Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Self-propelled Continuous Transport of Nanoparticles on A Wedge-Shaped Groove Track

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Section I: Calculation of the driving force for Stage II (-12<x≤-3.5 nm)

The contact area of the flake and substrate $A_{\text{f-s}}$ can be expressed as

$$A_{f-s} = W\left(-x-\frac{W}{2tan\frac{\varphi}{2}}+\frac{L}{2}\right)+\left[\left(-x-\frac{L}{2}\right)tan\frac{\varphi}{2}+\frac{W}{2}\right]\left(x+\frac{W}{2tan\frac{\varphi}{2}}+\frac{L}{2}\right)= -tan\frac{\varphi}{2}x^2+\frac{WL}{2}-\frac{W^2}{4tan\frac{\varphi}{2}}-\frac{L^2}{4}tan\frac{\varphi}{2}$$

Where, φ denotes the angle of the substrate, x denotes the local position of the CoM of the flake, W and L are the width and legnth of the flake, respectively. Thus, we can obtain the vdW interaction energy from the substrate

$$U_{sub} = -A_{f-s}E_{sub}$$

Therefore, the force exerted on the flake from the substrate is

$$F_{sub} = -\frac{\partial U_{sub}}{\partial x} = (- 2tan\frac{\varphi}{2}x - Ltan\frac{\varphi}{2} - W)E_{sub}$$

Section II: Calculation of the driving force for Stage III (-3.5<*x*<3.5 nm)

When the flake moves to the stage III (-3.5<*x*<3.5 nm), the contact area of the flake with the upper layer of the first and second track are

$$A_{up1} = \left(- x + \frac{L}{2}\right)W - \left(- x + \frac{L}{2}\right)^2 tan\frac{\theta}{2}$$

$$A_{up2} = (x + \frac{L}{2})W - \left(x + \frac{L}{2}\right)[\left(L_{rail} - \frac{L}{2} - x\right)tan\frac{\theta}{2} + L_{rail}tan\frac{\theta}{2}]$$

The total contact area between the flake and the upper layer is therefore obtained as

$$A_{up} = A_{up1} + A_{up2}$$

Therefore, the driving force from the upper layer is

$$F_{up} = -\frac{\partial(- A_{up}E_{up})}{\partial x} = - 2(L_{rail} - L)tan\frac{\theta}{2}E_{up}$$

The contact area of the flake with the substrate of the first and second track are

$$A_{sub1} = tan\frac{\varphi}{2}\left(- x + \frac{L}{2}\right)^2$$

$$A_{sub2} = W(x + \frac{L}{2})$$

The total contact area between the flake and the substrate is obtained as

$$A_{sub} = A_{sub1} + A_{sub2}$$

Thus, we get the driving force from the substrate

$$F_{sub} = -\frac{\partial(- A_{f - s}E_{sub})}{\partial x} = \left(2tan\frac{\varphi}{2}x - Ltan\frac{\varphi}{2} + W\right)E_{sub}$$