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Correction: Energetics, barriers and vibrational spectra of partially and fully hydrogenated hexagonal boron nitride

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Correction for 'Energetics, barriers and vibrational spectra of partially and fully hydrogenated hexagonal boron nitride' by J. M. H. Kroes *et al.*, *Phys. Chem. Chem. Phys.*, 2016, **18**, 19359–19367.

We would like to inform the reader of a correction that needs to be made to our previous publication. The bending rigidity, κ , is incorrectly reported to be 1.26 eV on page 19364 and in a label in Fig. 9. The correct value is 0.96 eV.

Thus the correct sentence should read "For pristine h-BN κ is found to be 0.96 eV."

The corrected version of Fig. 9 is given below.

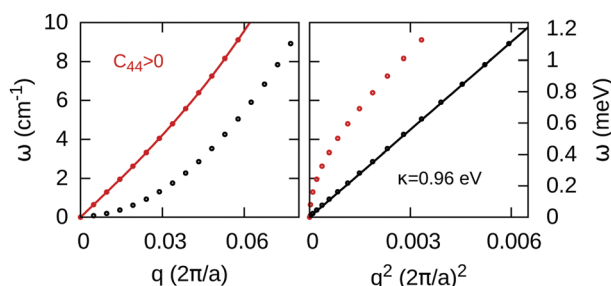


Fig. 9 Dependence of the ZA mode for pristine h-BN near Γ (M direction) on q (left) or q^2 (right). In black, results for the optimized cell showing $\omega \propto q^2$. The red curve shows the $\omega \propto q$ behaviour in a 0.2% larger cell.

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

