Electronic Supplementary Material (ESI) for Nanoscale.

Locally-Strained Hexagonal-Boron Nitride Nanosheets Quantified by Nanoscale Infrared Spectroscopy

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The DFT calculations were performed using an explicit van der Waals density functional, in our case vdW-DF2-B86r to consider the weak interaction between the layers of h-BN (from 1 to 5 layers). A two-atom cell of single layer of h-BN was used, with a G point centered mesh of 24 x 24 x 1 k points in the first Brillouin zone. The optimized value of 2.5148 Å of the lateral lattice constant was applied in the calculations, and 16 Å to separate the periodic images of the layers. The harmonic phonon frequencies and IR intensities were calculated using the density functional perturbation theory[1]. The Quantum ESPRESSO software[2], with energy cut-offs of 50 and 400 Ry for the wave functions and density, together with ultra-soft pseudo potentials, were employed. Calculations were carried out for one, two and five layers of h-BN with strain varying from -2% to 2%/ The results are presented in Figure S1.

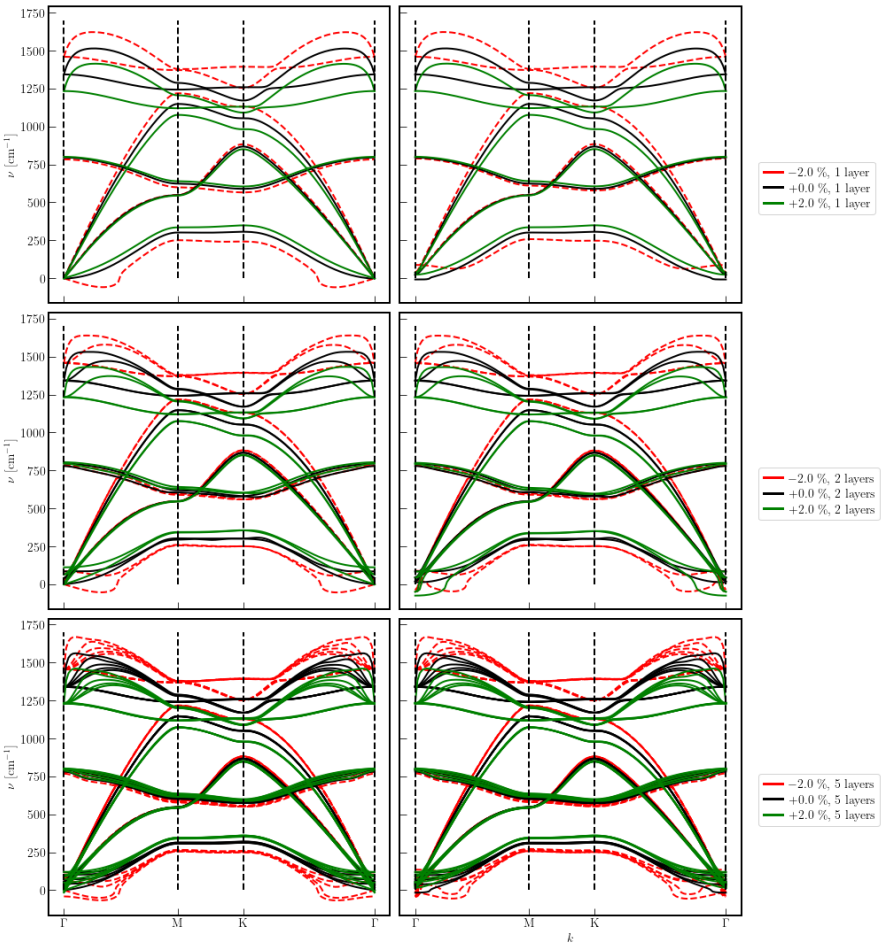

Figure S1: Computed phonon band structure in the one, two and five layers of h-BN at equilibrium and strain of +-0.5 %. In the left column acoustic sum rule was applied, in the right column not.

Very well converged parameters were used in our calculations. The convergence criteria on the self-consistency, total energy and forces acting on the atoms, the cut-off energies on the wave functions and the augmented charge density, the k point sampling and the number of q vectors were chosen to assure convergence from the beginning, as the calculations in these few-atom cells are very light in any case. We note that the convergence with respect to the k points and q vectors, for example, is much faster than in graphene, where the electronic and phonon band structures have more complicated structures close to the borders and corners of the first Brillouin zone.

Table S1: Correspondence of experimental frequencies to local strain, obtained by fitting the computed values to a linear line and shifting the line to the frequency at 1370 wavenumbers.

	Experimental position of the peak (cm^{-1})							
Nlayers	**1459**	**1389**	**1370**	**1353**	**1337**	**1318**	**1293**	**1276**
1	-1.571	-0.335	ref	0.300	0.582	0.918	1.359	1.659
2	-1.613	-0.344	ref	0.308	0.598	0.942	1.395	1.703
3	-1.627	-0.347	ref	0.311	0.603	0.951	1.408	1.719
4	-1.645	-0.351	ref	0.314	0.610	0.961	1.423	1.737
5	-1.668	-0.356	ref	0.319	0.618	0.975	1.443	1.762

Table S2: Computed frequencies from the DFT calculations at different values of strain from one to five layers.

Strain	**1L**	**2L**	**3L**	**4L**	**5L**
-2.0 %	1460	1457	1456	1456	1456
-1.5 %	1430	1427	1425	1428	1426
-1.0 %	1401	1398	1399	1397	1398
-0.5 %	1372	1370	1369	1369	1369
0 %	1343	1341	1341	1341	1341
+0.5 %	1315	1314	1313	1313	1313
+1.0 %	1288	1286	1286	1285	1286
+1.5 %	1261	1259	1259	1258	1258
+2.0 %	1234	1232	1232	1232	1231

Molecular simulations were carried out with LAMMPS. A 60 nm x 60 nm h-BN monolayer was considered with about 155,000 atoms. Time steps of 1 fs and total time of simulation of 10 ns were used. Equilibration time for unperturbed h-BN was 200 ps using statistical ensemble NVT. A Nose-Hoover thermostat was used for the simulation. The total energy vs time for a 10 ns NVT run is shown in Figure S2. The nearest neighbor distance (nnd) was determined using a custom algorithm. Boundaries for binning were determined based on the ranges indicated by the DFT results.

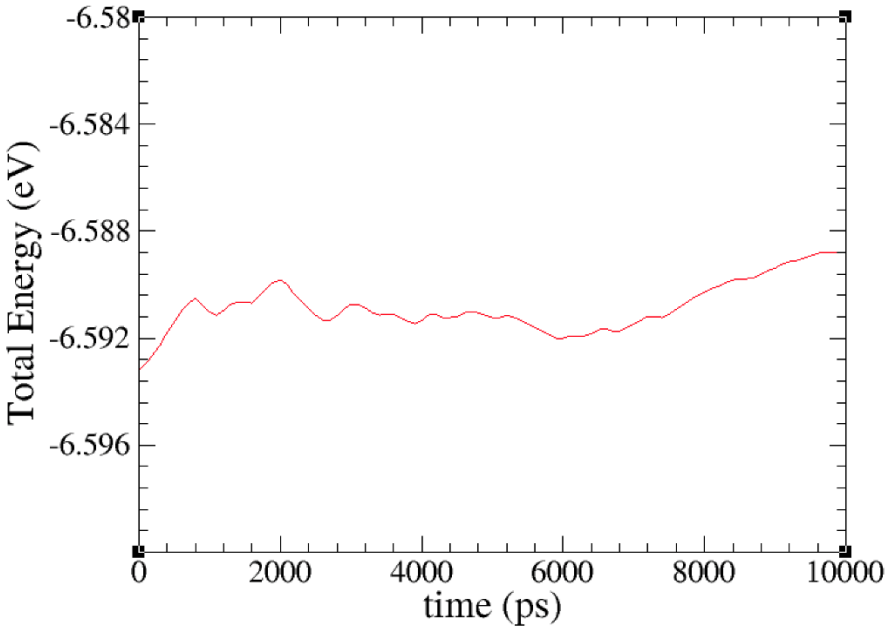

Figure S2: Total energy vs time for a 10 ns NVT run.

1. S. Baroni, S. de Gironcoli, A. Dal Corso and P. Giannozzi, *Reviews of Modern Physics*, 2001, **73**, 515-562.
2. P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. de Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P. Umari and R. M. Wentzcovitch, *Journal of Physics: Condensed Matter*, 2009, **21**, 395502.