SCIENTIFIC REPORTS

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Corrigendum: Hinge-like structure induced unusual properties of black phosphorus and new strategies to improve the thermoelectric performance

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Scientific Reports **4**:6946; doi: 10.1038/srep06946; published online 06 November 2014; updated on 04 March 2016

This Article contains errors in the insets of Figures 3(a), 3(b) and 3(c), where the stress values were incorrectly given as three times smaller than the correct GPa values. The correct Figure 3 appears below as Figure 1.

As such, in the Results section, under subheading 'Strain modulated electronic structure.' :

"The Young's modulus along x, y and z directions can be evaluated to be 49.89 GPa, 15.11 GPa and 15.68 GPa based on the slopes of the stress-strain curves plotted in the insets of Fig. 3, revealing that BP is indeed much harder in x direction than in y or z direction."

should read:

"The Young's modulus along x, y and z directions can be evaluated to be 149.7 GPa, 45.3 GPa and 47.0 GPa based on the slopes of the stress-strain curves plotted in the insets of Fig. 3, revealing that BP is indeed much harder in x direction than in y or z direction."

"If the compressive strain is large enough, i.e., about −10% (corresponding to an external pressure 7.67 GPa) or more, the gap vanishes and BP turns into a metal. With increasing the strain, the direct band gap goes to a maximum (about 0.6 eV) at 8% (corresponding to the tensile strength 2.63 GPa), and then the band gap becomes indirect and declines quickly."

should read:

"If the compressive strain is large enough, i.e., about −10% (corresponding to an external pressure 23.01 GPa) or more, the gap vanishes and BP turns into a metal. With increasing the strain, the direct band gap goes to a maximum (about 0.6 eV) at 8% (corresponding to the tensile strength 7.89 GPa), and then the band gap becomes indirect and declines quickly."

"The metal-semiconductor transition occurs at −5% strain (0.77 GPa external pressure), and the direct-indirect critical point is at 3% strain (0.44 GPa tensile strength), which are nearly one order of magnitude lower than the pressure needed for the strain along the *x* direction for such a transition."

should read:

"The metal-semiconductor transition occurs at −5% strain (2.31 GPa external pressure), and the direct-indirect critical point is at 3% strain (1.32 GPa tensile strength), which are nearly one order of magnitude lower than the pressure needed for the strain along the *x* direction for such a transition."

"A tensile strain does not turn the band gap of BP from direct into indirect within the range we considered (less than 10%), but makes the band gap increase linearly as the strain increases from 1% to 10%, while a small compressive strain (−3%, 0.58 GPa) turns the band gap from direct to indirect. "When the compressive strain reaches −7% (1.7 GPa), the band gap becomes zero and BP turns into a metal. It is interesting to note that Narita *et al.*[28,29] have observed experimentally a semiconducting to metallic transition of BP without phase change at the pressure around 1.70 GPa from the resistivity-pressure measurements. Our calculated results are nicely consistent with this experimental observation."

should read:

"A tensile strain does not turn the band gap of BP from direct into indirect within the range we considered (less than 10%), but makes the band gap increase linearly as the strain increases from 1% to 10%, while a small compressive strain (−3%, 1.74 GPa) turns the band gap from direct to indirect. When the compressive strain reaches −7% (5.1 GPa), the band gap becomes zero and BP turns into a metal. It is interesting to note that Morita *et al.*[28,29] have observed experimentally a semiconducting to metallic transition of BP without phase change at the pressure around 1.70 GPa along the puckered direction (the y direction here) from the resistivity pressure measurements. From Fig. 3 (b), the semiconducting to metallic transition arise around 4%–5% compressive strain (corresponding to 1.7–2.3 GPa) along y direction. Thus our calculated results are consistent with experimental observation."

In the Discussion section,

"This is confirmed by the anisotropic Young's modulus along the *x* (49.89 GPa) and *y* (15.11 GPa) directions obtained by the DFT calculations. It is interesting to find that the Young's modulus along the *y* direction is very close to that along the *z* direction (15.68 GPa)."

should read:

"This is confirmed by the anisotropic Young's modulus along the *x* (149.7 GPa) and *y* (45.3 GPa) directions obtained by the DFT calculations. It is interesting to find that the Young's modulus along the *y* direction is very close to that along the *z* direction (47.0 GPa)."

"The compressive pressure needed for the metal-semiconductor transition in BP is 7.67 GPa (*x* direction), 0.77 GPa (*y* direction), and 1.70 GPa (*z* direction)."

should read:

"The compressive pressure needed for the metal-semiconductor transition in BP is 23.0 GPa (*x* direction), 2.3 GPa (*y* direction), and 5.1 GPa (*z* direction)."

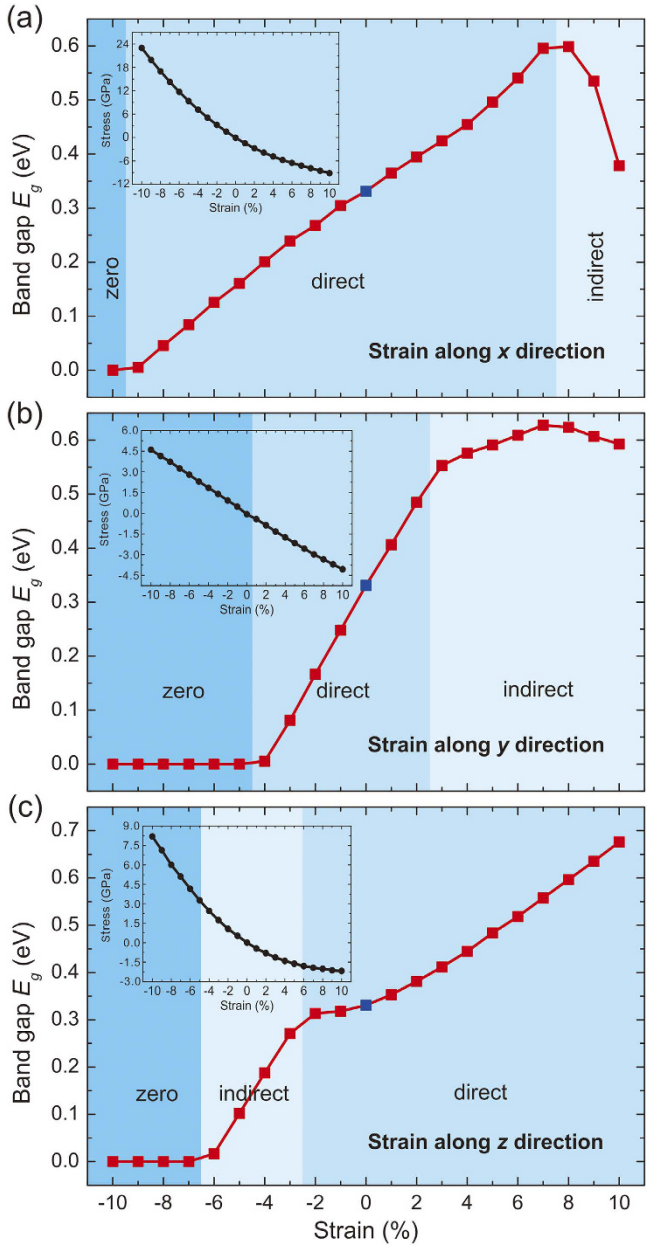

Figure 1.