Supplementary Information: Wetting and Strain Engineering of 2D Materials on Nanopatterned Substrates

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I. ENERGY CONTRIBUTIONS

We use a similar ansatz to Ref. 1 to describe the geometric profile of the 2D material overlaid on nanopillar arrays and grating structures:

$$y(x) = A_0 + \sum_{n=1}^{N} A_n \cos\left(\frac{n\pi x}{a}\right). \tag{S1}$$

Upon enforcing boundary conditions, this representation simplifies to:

$$y(x) = h_a + \sum_{n=1}^{N} A_n[\cos\left(\frac{n\pi x}{a}\right) - \cos(n\pi)]. \tag{S2}$$

Here, h_a denotes the height of the 2D material at $x = a$ (see Fig. 1), while $2a$ represents the period of the structure, and A_n signifies the Fourier coefficient. In this section, we discuss the components that contribute to the total energy of the 2D profile, encompassing the stresses, bending, and van der Waals adhesion energies.

A. 2D Materials on Nanopillar Arrays

To elucidate the underlying energy expressions that govern this configuration, we present the following equations.

The quantification of strain energy is expressed as:

$$E_{\text{strain}} = \pi Y \int_0^a x\varepsilon(x)^2 dx, \tag{S3}$$

where Y represents the Young's modulus.

The energy associated with bending is articulated as:

$$E_{\text{bending}} = \pi\chi \int_0^a x \frac{y''(x)^2}{(1+y'(x)^2)^3} dx, \tag{S4}$$

with χ denoting the bending stiffness. The values for Y and χ in various materials are provided in Table S1.

To evaluate adhesion energy, we employ the Morse potential[2] between layers:

$$\begin{aligned} E_{\text{adhesion}} =& \pi 4a^2\gamma + (4-\pi)a^2 U_{2D}(y(a)) \\ &+ 2\pi \int_0^a x\ U_{2D}(y(x))dx, \end{aligned} \tag{S5}$$

where γ represents the interfacial adhesion energy between the 2D material and the substrate. $U_{2D}(y)$ is given by:

$$\begin{aligned} U_{2D}(y) =& \frac{1}{A_C}\int U(x,y,z)\ dxdz \\ =& \gamma\left(e^{-2\sqrt{5}((y/h_0)^2-1)} - 2e^{-\sqrt{5}((y/h_0)^2-1)}\right), \end{aligned} \tag{S6}$$

where the interatomic pair Mosre potential, $U(x,y,z)$, is:

$$U(x,y,z) = u_0[e^{-2\lambda(x^2+y^2+z^2)} - e^{-\lambda(x^2+y^2+z^2)}]. \tag{S7}$$

Here, $u_0 = 2\lambda\gamma A_C^2/\pi$ and $\lambda = \sqrt{5}/h_0^2$. A_C and $h_0 = 0.34\ nm$ stand for the area per atom and the equilibrium distance between layers, respectively. Within these equations, $y'(x)$ and $y''(x)$ represent the first and second derivatives of the shape of the 2D material, respectively. This comprehensive ensemble of energy components collectively serves to elucidate the intricate mechanical interactions between 2D materials and nanopillar arrays.

TABLE S1. Mechanical Characteristics of Various Materials, including Young's Modulus (Y), Bending Stiffness (χ), and Monolayer Thickness (d)[3,4].

Materials	**Y (GPa)**	χ **(eV)**	d **(nm)**
$MoSe_2$	177	9.96	0.700
Graphene	1000	1.40	0.335
hBN	865	0.86	0.334

B. 2D Material on rectangular grating substrate

Another intriguing configuration involves positioning 2D materials over a grating structure. The fundamental energy expressions governing this configuration are described in detail below.

The strain energy can be obtained by:

$$E_{\text{strain}} = Ya \int_0^a \varepsilon(x)^2 dx. \tag{S8}$$

To calculate the bending energy, we employ:

$$E_{\text{bending}} = a\chi \int_0^a \frac{h''(x)^2}{(1+h'(x)^2)^3} dx. \tag{S9}$$

Finally, we calculate the adhesion energy using:

$$\begin{aligned} E_{\text{adhesion}} =& 4a^2\gamma + 4a\int_0^a U_{2D}(y(x))dx \\ &+ 4a\int_0^a dx\int_{-r}^{r}\big(U_{1D}(x-x', y(x)-r) \\ &- U_{1D}(x-x', y(x))\big)dx' \\ &+ 4a\int_0^a dx\int_0^r U_{1D}(x-r, y(x)-y')dy', \end{aligned} \tag{S10}$$

where $U_{1D}(x,y)$ is described as:

$$\begin{aligned} U_{1D}(x,y) =& \gamma\frac{2\times 5^{1/4}}{\sqrt{\pi}h_0}\times \\ & \left(\frac{1}{\sqrt{2}}e^{-2\sqrt{5}((x^2+y^2)/h_0^2-1)} - e^{-\sqrt{5}((x^2+y^2)/h_0^2-1)}\right). \end{aligned} \tag{S11}$$

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