Scientists Reveal "Magic Boron Clusters" on Monolayer Borophene

Boron, a chemical element located adjacent to carbon in the periodic table, has one less electron than carbon. This electron deficiency results in its strong bonding ability and diverse boron polymorphs. Despite their variations, all boron polymorphs have B12 clusters as their building blocks, which possess an icosahedral cage structure. Nonetheless, research combining experimental and theoretical approaches has revealed that small boron clusters in the gas phase, such as B_n (n = 3 to 12, 36), are planar or quasi-planar. This feature has enabled the possibility of two-dimensional (2D) boron, also known as borophene. The unique properties of borophene, such as its mechanical flexibility, metallic Dirac fermions, and superconductivity, have generated significant experimental and theoretical interest.

The planar structure motifs of boron clusters benefit from the strong two-center-two-electron (2c–2e)σ bonds and multicenter-two-electron (nc–2e) bonds, which results in electron delocalization that enhances their chemical stability. Since the formation and arrangement of small boron clusters on a surface represent the initial stage of borophene growth, these clusters can serve as fundamental building blocks and play a crucial role in the formation of monolayer and bilayer borophenes. Moreover, the polymorphic nature of borophene suggests that the growth of boron clusters on metal surfaces can strongly influence the structure of borophene. However, previous experimental studies have mainly focused on small boron clusters in the gas phase, and only a few theoretical studies have investigated the evolution of boron clusters from small clusters to 2D sheets on surfaces. Recently, researchers from the Institute of Physics, Chinese Academy of Sciences, and the University of Science and Technology of China, including Chen Caiyun in Prof. CHEN Lan and Prof. WU Kehui's groups and LV Haifeng in Prof. WU Xiaojun's group, have revealed the formation of boron clusters with magic numbers on monolayer borophene and observed the evolution process from monolayer borophene with adsorbed boron clusters into bilayer borophene.

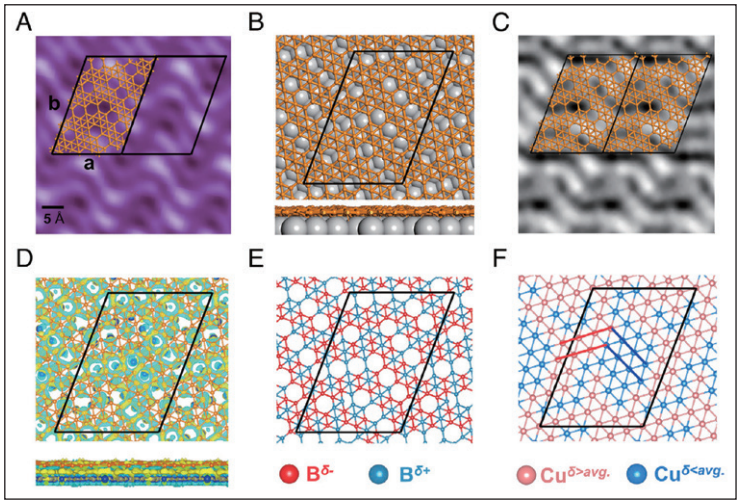

Figure 1: The STM characterization, structural motifs, simulated STM image and charge redistribution of monolayer borophene on Cu(111). (Image by Institute of Physics)

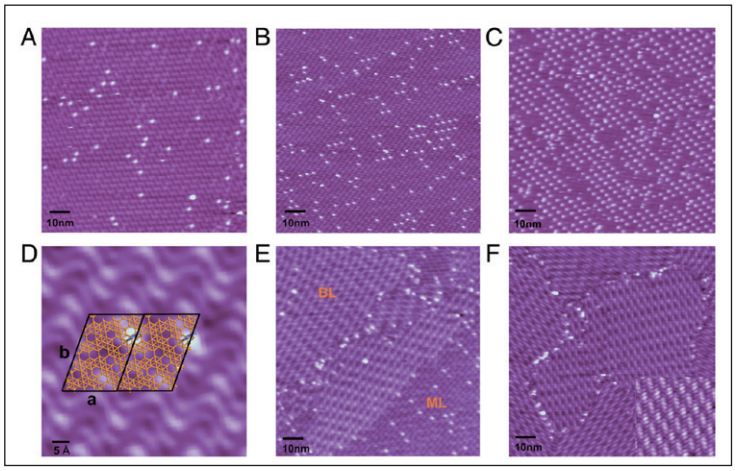

Figure 2: The STM characterization of boron clusters on monolayer borophene and their evolution to bilayer borophene. (Image by Institute of Physics)

Through their research, the scientists discovered that by evaporating boron on a Cu(111) surface

covered with a monolayer of borophene, they could create boron clusters with a unique size distribution. Each boron cluster selectively binds to specific sites in each unit cell of the monolayer borophene, resulting in periodic arrangements. Density functional theory (DFT) calculations identified the chemically adsorbed boron clusters as B_5 clusters, and the formation and arrangement of these clusters on the surface were found to be the result of the in-plane charge distribution and electron delocalization in the monolayer borophene. Additionally, the close-packed adsorption of B_5 clusters on the monolayer borophene was observed to result in the spontaneous transformation into bilayer borophene.

This study entitled "*Selective binding and periodic arrangement of magic boron clusters on monolayer borophene*" was published in *Proceedings of the National Academy of Sciences* (*PNAS*).

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Contact:
Dr. CHEN Lan
Institute of Physics, CAS
Email: lchen@iphy.ac.cn

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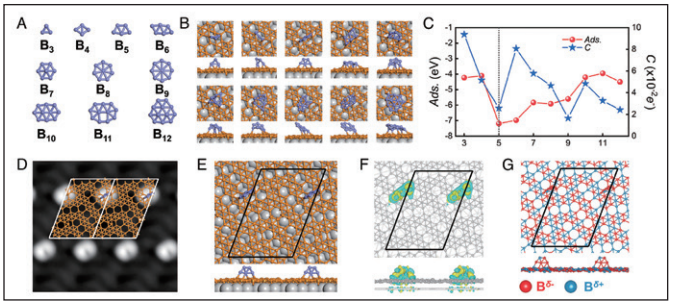

Figure 3: The structures of boron clusters (B_n), calculated structural motifs of monolayer borophene with adsorbed B_n, simulated STM image and the charge redistribution. (Image by Institute of Physics)

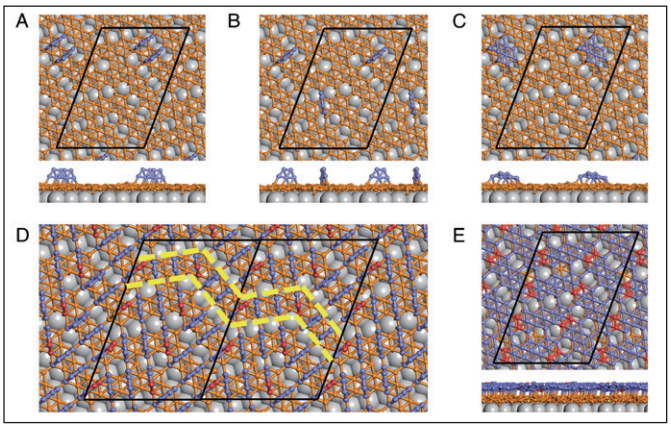

Figure 4: The close-packed adsorption of B_5 clusters on monolayer borophene and their transformation to bilayer borophene. (Image by Institute of Physics)