Interlayer Registry Determines the Sliding Potential of Layered Metal Dichalcogenides: The case of *2H*-MoS2

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Supporting Information: Coordinates of some representative structures

$2H$-MoS$_2$ is a layered crystal, where each layer consists of three sub-layers of S-Mo-S (Fig. S1). The crystal unit cell has the symmetry of the P6$_3$/mmc space group, with lattice parameters of $a = b = 3.1612$ Å and $c = 12.2985$ Å.[1-2,3] For the construction of the bilayer system studied in the present manuscript we used the following partial coordinates representation:[4-5]

Mo: $(1/3)A+(2/3)B+(1/4)C$

S: $(2/3)A+(1/3)B-(1/2-u)C$

S: $(2/3)A+(1/3)B+(1-u)C$

Mo: $(2/3)A+(1/3)B+(3/4)C$

S: $(1/3)A+(2/3)B+uC$

S: $(1/3)A+(2/3)B+(1.5-u)C$

Where: $A = \left(-\sqrt{3}\frac{a}{2}, \frac{a}{2}, 0\right)$, $B = \left(\sqrt{3}\frac{b}{2}, \frac{b}{2}, 0\right)$, $C = (0, 0, c)$, $u = 0.621$
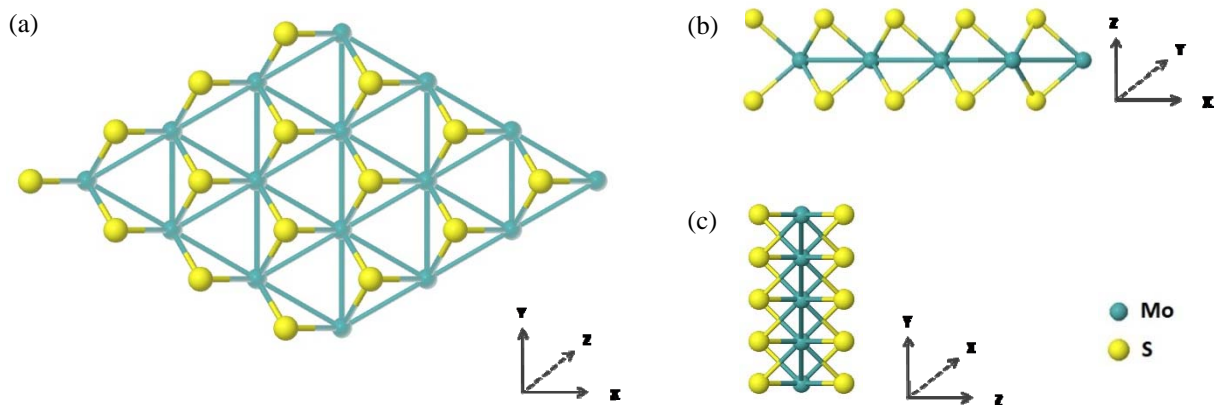

(a)   (b)   (c)

Fig. S1 Different views of MoS$_2$ crystal structure: (a) X-Y plain, (b) Y-Z plain and (c) X-Z plain.

The resulting coordinates of some high symmetry configurations (see Fig. 3 of the main text) are given below:

AA' configuration:

S   (-0.912560,   4.741800,   1.488119)
Mo   (0.912560,   4.741800,   3.074625)
S   (-0.912560,   4.741800,   4.661132)
S   (0.912560,   4.741800,   7.637369)
Mo   (-0.912560,   4.741800,   9.223875)
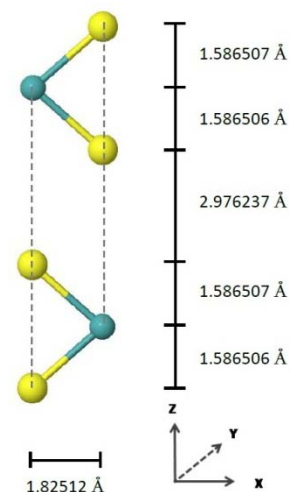S   (0.912560,   4.741800, 10.810382)

Fig. S2 (a) AA'

AB$_1$ configuration:

S   (-0.912560,   4.741800,   1.488119)
Mo   (0.912560,   4.741800,   3.074625)
S   (-0.912560,   4.741800,   4.661132)
S   (2.737680,   4.741800,   7.637369)
Mo   (0. 912560,   4.741800,   9.223875)
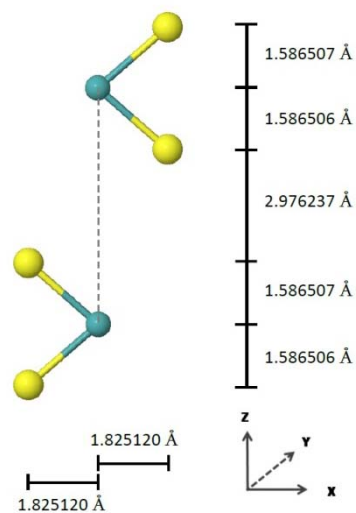S   (2.737680,   4.741800, 10.810382)

Fig. S2 (b) AB$_1$

AB$_2$ configuration:

S   (-0.912560,   1.580600,   1.488119)
Mo   (0.912560,   1.580600,   3.074625)
S   (-0.912560,   1.580600,   4.661132)
S   (1.837043,   6.321606,   7.637369)
Mo   (0.011923,   6.321606,   9.223875)
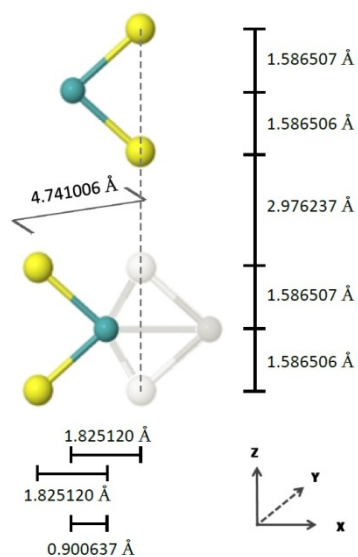S   (1.837043,   6.321606, 10.810382)

Fig. S2 (c) AB$_2$

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