

## Supplementary materials

for:

### Vertical ferroelectric switching by in-plane sliding of two-dimensional bilayer WTe<sub>2</sub>

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Table S1. The input parameters for our DFT VASP calculations.

	Structural relaxation	Self-consistent calculation
ISM EAR	0	0
SIGMA	0.05	0.05
ENCUT	500	500
PREC	High	High
NBANDS	144	144
ALGO	Fast	Fast
IVDW	12	12
EDIFFG	-1E-03	-1E-03
EDIFF	1E-06	1E-08
LWAVE	TRUE	TRUE
LCHARG	TRUE	TRUE
KPOINTS	21×11×1	21×11×1
POTCAR	W: PAW_PBE 08Apr2002 Te: PAW_PBE 08Apr2002	W: PAW_PBE 08Apr2002 Te: PAW_PBE 08Apr2002

Atomic coordinates of **State\_1**

WTe<sub>2</sub>

```

1.0000000000000000
  3.4800000000000000    0.0000000000000000    0.0000000000000000
  0.0000000000000000    6.2658415999999999    0.0000000000000000
  0.0000000000000000    0.0000000000000000    28.2758666514528016

```

```

W      Te
  4      8

```

Direct

```

0.0000000000000000    0.5930976920249637    0.6241994171249241
0.0000000000000000    0.0529567466930580    0.3757067768080196
0.5000000000000000    0.6973953164741969    0.3834928460982238
0.5000000000000000    0.2376039827483803    0.6165964024407248
0.0000000000000000    0.9879441279508380    0.6725676175285693
0.5000000000000000    0.3019925156283895    0.4303413470623557
0.0000000000000000    0.7987821583883001    0.4535993536592476
0.5000000000000000    0.4943603827839169    0.6942899806610525
0.0000000000000000    0.4482209273989674    0.3274062534855166
0.5000000000000000    0.8427337785666679    0.5696006202680761
0.0000000000000000    0.3367889535816304    0.5464136983215955
0.5000000000000000    0.9537699249510562    0.3056776700331256

```

Atomic coordinates of **State\_2**

WTe2

1.0000000000000000		
3.4800000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	6.2658415999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.2758666514528016

W	Te
4	8

Direct

0.0000000000000000	0.5120240468921223	0.6243040325411172
0.0000030800099893	0.0518408180692860	0.3758063785029856
0.5000000000000000	0.6963483650943866	0.3834111992516360
0.5000030800099893	0.1564645147748022	0.6165188900300882
0.0000014313118015	0.9072878057163551	0.6726053644568255
0.5000014278625713	0.3014754251268728	0.4304055294860192
0.0000008227117831	0.7955441795202169	0.4535938062558167
0.5000008140472119	0.4128417490424076	0.6943341637589349
0.0000008140472119	0.4466894499847104	0.3274390222113616
0.5000008227117831	0.7610636778449854	0.5696702499823526
0.0000014278625713	0.2578398803032543	0.5464117792722989
0.5000014313117873	0.9531019181687220	0.3057165039510268