Electronic Supporting Information

Exfoliation of boron carbide into ultrathin nanosheets

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1. Computationally Relaxed Structures

The images in this section show computationally relaxed structures of B_4C cleaved along different planes but terminated at different heights. The surfaces have been allowed to relax, and different rearrangements or reconstructions of the atoms are seen. In all these images, the boron atoms are green while the carbon atoms are red.

1.1. (001) plane



Figure S1: Relaxed structures for different terminations for cleavage along the (001) plane.

1.2. (101) plane



Figure S2: Relaxed structures for different terminations for cleavage along the (101) plane.

1.3. (012) plane



Figure S3: Relaxed structures for different terminations for cleavage along the (012) plane.

2. Additional Raman spectra



Figure S4. Example of B_4C flakes with different intensity ratios between the 481 and 533 cm⁻¹ peaks. (a) Optical microscope image of two B_4C nanosheets produced by tip sonication in IPA for 2 hours, and then spin coated three times at 3,000 rpm on a sapphire substrate, and then annealed at 500°C for 5 h. (b) Raman spectra of flakes A and B labeled in panel (a), compared to the spectrum of bulk B_4C powder. Flake A shows no carbon peaks (in the range ~1300 to ~1600 cm⁻¹), and the intensity ratio (I_{481} / I_{533}) is close to 1. Flake B shows prominent carbon peaks and the I_{481} / I_{533} ratio is close to 2. Other characteristic B_4C peaks are seen in both Flakes A and B. The I_{481} / I_{533} ratio is also close to 2 in the bulk B_4C powder.



Figure S5. Each trace shows the change in the ratio of the area of the D band at 1350 cm⁻¹ and the area of the B_4C peak at 1080 cm⁻¹ for an individual B_4C nanosheet as a function of laser irradiation time. Panels (a)-(d) show the four types of time evolution as described in the main text. There are 50 total B_4C nanosheets shown.

3. Stability of B₄C nanosheets



Figure S6. Comparison of Raman spectra for LPE-produced B_4C flakes under different conditions/environments. The main peaks from B_4C are labelled with numbers indicating their wavenumber positions and are also indicated by the vertical dashed lines. The boric acid peaks are marked with *.