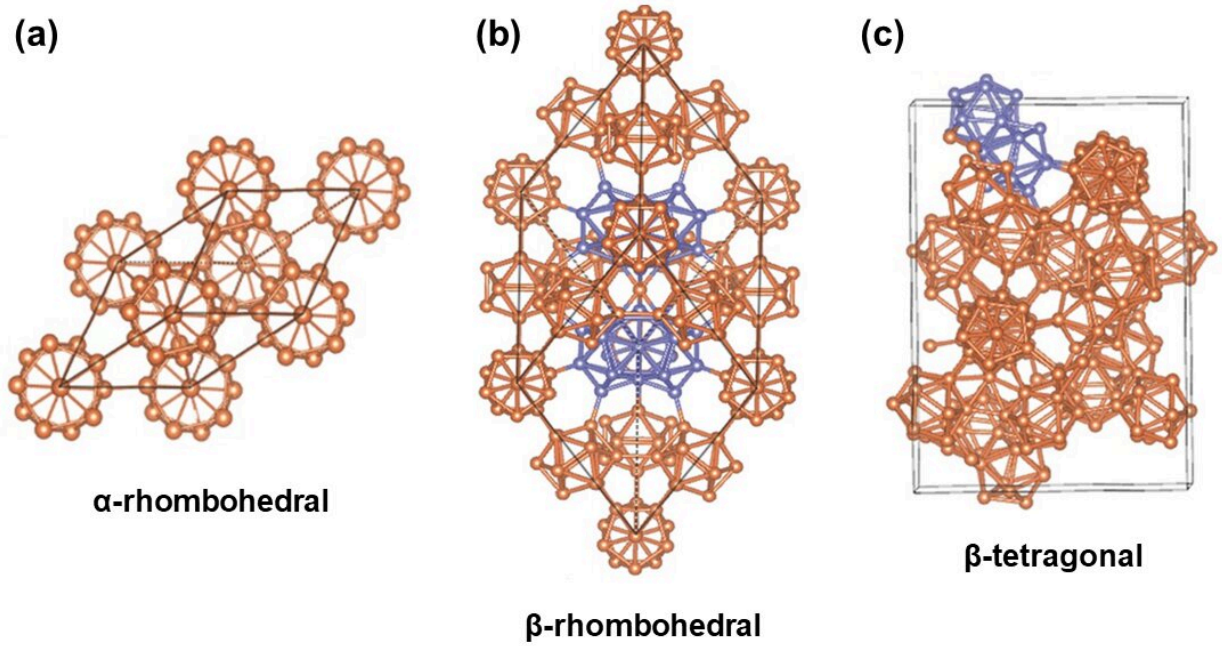

Figure 1: The structure of Boron allotropes: bulk polymorphs of (a) α-rhombohedral Boron, (b) β- rhombohedral Boron, and (c) β-tetragonal Boron. Credit: *Advanced Functional Materials* (2016). DOI: 10.1002/adfm.201603300

Initially, one of the underlying reasons for limited experimental investigations of 2D boron sheets was the use of costly and toxic precursors, e.g., diborane. Later, atomically thin borophene sheets were grown under ultrahigh-vacuum conditions using a solid boron atomic source of 99.9999% purity to circumvent the difficulties caused by poisonous precursors.

Recently, borophene has drawn tremendous attention for its ultralow molar mass. Unlike graphene, borophene comes with different polymorphs, such as striped, β_{12}, X_3, and honeycomb, and until now, all of them turned out to be metallic. However, bulk boron is semiconducting. Naturally, researchers want to explore the semiconducting 2D phase of boron.

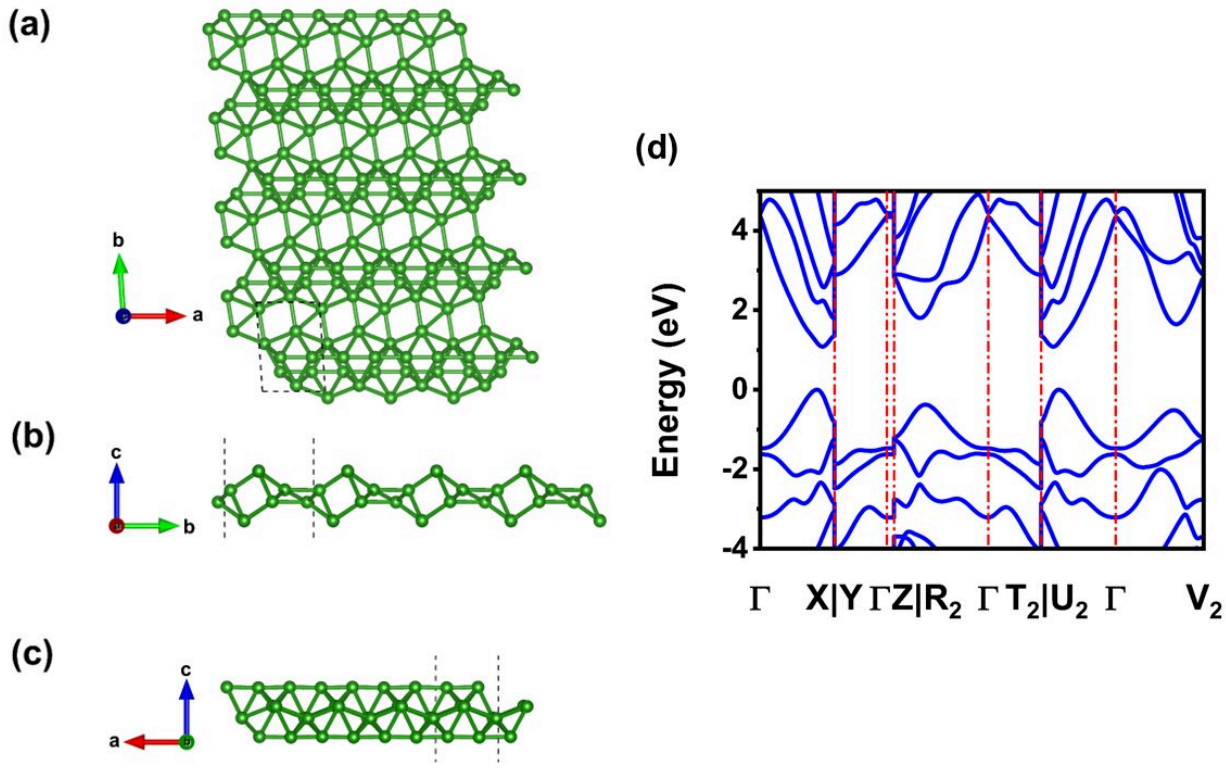

Figure 2: Structure and band dispersion of clustered-P1 borophene. (a) Top and (b, c) side views of CP1 borophene. (d) Electronic band dispersion. Credit: *ACS Applied Materials & Interfaces* (2023). DOI: 10.1021/acsami.2c20055

Semiconductors play a crucial role in the design of transistors and integrated circuits built with them. The use of silicon as a base semiconducting material in a transistor has revolutionized the electronics industry. With time, downscaling of transistor size has enabled engineers to pack millions of transistors in a unit area of silicon wafer.

However, researchers predict that the downscaling of silicon technology will reach its bottleneck within the next few years. Therefore, the semiconductor industry needs to explore 2D materials as an alternative

to silicon, as researchers declare that 2D materials may provide optimum electrostatic integrity for transistors.

After the discovery of graphene in 2004, a dozen 2D semiconductors (e.g., germanane, tellurene, phosphorene, etc.) have been investigated experimentally for transistor channel application. However, exploring 2D materials experimentally from their infinite space is unfeasible. Therefore, with the advancement in computational science and technology, the discovery of the relevant transistor material from the enormous 2D material space is in demand.

So far, the reported semiconducting phases of borophene exhibit small bandgaps, which make them inappropriate as transistor channel material. In our work, we have discovered a hyper-coordinated 2D network of boron atoms named clustered-P1 borophene. It shows a bulk silicon-like band gap, yet lower and symmetric effective masses along the transport direction.

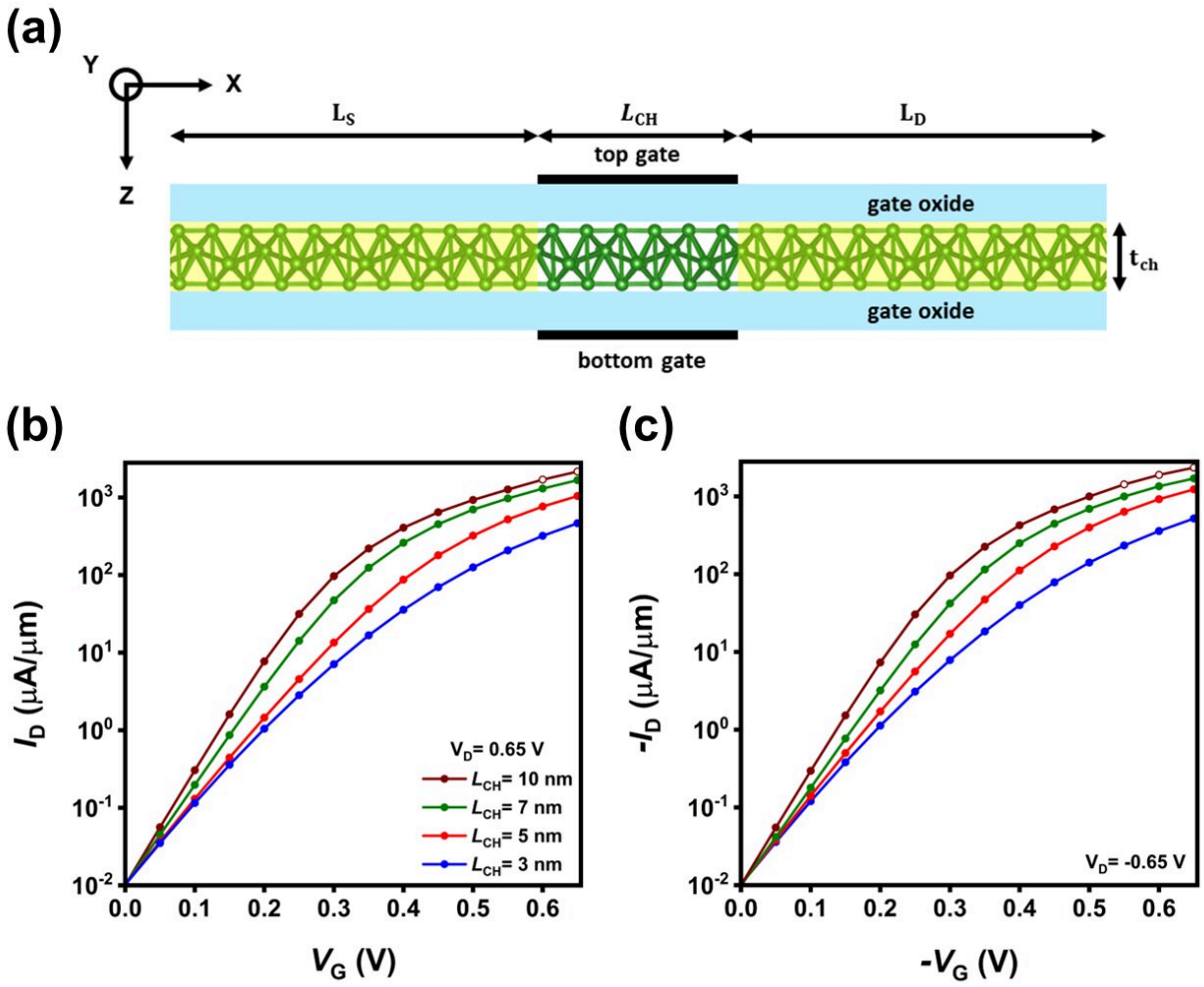

Figure 3: Device schematic and transfer characteristics. (a) Schematic of the cross-sectional (x-z plane) view of the simulated MOSFET. The channel is undoped, whereas the source and drain regions (shaded) are uniformly doped. Transfer characteristics (I_D-V_G) of (b) n-type and (c) p-type MOSFETs at a drain bias of |V_D |= 0.65 V for L_CH= 10 nm to 3 nm. Credit: *ACS Applied Materials & Interfaces* (2023). DOI: 10.1021/acsami.2c20055

In our recent work, which is published in *ACS Applied Materials and Interfaces* ("Discovery of Clustered-P1 borophene and Its Application as the Lightest High-Performance Transistor"), we begin the study with a

first-principles-based search of boron's 2D space, employing an evolutionary algorithm. It yields the exceptional semiconducting borophene phase, clustered-p1 borophene, that exhibits a total energy close to the global minimum of all borophene phases.

After that, we have predicted the performance characteristics of conventional MOSFETs (metal-oxide-semiconductor field-effect transistors) implemented with clustered-P1 borophene for 10-nm to 3-nm channel lengths. We have performed this work using an in-house, GPU-based, self-consistent quantum transport simulator. The performance of these MOSFETs has been found to meet the IRDS (international roadmap for devices and systems) requirements for several benchmark metrics.

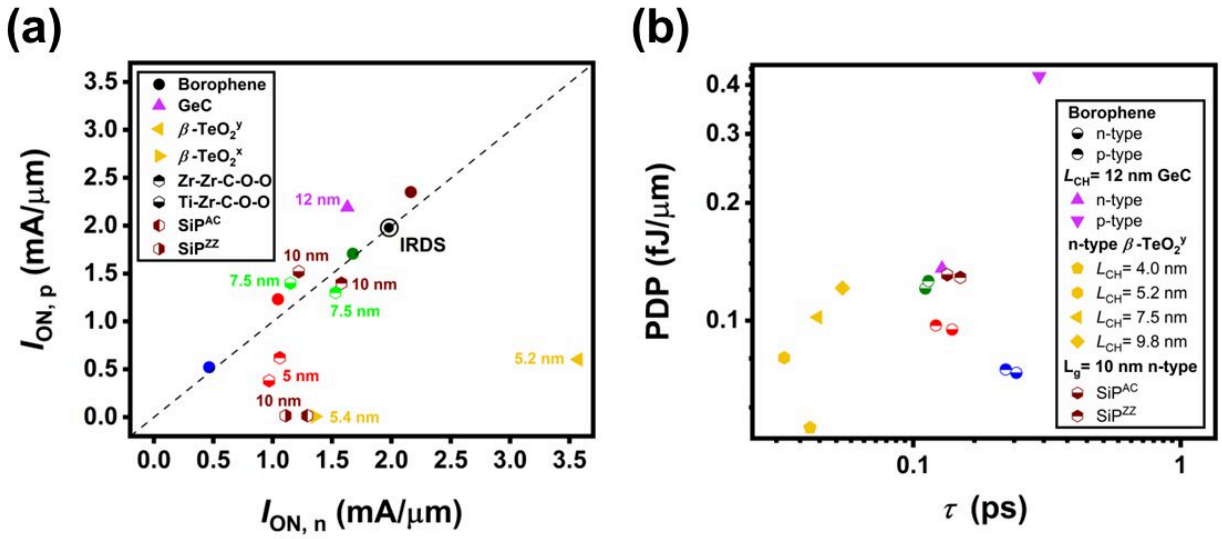

Figure 4: Performance evaluation of n- and p-type transistors. Performance is evaluated (a) in terms of ON-state current (I_ON), (b) in the PDP-τ plane against other reported 2D material-based transistors. Credit: *ACS Applied Materials & Interfaces* (2023). DOI: 10.1021/acsami.2c20055

The clustered-p1 borophene shows remarkable thermodynamic, structural, and dynamic stability. As shown in our work, it is noteworthy that even a transistor of 3-nm channel length can deliver 10^4 ON-to-OFF current ratio. On the other hand, the balanced-mode operation of n- and p-type MOSFETs makes it suitable for CMOS (complementary metal-oxide semiconductor) circuit performance. Keeping these beneficial outcomes in mind, we have predicted that the clustered-P1 borophene MOSFET may lead to a good option for possibly the lightest high-performance transistor.

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More information: Sirsha Guha et al, Discovery of Clustered-P1 Borophene and Its Application as the Lightest High-Performance Transistor, *ACS Applied Materials & Interfaces* (2023). DOI: 10.1021/acsami.2c20055

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