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

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We would like to inform the reader of a correction that needs to be made to our previous publication. The bending rigidity, \( \kappa \), 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 \( \kappa \) is found to be 0.96 eV."

The correct version of Fig. 9 is given below.

Fig. 9  Dependence of the ZA mode for pristine h-BN near \( I \) (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.