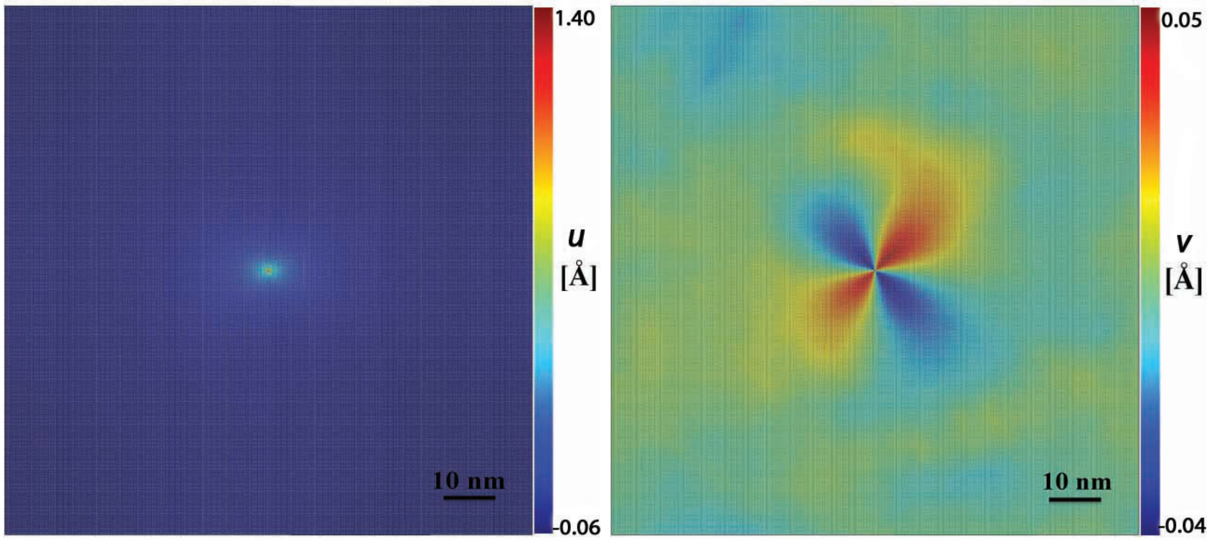
Electronic Supplementary Material (ESI) for Nanoscale

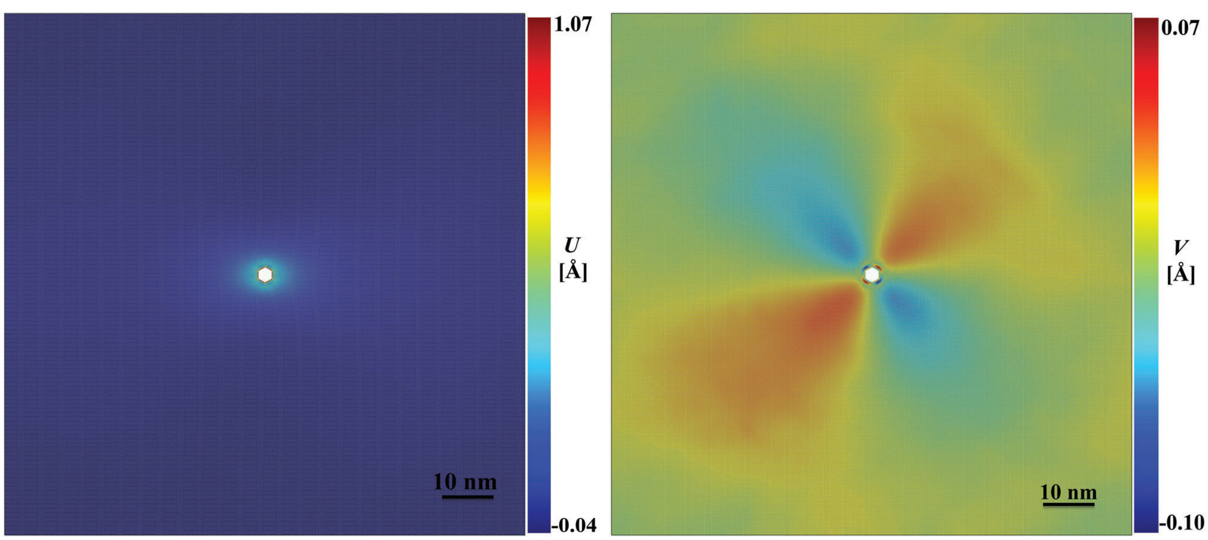
Supplementary Information

S1. SLIP DISPLACEMENT FIELDS OF BLG IN 100 × 100 NM SUPERCELL



(a) (b)

Figure S1: (a) and (b): Displacement fields of BLG along x-axis, u, and along y-axis, v, in 100 nm × 100 nm supercell with one central atom pair fixed as A-A stacking.



(a) (b)

Figure S2: (a) and (b): Displacement fields of BLG along x-axis, u, and along y-axis, v, in 100 nm × 100 nm supercell with hexagonal BLG nanopore.

S2. ANALYTICAL EXPRESSION TO FIT BLG GSF (γ-SURFACE)

The γ-surface of given plane of materials is a 2D periodic function, so it can be represented by a 2D Fourier series with the aid of reciprocal lattice vectors g_n,

$$\gamma(\mathbf{r}) = \sum_{\mathbf{n}} \mathbf{C_n} e^{\mathbf{i g_n \cdot r}} \tag{1}$$

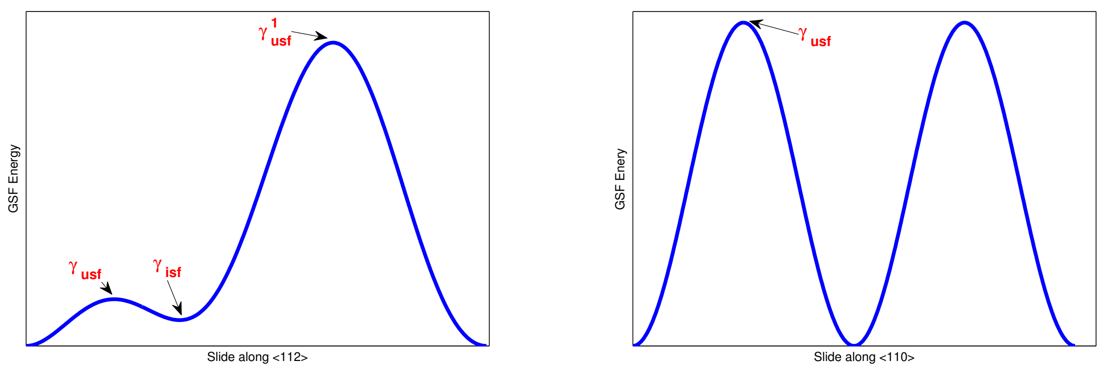
For graphene, we adopt the first three items to describe γ-surface:

$$\begin{aligned} \gamma(u,v) = C_0 + & C_1 \left[\cos(2\psi) + 2\cos(\psi)\cos(\phi)\right] \\ & + C_2 \left[\sin(2\psi) - 2\sin(\psi)\cos(\phi)\right] \end{aligned} \tag{2}$$

where

$$\psi = \frac{2\pi u}{3A_0}, \phi = \frac{2\pi v}{\sqrt{3}A_0} \tag{3}$$

Here A_0 is the bond length of graphene; u and v is the displacement along x-axis and y-axis defined in Figure 1 (a) of main text, respectively. Using Equation (2), GSF profiles along certain special directions are displayed in Figure S3, where γ_{isf}, γ_{usf} and γ^1_{usf} is intrinsic stacking fault energy, unstable stacking fault energy and second unstable fault energy, respectively.



(a) (b)

Figure S3: GSF profile along $\langle 112 \rangle$ and $\langle 110 \rangle$ of bilayer graphene.

Then we find out the expressions of the coefficients (C_0, C_1 and C_2). Because $\gamma(0,0) = 0$, so $C_0 = -3C_1$. For extreme-points of GSF curve along $\langle 112 \rangle$ (γ_{isf}, γ_{usf} and γ^1_{usf}), the corresponding ψ are

$$\begin{cases} \psi_0 = \frac{2\pi}{3}, \psi_1 = \frac{4\pi}{3}, \psi_2 = 2\pi - 2\arctan\left(\frac{C_1}{C_2}\right) & \text{when} \quad C_1 C_2 > 0 \\ \psi_0 = 2\arctan\left(-\frac{C_1}{C_2}\right), \psi_1 = \frac{2\pi}{3}, \psi_2 = \frac{4\pi}{3} & \text{when} \quad C_1 C_2 < 0 \end{cases} \tag{4}$$

Inserting Equation (4) into (2) we get

$$\begin{cases} \gamma_{\mathrm{usf}} = -\frac{4{C_1}^3}{{C_1}^2+{C_2}^2} \\ \gamma_{\mathrm{isf}} = \frac{3\sqrt{3}}{2}C_2 - 4.5C_1 \qquad \text{when} \quad C_1C_2 > 0 \\ \gamma_{\mathrm{usf}}^1 = -\frac{3\sqrt{3}}{2}C_2 - 4.5C_1 \end{cases} \tag{5}$$

$$\begin{cases} \gamma_{\mathrm{usf}} = -\frac{4{C_1}^3}{{C_1}^2+{C_2}^2} \\ \gamma_{\mathrm{isf}} = -\frac{3\sqrt{3}}{2}C_2 - 4.5C_1 \qquad \text{when} \quad C_1C_2 < 0 \\ \gamma_{\mathrm{usf}}^1 = \frac{3\sqrt{3}}{2}C_2 - 4.5C_1 \end{cases} \tag{6}$$

We just use Equation (6), then the coefficients are

$$C_1 = \frac{1}{3}\gamma_{\mathrm{usf}}\left[1 + \left(1 - \frac{\gamma_{\mathrm{isf}}}{\gamma_{\mathrm{usf}}}\right)^{\frac{1}{3}} + \left(1 - \frac{\gamma_{\mathrm{isf}}}{\gamma_{\mathrm{usf}}}\right)^{\frac{2}{3}}\right] \tag{7}$$

$$C_2 = \frac{2\sqrt{3}}{9}\gamma_{\mathrm{isf}} - \frac{\sqrt{3}}{3}\gamma_{\mathrm{usf}}\left[1 + \left(1 - \frac{\gamma_{\mathrm{isf}}}{\gamma_{\mathrm{usf}}}\right)^{\frac{1}{3}} + \left(1 - \frac{\gamma_{\mathrm{isf}}}{\gamma_{\mathrm{usf}}}\right)^{\frac{2}{3}}\right] \tag{8}$$

Then we plot GSF of BLG obtained from atomic simulations along certain directions in Figure S4, which shows that $\gamma_{\mathrm{isf}} \approx 0$. So $C_2 \approx -\sqrt{3}C_1 = -\sqrt{3}\gamma_{\mathrm{usf}}$ for graphene. In addition, if u and v are both small, along some direction $\vec{l}$ we have

$$\nabla_{\vec{l}}\gamma = \frac{8\pi^2 C_1}{3{A_0}^2}s \tag{9}$$

Here s is the displacement along direction $\vec{l}$. We also have,

$$\nabla_{\vec{l}}\gamma = \frac{G_\perp}{h_0}s \tag{10}$$

which is exactly the Hook's law. Here h_0 represents the inter-layer distance and $G_\perp$ is effective shear modulus between two layers. From the above two equations we know

$$G_\perp = \frac{8\pi^2 C_1 h_0}{3{A_0}^2} \tag{11}$$

Combing (2), (3),(7), (8) and (11) we can get the expression of γ-surface as

$$\gamma(u,v) = \frac{3{A_0}^2 G_\perp}{2\pi^2 h_0}\left[\cos^2\left(\frac{2\pi u}{3A_0} - \frac{2\pi}{3}\right) + \cos\left(\frac{2\pi v}{\sqrt{3}A_0}\right)\cos\left(\frac{2\pi u}{3A_0} - \frac{2\pi}{3}\right) + \frac{1}{4}\right] \tag{12}$$

To fit GSF obtained from atomic simulations in Figure 3 (a) in main text, we set

$$G_\perp = 1.588\mathrm{meV}/\mathrm{\mathring{A}}^3 = 254.1\mathrm{MPa} \tag{13}$$

Using this value, the results of Equation (12) is shown in Figure 3 (b) in main text for the whole 2D GSF and Figure S4 for GSF along certain directions.

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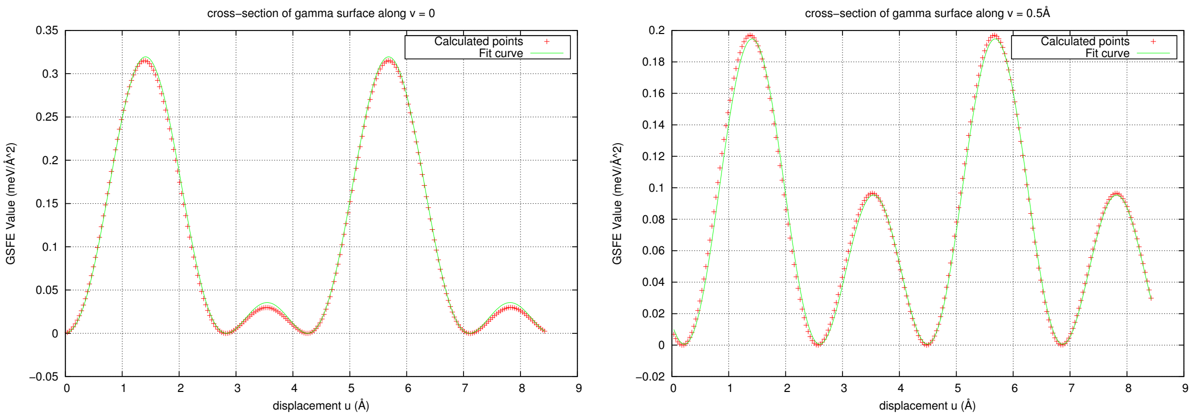


(a) (b)

Figure S4: GSF curves obtained from atomic simulations and Equation (12). (a) along v=0. (b) along v=0.5Å.

S3. ANALYTICAL SOLUTIONS OF CONTINUUM MODEL

If we perform Fourier transformation to both side of Equations (5) in the main text, we have

$$\begin{cases} w^2U(w,s)+\frac{1-\nu}{2}s^2U(w,s)+\frac{1+\nu}{2}swV(w,s)+k_0^2U(w,s)=\frac{a}{2\pi} \\ s^2V(w,s)+\frac{1-\nu}{2}w^2V(w,s)+\frac{1+\nu}{2}swU(w,s)+k_0^2V(w,s)=\frac{b}{2\pi} \end{cases} \tag{14}$$

Here (w,s) is the coordination in reciprocal space. Solving U and V from the above equations, we obtain

$$\begin{cases} U(w,s)=\frac{\frac{a}{2\pi}}{k_0^2+\frac{1-\nu}{2}(w^2+s^2)}-\frac{1+\nu}{4\pi}\frac{aw^2+bsw}{(k_0^2+\frac{1-\nu}{2}(w^2+s^2))(w^2+s^2+k_0^2)} \\ V(w,s)=\frac{\frac{b}{2\pi}}{k_0^2+\frac{1-\nu}{2}(w^2+s^2)}-\frac{1+\nu}{4\pi}\frac{asw+bs^2}{(k_0^2+\frac{1-\nu}{2}(w^2+s^2))(w^2+s^2+k_0^2)} \end{cases} \tag{15}$$

Using the polar coordination $[w=\rho\cos(\phi),\ s=\rho\sin(\phi)]$ and $[x=r\cos(\theta),\ y=r\sin(\theta)]$, We can get

$$\begin{aligned} &u(r,\theta) \\ =&\frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-i(wx+sy)}U(w,s)\mathrm{d}w\mathrm{d}s \\ =&\frac{a}{2\pi}\int_0^{\infty}\frac{\rho J_0(\rho r)}{k_0^2+\frac{1-\nu}{2}\rho^2}\mathrm{d}\rho-\frac{1+\nu}{8\pi^2}\int_0^{\infty}\frac{\rho^3F(\rho r,\theta)}{\left(k_0^2+\frac{1-\nu}{2}\rho^2\right)\left(k_0^2+\rho^2\right)}\mathrm{d}\rho \end{aligned} \tag{16}$$

Here we take the following relation of Bessel function into account[1]

$$\int_0^{2\pi}e^{-i\rho r\cos(\phi-\theta)}\mathrm{d}\phi=2\pi J_0(-\rho r)=2\pi J_0(\rho r) \tag{17}$$

and define

$$\begin{aligned} F(\rho r,\theta)=&\int_0^{2\pi}(a\cos^2(\phi)+b\sin(\phi)\cos(\phi))e^{-i\rho r\cos(\phi-\theta)}\mathrm{d}\phi \\ =&\pi aJ_0(\rho r)+f_1(\theta)\int_0^{2\pi}\cos(2\phi)e^{-i\rho r\cos(\phi)}\mathrm{d}\phi+g_1(\theta)\int_0^{2\pi}\sin(2\phi)e^{-i\rho r\cos(\phi)}\mathrm{d}\phi \end{aligned} \tag{18}$$

where

$$\begin{cases} f_1(\theta)=\frac{a}{2}\cos(2\theta)+\frac{b}{2}\sin(2\theta) \\ g_1(\theta)=-\frac{a}{2}\sin(2\theta)+\frac{b}{2}\sin(2\theta) \end{cases} \tag{19}$$

In addition, we have[2]

$$\int_0^{2\pi}\sin(2\phi)e^{-i\rho r\cos(\phi)}\mathrm{d}\phi=0 \tag{20}$$

and

$$\int_0^{2\pi} \cos(2\phi) e^{-i\rho r \cos(\phi)} \mathrm{d}\phi = 2\pi \left[J_0(\rho r) - 2\frac{J_1(\rho r)}{\rho r} \right] \tag{21}$$

Substituting these into Equation (18), we get

$$F(\rho r, \theta) = 2\pi \left[T_1(\theta) J_0(\rho r) - 2 f_1(\theta) \frac{J_1(\rho r)}{\rho r} \right] \tag{22}$$

where

$$T_1(\theta) = \frac{a}{2} + f_1(\theta) \tag{23}$$

Using the equations of Bessel functions below[2],

$$\int_0^{\infty} \frac{\rho J_0(\rho r)}{k_0^2 + \rho^2} \mathrm{d}\rho = K_0(k_0 r) \tag{24}$$

$$\int_0^{\infty} \frac{\rho J_0(\rho)}{(k_0^2 + \rho^2)^2} \mathrm{d}\rho = \frac{K_1(k_0)}{2k_0} \tag{25}$$

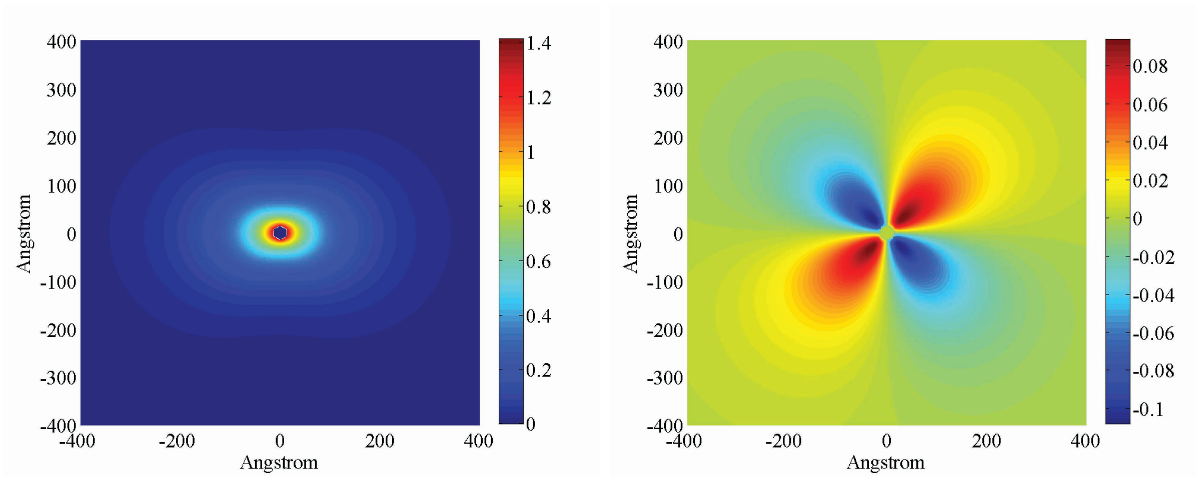
$$\int_0^{\infty} \frac{J_1(\rho)}{k_0^2 + \rho^2} \mathrm{d}\rho = \frac{1}{k_0^2} - \frac{K_1(k_0)}{k_0} \tag{26}$$

we finally get analytical expressions of displacement fields in polar coordination as the following

$$\begin{cases} u(r, \theta) = a u_1(r, \theta) + b u_2(r, \theta) \\ v(r, \theta) = a v_1(r, \theta) + b v_2(r, \theta) \end{cases} \tag{27}$$

Here u_1/u_2 and v_1/v_2 are the Green's functions of the system due to the reduced external force $[a, b]$ to produce the displacement at the point of origin. Their detail forms are written in Equation (7) and (8) of main text.

S4. NUMERICAL SOLUTIONS OF CONTINUUM MODEL OF HEXAGONAL BLG NANOPORE



(a) (b)

Figure S5: (a) and (b): Displacement fields of BLG along x-axis, u, and along y-axis, v, for hexagonal BLE nanopore with diameter of 3 nm from numerical solutions of Equation 9 in main text.

[1] G. Watson, *A treatise on the theory of Bessel functions* (University press, 1922).

[2] I. Gradshteĭn, I. Ryzhik, and A. Jeffrey, *Table of integrals, series, and products* (Academic Press, 2000).