

Correction

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Correction for “Ultrasensitive gas detection of large-area boron-doped graphene,” by Ruitao Lv, Gugang Chen, Qing Li, Amber McCreary, Andrés Botello-Méndez, S. V. Morozov, Liangbo Liang, Xavier Declerck, Nestor Perea-López, David A. Cullen, Simin Feng, Ana Laura Elías, Rodolfo Cruz-Silva, Kazunori Fujisawa, Morinobu Endo, Feiyu Kang, Jean-Christophe Charlier, Vincent Meunier, Minghu Pan, Avetik R. Harutyunyan, Konstantin S. Novoselov, and Mauricio Terrones, which appeared in issue 47, November 24, 2015, of *Proc Natl Acad Sci USA* (112:14527–14532; first published November 2, 2015; 10.1073/pnas.1505993112).

The authors note that, due to a printer’s error, the legend for Fig. 3 appeared incorrectly. Specifically, “Two-dimensional peak” should instead appear as “2D peak.” The figure and its corrected legend appear below.

The authors also note that, due to a printer’s error, on page 14530, right column, first full paragraph, lines 18–19, “to reach detection limits of 95 and 60 ppb” should instead appear as “to reach detection limits of 95 ppt and 60 ppb.”

The authors also note that on page 14530, left column, first paragraph, line 1, “Figs. 2C and 3D” should instead appear as “Fig. 2 C and D.”

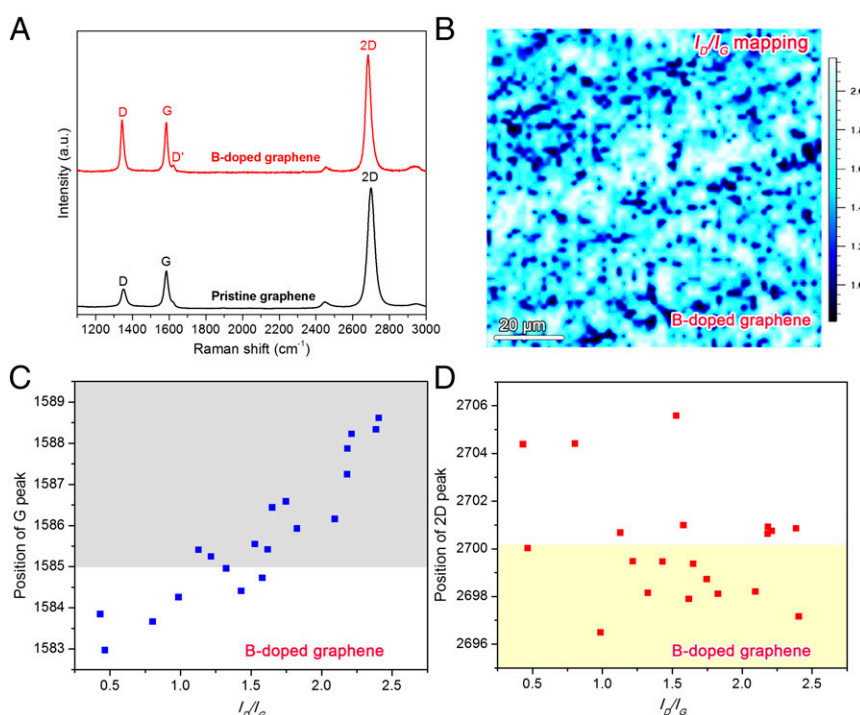


Fig. 3. Raman analysis of as-transferred BG sheets on SiO₂/Si substrate. (A) Typical Raman spectra of PG (nondoped) and BG sheets. The Raman laser line is 514 nm. (B) D-peak over G-peak intensity ratio (I_D/I_G) mapping of BG. (C) Position distributions of G peak and (D) 2D peak with the corresponding I_D/I_G ratios of BG sheets.

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Ultrasensitive gas detection of large-area boron-doped graphene

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Heteroatom doping is an efficient way to modify the chemical and electronic properties of graphene. In particular, boron doping is expected to induce a *p*-type (boron)-conducting behavior to pristine (non-doped) graphene, which could lead to diverse applications. However, the experimental progress on atomic scale visualization and sensing properties of large-area boron-doped graphene (BG) sheets is still very scarce. This work describes the controlled growth of centimeter size, high-crystallinity BG sheets. Scanning tunneling microscopy and spectroscopy are used to visualize the atomic structure and the local density of states around boron dopants. It is confirmed that BG behaves as a *p*-type conductor and a unique croissant-like feature is frequently observed within the BG lattice, which is caused by the presence of boron-carbon trimers embedded within the hexagonal lattice. More interestingly, it is demonstrated for the first time that BG exhibits unique sensing capabilities when detecting toxic gases, such as NO₂ and NH₃, being able to detect extremely low concentrations (e.g., parts per trillion, parts per billion). This work envisions that other attractive applications could now be explored based on as-synthesized BG.

graphene | boron-doped | STM | gas sensor | B-C trimers

Graphene is a fascinating material that has created an unprecedented impact in condensed-matter physics, chemistry, materials science, and industry (1–6). According to theory, the valence and conduction bands of pristine (nondoped) graphene (PG) touch at the *K* point in the Brillouin zone, thus making it behave as a zero-overlap semimetal (7). This lack of band gap limits graphene applications in some areas including semiconductor electronics. Therefore, it is crucial to tailor the electronic properties of graphene and eventually be able to open an electronic band gap. Doping, especially chemical doping, constitutes an efficient way to modify the electronic, chemical, and magnetic properties of materials. Recently, exciting progress has been achieved regarding graphene chemical doping, and more detailed information can be found in the literature (8, 9). Among different dopants, the two most adjacent neighbors of carbon in the periodic table of the elements (i.e., B and N) have attracted the attention of numerous scientists because of their similar atomic sizes with C and potential to induce *p*-type (boron) and *n*-type (nitrogen) conduction in graphene. In particular, the synthesis of N-doped graphene (NG) (10–14), as well as its atomic scale characterization (15–18) and possible applications (19–21), have been well explored. However, experimental progress on boron-doped graphene (BG) (22–27) is still very scarce compared with that on NG. Actually, theoretical work on BG has been extensively carried out to demonstrate the properties of BG and its possible applications, including field-effect transistors

(FETs) (28), hydrogen storage (29), and Li-ion batteries (LIBs) (30). In particular, density functional theory (DFT) calculations predicted that FETs fabricated with BG could exhibit high ON/OFF ratios and low subthreshold swings (28). Moreover, B atoms embedded within the graphene lattice can lead to improved hydrogen storage capacity by decreasing the H₂ adsorption energy dramatically (29). Compared with PG, more Li ions could be captured around boron-doping sites in BG because of the formation of an electron-deficient structure. In this context, Yakobson et al. have demonstrated that the substitutional doping of boron in graphene could lead to much improved Li storage performance with small volume variation during discharge/charge cycles and a capacity of 857 mAh/g (as Li_{1.5}C₃B), which is two times higher than that of graphite (372 mAh/g) (30). Besides that, it has been theoretically demonstrated that BG could break the symmetry of spin-up and spin-down transmittance channel, thus leading to a metallic-to-semiconductor transition. In this sense, it is believed that BG

Significance

The gas-sensing performance of graphene could be remarkably enhanced by incorporating dopants into its lattice based on theoretical calculations. However, to date, experimental progress on boron-doped graphene (BG) is still very scarce. Here, we achieved the controlled growth of large-area, high-crystallinity BG sheets and shed light on their electronic features associated with boron dopants at the atomic scale. As a proof-of-concept, it is demonstrated that boron doping in graphene could lead to a much enhanced sensitivity when detecting toxic gases (e.g. NO₂). Our results will open up new avenues for developing high-performance sensors able to detect trace amount of molecules. In addition, other new fascinating properties can be exploited based on as-synthesized large-area BG sheets.

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The authors declare no conflict of interest.

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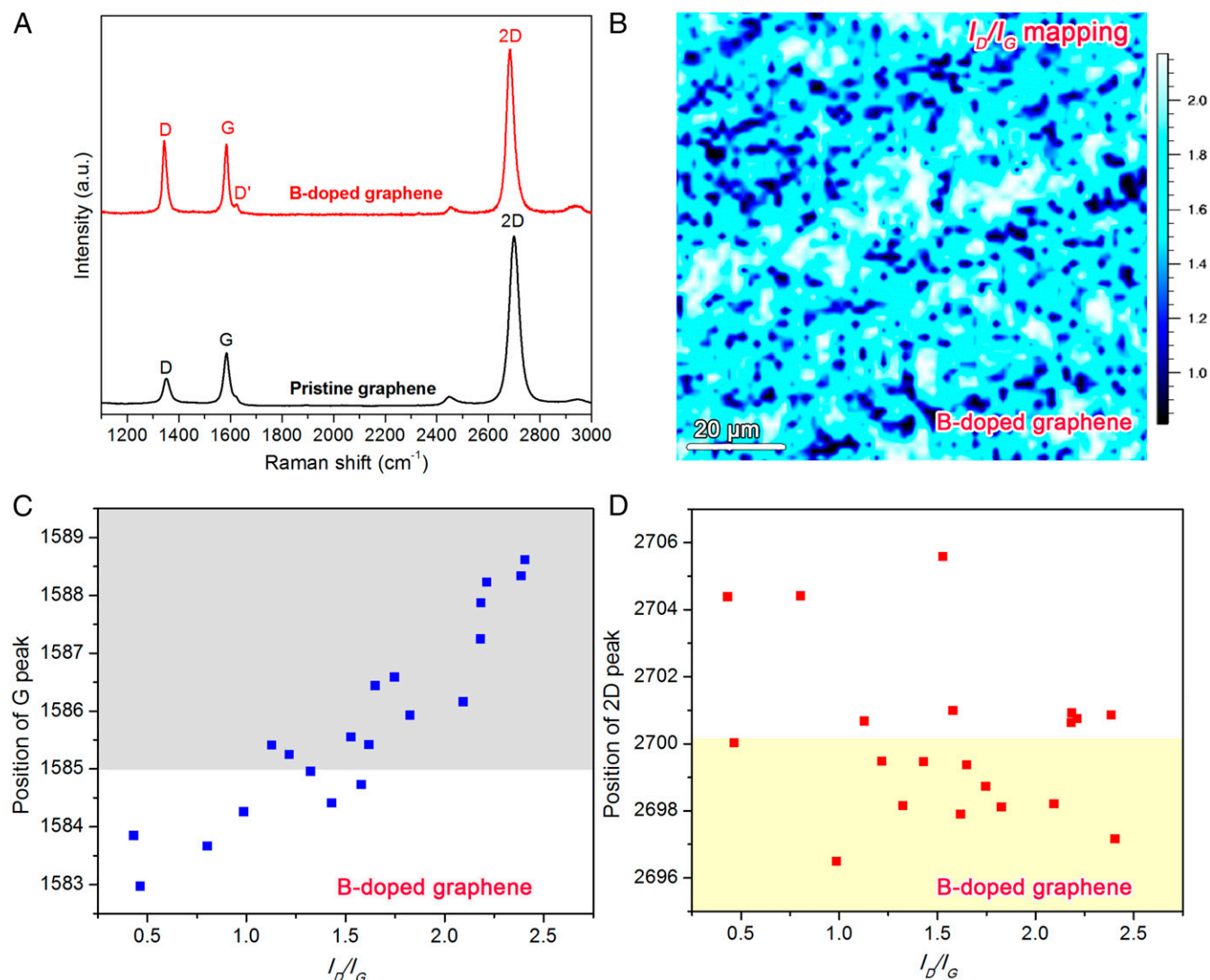


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scanning transmission electron microscope (STEM) image of as-synthesized BG sheets. The monolayer region is shown in green. Based on both STEM and AFM measurements, it can be confirmed that the synthetic strategy can remarkably promote the growth of monolayer BG sheets. Furthermore, the size of as-synthesized BG is just determined by that of the Cu foil substrates considering the conformal coverage of BG. In addition, the aberration-corrected STEM image (Fig. 1C) and selected-area electron diffraction (SAED) pattern (Fig. 1D) of BG sheets clearly display the hexagonal lattice of graphene. The grain sizes of PG and as-synthesized BG sheets were analyzed by dark-field transmission electron microscopy (DF-TEM) observation, as shown in [SI Appendix, Figs. S5–S7](#). DF-TEM images revealed that both PG and BG are composed of grains ranging from ~ 100 nm to over $1\text{ }\mu\text{m}$ ([SI Appendix, Figs. S5 and S6](#)). According to low-magnification DF-TEM image from BG ([SI Appendix, Fig. S7](#)), $\sim 7\text{ }\mu\text{m}$ of large domain was observed. X-ray photoelectron spectroscopy (XPS) and STM/STS studies were performed to confirm the presence of B and to clearly identify B atoms within the lattice (see below). The XPS survey scan of freshly synthesized BG samples on copper foil substrates is shown in [SI Appendix, Fig. S8A](#). The B-doping level in the as-synthesized BG sample is ~ 1.75 atomic % (more details can be found in the [SI Appendix](#)). The C1s fine-scan results of BG and PG sample are

shown in *SI Appendix, Fig. S8 B and C*, respectively. No obvious difference of C1s spectra can be found in these two samples, except for a small increase in the full-width at half maximum (FWHM) of the peaks. However, from the B1s spectra shown Fig. 1E, one can clearly see the difference between BG and PG samples. In the case of PG, no B signal in the B1s line scans can be detected (Fig. 1E). For BG, two prominent peaks located at approximately 186.4 and 190.3 eV are identified in the B1s line scans (Fig. 1E), which could be assigned to the substitutional boron atoms embedded within the graphene lattice and edge oxidized boron, respectively (36, 37).

The electronic and chemical properties of doped graphene highly depend on the atomic details of how the foreign atoms incorporate into the honeycomb lattice. Indeed, for the case of nitrogen-doped graphene, the local electronic properties can change dramatically depending on how nitrogen binds to the host crystal (18). Therefore, atomic characterization is mandatory. Fig. 2A illustrates the characteristic STM topography of the synthesized BG samples. The peculiar feature detailed in Fig. 2B is consistently observed throughout the sample. Considering the length scale and its symmetry, it is inferred that the defect should be more complex than a simple B substitution. *Ab initio* STM simulations provide several candidates with the same symmetry (*SI Appendix, Fig. S9*); however, to unambiguously identify the defect, a comparison of

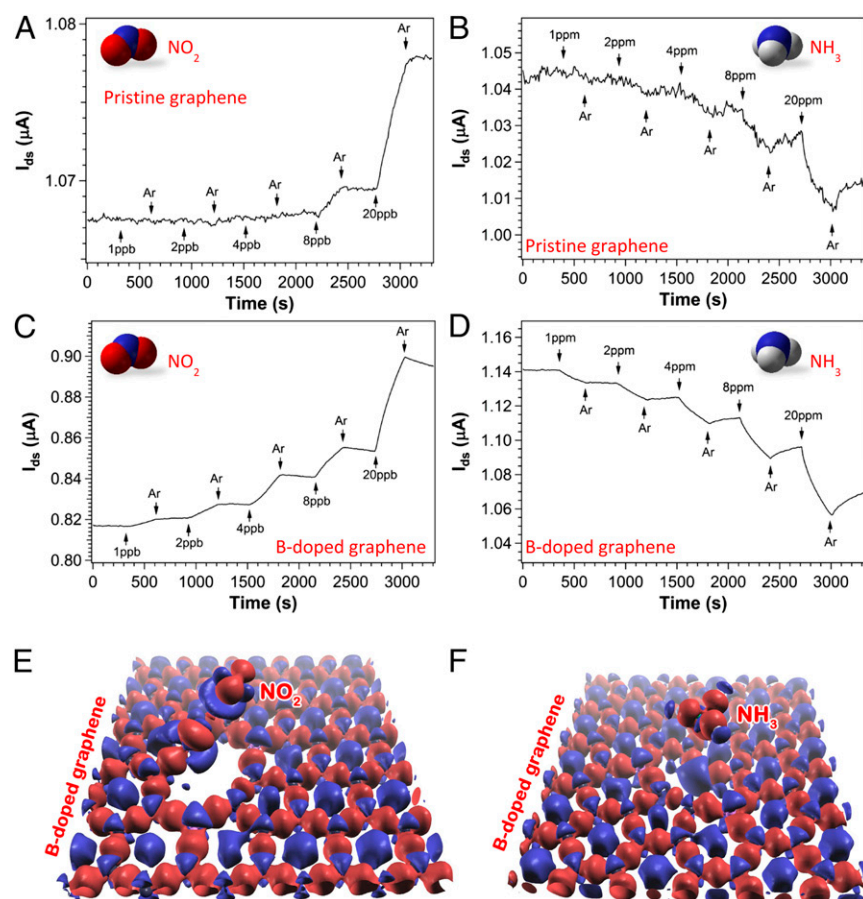


Fig. 4. Comparison of sensor response between PG (nondoped) and BG sheets. (A and B) Sensor response of PG sheets versus time recorded with the sensor exposed to NO_2 (A) and NH_3 (B). (C and D) Corresponding gas sensing on BG sheets when the sensor was exposed to NO_2 (C) and NH_3 (D). All experiments were carried out under in situ UV light illumination. Successive experiments were done after the device had been recovered. E and F demonstrate the difference of charge density with respect to the isolated atoms for the B_3 -doped graphene with NO_2 and NH_3 molecules, respectively.

the STS should also be carried out. Figs. 2C and 3D exhibit the simulated STM and STS of the candidate that best matches the experimental observations. The effect of phonon-assisted tunneling (PAT) has been included in the simulation of the STS (38). The feature at -0.42 eV is consistent with the experimental STS measurement depicted in Fig. 2E. Therefore, although the comparison is not perfect, the defect is attributed to the geometry shown in Fig. 2C. The discrepancies might arise from the Tersoff–Hamann approximation (i.e., the effect of the shape of the tip might be more important than expected) and from interaction with the substrate.

Raman spectroscopy is a powerful technique for characterizing doping in graphene-like materials. The typical Raman spectra of as-synthesized BG and PG are shown in Fig. 3A. An enhanced D-band and a prominent D'-band can be observed in BG compared with bands characteristic of PG. It is well known that the D-band of graphene is caused by the breathing modes of six-atom rings and a defect is necessary for its activation. The D'-band could be attributed to a double resonance occurring by an intravalley process (39). The D-peak intensity (I_D) over the G-peak intensity (I_G) mapping is shown in Fig. 3B. The significant intensity of the D-band in BG could be attributed to the presence of defects caused by in-plane doping of B atoms embedded within the graphene hexagonal lattice. Furthermore, B doping will modify the Fermi surface of graphene and lead to a shift of the Raman peak positions. Previous work has demonstrated that the G-band will upshift for both hole and electron doping. In this study, B is expected to induce hole doping in graphene and a dominant upshift can be seen in the G-band of BG (Fig. 3C), which is in agreement with the hole doping by applying a gate voltage (40). However, the 2D band (also known as G'-band) responds differently to holes and electron doping. In previous work on NG, a remarkable downshift (7 cm^{-1}) was reported in NG compared with that of PG (18). For BG, dominant downshifts and some upshifts can be monitored, as shown in Fig. 3D. Another obvious difference

between BG and PG is the I_{2D}/I_G ratio. From Fig. 3A, the I_{2D}/I_G ratio of BG is lower than that of PG. From the mapping results shown in *SI Appendix*, Fig. S10, some parts of the BG sheets show I_{2D}/I_G ratio less than 2 (see dark blue parts in *SI Appendix*, Fig. S10). This is in agreement with the AFM studies which demonstrated that some multilayer regions coexist with monolayer graphene in BG samples.

To investigate the effect of B doping on graphene's gas sensitivity, comparative studies on NO_2 and NH_3 under similar detection environment were carried out. It is known that the interaction between adsorbed molecules and graphene will alter the electronic structure of graphenes as reflected by the change of current. The sensing experiments were carried out at a fixed drain to source voltage (V_{ds}) of 10- and 1-mV under continuous in situ UV light illumination for BG and PG sensors, respectively. The results are shown in Fig. 4A–D. For NO_2 detection, PG cannot detect any obvious signal until the NO_2 concentration reaches 8 ppb, where a signal-to-noise ratio (s/n) of 9.4 is registered. In comparison, a clean signal with s/n = 31.5 at 1 ppb of NO_2 exposure to BG was observed. The same kind of improvement has been observed for NH_3 detection (e.g., PG can detect 20 ppm of NH_3 with s/n = 9.5, whereas B-doped graphene can easily sense 1 ppm with s/n = 50.1). Assuming a linear extrapolation, the sensitivity can be defined as the signal-to-noise ratio divided by gas concentration at the lowest tested concentration, such that B doping of graphene has enhanced its sensitivity 27 and 105 times to reach detection limits of 95 and 60 ppb (s/n = 3), respectively, for NO_2 and NH_3 detections.

Compared with typical sensing performance of graphene-based devices reported in the literature (Table 1), the CVD grown graphene sensors presented here, both with and without B doping, have very high sensitivities. Note that the current experiments were performed under continuous in situ UV light illumination. As reported previously (41, 42), UV light induced molecular desorption that dynamically keeps the sensor surface fresh, and UV light is believed to contribute to the overall sensor performance. Because PG and

minimize experimental errors, gas dilution was restricted to a simple one-step mixing of carrier and analyte gases controlled by two digital mass flow controllers (MFCs) (model no. 5850S; Brooks). Both MFCs were calibrated using a multipoint calibration curve with gas measurement equipment (DHI) accurate to 0.01 mL/min. The flow accuracy of these MFCs is $\pm 0.7\%$ of flow rate and $\pm 0.2\%$ of full scale. Based on these specifications and the gas flow rates used, the gas concentration error after dilution is estimated to be no more than 20% for the detection range used in this study. Two electrical contacts (Au/Ti with thicknesses of 120 nm/30 nm) were applied on top of the graphene through vacuum thermal deposition. Gas sensing measurements were done on a customized flowing cell that has electrical feedthrough connections for temperature and electrical measurements. The current was monitored with a Keithley 4200-SCS instrument at atmospheric pressure and a fixed room temperature of 25 °C through a temperature controller equipped with automatic heating and cooling assemblies. In situ UV light ($\lambda = 253.7$ nm and I of ~ 1.7 mW/cm²) was applied through a quartz window onto the device for all gas detection experiments.

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