Supplementary information: Mechanical metal-insulator transition in 2D graphene phononic crystals

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Finite element method simulations (FEM)

For all FEM-simulations presented in the main paper, we use the solid mechanics module of Comsol Multiphysics (Version 5.5).

Band structure calculations for an infinite lattice

The infinite model for the band structure calculations is based on two studies within the same model. In the first step we simulate the tension redistribution upon pattering (stationary study), which we use as input for a second study step in which we apply periodic boundary conditions to the unit cell and calculate the eigenfrequencies, which gives us the band structure. For all details see Ref. [1]. To assure that our simulations properly capture the phononic band gaps, we extend our calculations to more high symmetry points. For the unit cell shown in Fig. S1a, we plot the extended band structure for $\sigma_{xx}/\sigma_{yy} = 1$ and $\sigma_{xx}/\sigma_{yy} = 1.7$ inside the 1.Brillouin zone, Fig. S1b,c. We find that the valence band maximum between Γ and X and the conduction band minimum at X, and it is therefore sufficient to focus on the high symmetry points shown in the main paper.

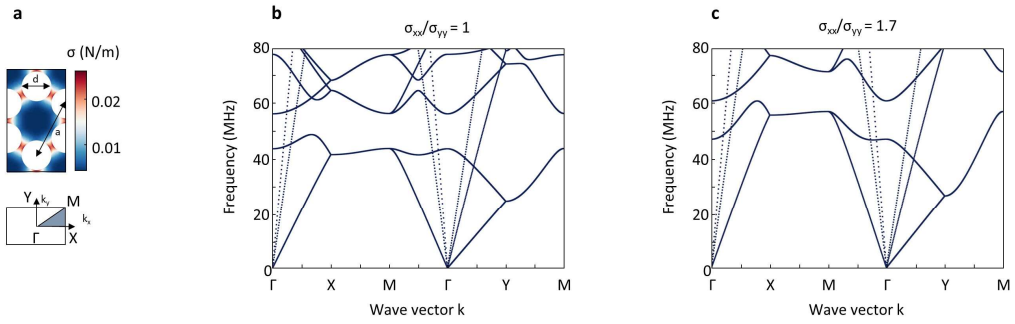

Figure S1 | Extended band structure. a, Unit cell of the honeycomb lattice with redistributed tension (top) and the corresponding first Brillouin zone (bottom). **b,c**, Extended phononic band structure for the unit cell shown in (a) with entirely uniform tension (σ_{xx}/σ_{yy} =1.) and implemented uniaxial tension σ_{xx}/σ_{yy} =1.7.

Transmission studies

To perform our transmission studies, we use a pre-stressed frequency domain study. In this study the phononic device is clamped along its perimeter (Fig. S2) and in a first study step we again calculate the tension redistribution upon patterning. In a second step, we add a time depended pressure in z direction at area A, which simulates an optothermal drive. For the transmission study, we then sweep the frequency of this time depended perturbation and calculate the response of the entire geometry (compare Eq. 1 main text). For this study step, we add isotropic damping ($\eta = 0.01$) to the graphene, which reproduces the quality factors ($Q \sim 100$) typically observed for graphene resonators at room temperatures. To simulate the effect of electrostatic pressure to the transmission studies, we add a boundary load to the entire device (including A and B) in z-direction and repeat the frequency sweep.

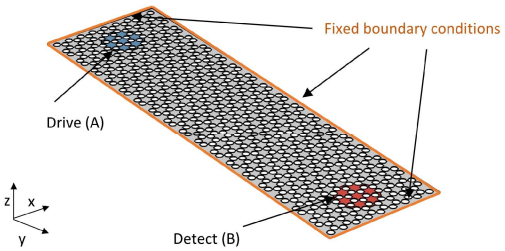

Figure S2 | Transmission geometry. The phononic device is clamped at its perimeter via fixed boundary conditions and motion is excited at A (blue) and detected at B (red).

Transmission circular reference device

As a comparison to the presented mMIT in the main text we perform transmission studies on a circular device under applied pressure which is excited at its centre and probed on the outside. The device geometry and resulting transmission spectra are shown in Fig. S3a,b, where we find clear band gap features (shaded area) with (red) and without (blue) applied pressure. In circular devices we find band gap features up to at least 30 kPa applied pressure in agreement with previous work.[1]

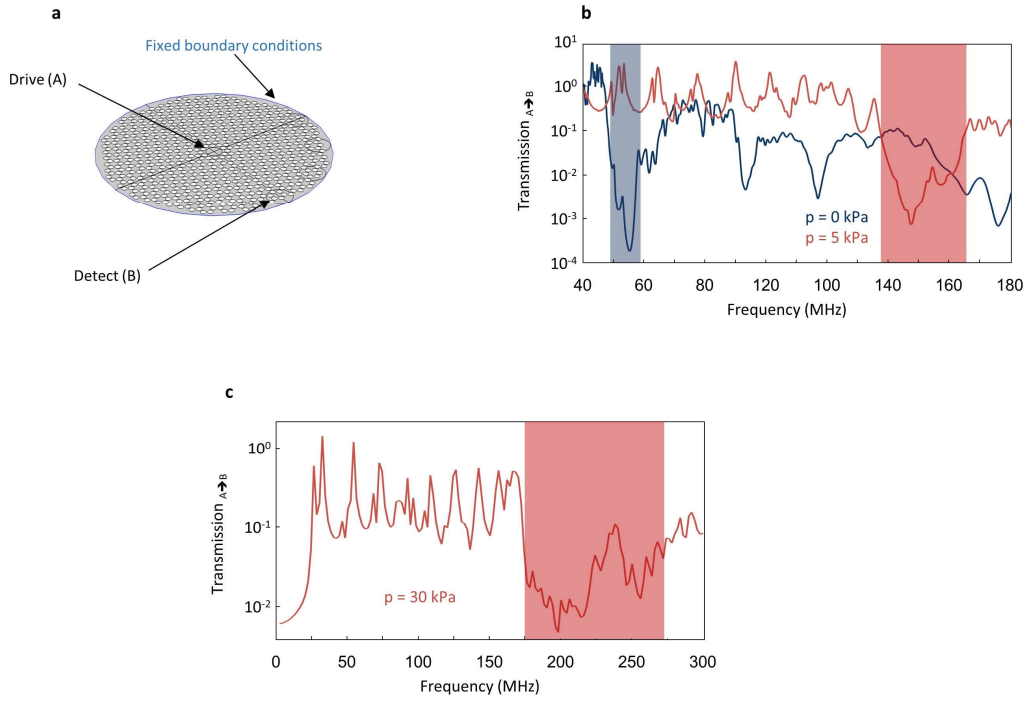

Figure S3 | Transmission circular reference device. a, Transmission geometry for a rectangular phononic device. At point A mechanical motion is excited by a frequency modulated laser, which than travels through the device and is detected at point B by a second laser spot. **b,c** Transmission from A to B vs. excitation frequency for the device shown in a) for 0, 5 and 30 kPa applied pressure. A clear bandgap region is visible for all cases.

Phononic bandgap vs. uniform residues

In addition the added pieces of mass (Fig. 4 main text), we also investigate the effect of a uniform layer of resist, which could be present on a device after thermal annealing. In Fig. S4 we plot transmission for a device made from clean graphene (blue) and one contaminated with a 3 nm layer of PDMS (green). For both cases we find a clear bandgap, the added PDMS however causes a downshift in frequency as the entire device becomes heavier. Also the bandgap is slightly less pronounced, but still clearly noticeable. For PDMS we assume a Young's modulus of 0.75 MPa, a Poisson's ratio of 0.49 and a density of 970 kg/m³.

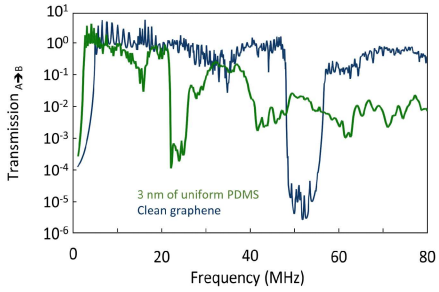

Figure S4 | Phononic bandgap vs. uniform residues. Transmission vs. frequency for a phononic device made from clean graphene (blue) and with a 3 nm uniform layer of PDMS residues (green).

Phononic bandgap vs. tension disorder

To represent a random but smooth enough spatial tension distribution in our devices we use a sum of plane waves with randomized amplitude $a(m,n)$ (between -1 and 1) and phase $\phi(m,n)$ (between 0 and π) of each mode:

$$\sigma(x,y) = p \sum_{m=-M}^{M} \sum_{n=-N}^{N} a(m,n)\cos\left(2\pi(mx+ny)+\phi(m,n)\right)$$

The factor p controls the disorder strength.

Phononic band gap vs. layer number

As a potential approach to overcome challenges associated with the fabrication of uniform and residue free suspended graphene devices for phononic pattering, we suggest to use thin multilayers. For this we have to check, if the bandgap persist also for thicker devices. We thus perform band structure calculations for various thickness (maintaining a constant stress in the device) and extract the band gap (Fig. S5). We find a bandgap up to ~350 layers of graphene.

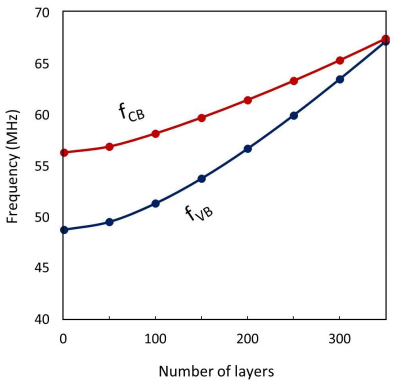

Figure S5 | Phononic band gap vs. layer number. Valence band maximum (f_{VB}) and conduction band minimum (f_{CB}) vs. number of graphene layers extracted from band structure calculations.

References

1. Kirchhof, J. N. *et al.* Tunable Graphene Phononic Crystal. *Nano Lett.* **21**, 2174–2182 (2021).