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Correction: First-principles prediction on bismuthylene monolayer as a promising quantum spin Hall insulator

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Correction for 'First-principles prediction on bismuthylene monolayer as a promising quantum spin Hall insulator' by Run-Wu Zhang, *et al.*, *Nanoscale*, 2017, **9**, 8207–8212.

The authors wish to make the following amendments to the manuscript text.

In this paper, we discuss in Fig. 1d the total energy differences of bismuthylene with respect to buckled Bi (111) and *f*-Bi films. However, in our recent further research, we realized after accurate calculations that the total energy of our optimized buckled Bi(111) contained a certain error. It has been found that the buckled Bi(111) bilayer has an 89 meV lower energy than bismuthylene, as shown in the revised Fig. 1d.

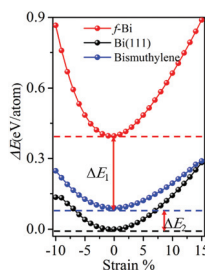


Fig. 1d Total potential energy of flattened Bi and buckled Bi (111) with respect to bismuthylene under in-plane strain, $\Delta E_1 = 307$ meV per atom and $\Delta E_2 = 89$ meV per atom.

Furthermore, the authors have also revised the corresponding descriptions in the manuscript.

In the abstract the sentences beginning “Analysis of the electronic structures reveal that bismuthylene is a native QSH state with a band gap as large as 0.28 eV at the Γ point, which is larger than that (0.2 eV) of the buckled Bi (111) and suitable for room temperature applications. Note that it has a much lower energy than buckled Bi (111) and flattened Bi films...” should be revised as “Analysis of the electronic structures reveals that bismuthylene is a native QSH state with a band gap as large as 0.28 eV at the Γ point, which is smaller than that (0.50 eV) of the buckled Bi (111) and suitable for room temperature applications. Notably, it has a much lower energy than flattened Bi and a higher energy than buckled Bi (111)...”

In the fourth paragraph the sentence beginning “Note that it is more stable than buckled Bi (111) and flattened Bi films...” should be revised as “Note that it is more stable than flattened Bi film”;

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In the sixth paragraph the sentence ending "...and the energy difference is 199 meV (ΔE_1) and 45 meV (ΔE_2) for buckled Bi (111) and *f*-Bi, respectively." should be revised as "...and the energy difference is 307 meV (ΔE_1) and -89 meV (ΔE_2) for *f*-Bi and buckled Bi (111), respectively."

In the eleventh paragraph the sentence beginning "Unexpectedly, it has a much lower energy than buckled Bi (111) and *f*-Bi films..." should be revised as "Unexpectedly, it has a much lower energy than the *f*-Bi film. Furthermore, F. Reis *et al.*³² have also reported the new high-temperature QSH paradigm on bismuthylene under a SiC(0001) substrate in their experiments. These findings provide good guidance for realizing bismuthylene in future experiments."

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

