Electronic Supplementary Material (ESI) for Nanoscale.

Frictionless nanohighways on crystalline surfaces

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I. DIRECTIONAL STRUCTURAL LUBRICITY IN WSE_2 ON CUF(001)

An example of B-like realistic interface based on the materials reported in Ref. [1]. The adsorbate is a flake of WSe_2 (lattice spacing $a = 0.3316\,\mathrm{nm}$) and the substrate is a CuF(001) (lattice spacing $b = 0.3747\,\mathrm{nm}$). The adosrbate and substrate are mutually rotate of $\theta_o = 3.317°$. The frictional behaviour is summaries in Fig. 1, which presents a similar investigation of the frictional regime as a function of size as that in the main text (Figures 5 and 6) for different systems.

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[1] N. Mounet, M. Gibertini, P. Schwaller, D. Campi, A. Merkys, A. Marrazzo, T. Sohier, I. E. Castelli, A. Cepellotti, G. Pizzi, and N. Marzari, Nature Nanotechnology **13**, 246 (2018).

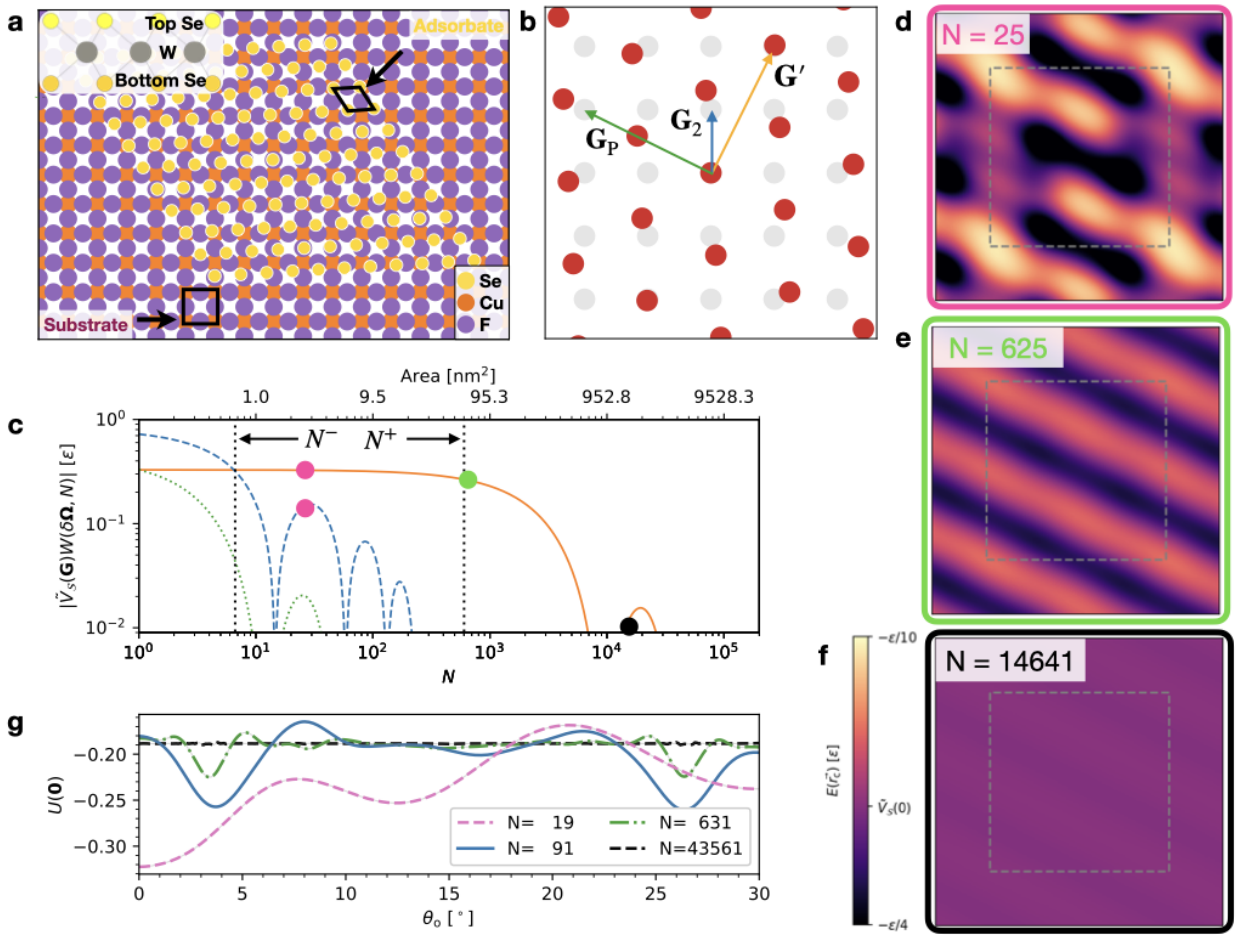

FIG. 1. **A realistic interface with approximate directional structural lubricity.** (a) The interface: a monolayer WSe_2 flake (yellow dots=bottom Se atoms) deposited on a CuF(001) surface (orange dots=Cu atoms; purple dots=F atoms). The angular misalignment is $\theta_o = 3.317°$. The interlocking potential is computed considering the interface between the CuF surface and the bottom Se layer, indicated in the top left inset. (b) Reciprocal lattices of the adsorbate ($\mathcal{Q}$, red) and substrate ($\mathcal{G}$, gray), with marked a CMV $\mathbf{G}' = 2\pi/b(1,2)$ (orange arrow), a perpendicular reciprocal vector $\mathbf{G}_P = 2\pi/b(-2,1)$ (green arrow), and the vector $\mathbf{G}_2 = 2\pi/b(0,1)$ (blue arrow) yielding a sizable Fourier component at small flake size. (c) The size dependence of the Fourier components associated to $\mathbf{G}'$ (orange solid line), $\mathbf{G}_P$ (green dotted), and $\mathbf{G}_2$ (blue dashed). The vertical lines mark the $\mathbf{G}'$ critical sizes $N^- \simeq 7$ and $N^+ = 611$ defined in Sec. 5D in the main text (d,e,f) Maps of the interlocking potential $U(\mathbf{r}_c)$ in the $[-b,b] \times [-b,b]$ square for the three selected flake sizes marked as matching-colored dots in panel (c); the energy scale is indicated at the left of panel f. The dashed gray square delimits the Wigner-Seitz cell of the substrate lattice $\mathcal{S}$. (g) Potential energy $U(\mathbf{r}_c)$, Eq. 2 in the main text, as a function of the misalignment angle θ_o for hexagonal clusters of the sizes reported in the legend; the center of mass is fixed at $\mathbf{r}_c = \mathbf{0}$.