Table I Lattice parameters and atomic positions of bulk TiS_2.

Atomic positions (*x, y, z*)			Lattice constants (Å)		
	EXP	GGA+U		EXP	GGA+U
S	1/3, 2/3, 0.25	1/3, 2/3, 0.234	*a, b*	3.41	3.45
S	2/3, 1/3, 0.75	2/3, 1/3, 0.766	*c*	5.69	6.02
Ti	0, 0, 0	0, 0, 0	Ti-S bond length	2.43	2.44

Table II Lattice parameters and atomic positions of TiS_2 nanosheets. All the supercells have *P*-3*m*1 symmetry and the equivalent atoms are not listed. For all the supercells, $a=b=3.41$Å and $c=(n+4)\times5.69$ Å, where n is the number of the layers in the nanosheet. For example, for 2 layers nanosheet, $c=(2+4)\times5.69=34.14$ Å. Here the experimental values of lattice constants are used.

Atomic positions of the nanosheet supercells

monolayer				12 layers				14 layers			
c=28.45 Å				*c*=91.04 Å				*c*=102.42 Å			
Ti	0	0	0.5	Ti	0	0	0.176	Ti	0	0	0.158
S	1/3	2/3	0.45	Ti	0	0	0.235	Ti	0	0	0.211
				Ti	0	0	0.294	Ti	0	0	0.263
2 layers				Ti	0	0	0.353	Ti	0	0	0.316
c=34.14 Å				Ti	0	0	0.412	Ti	0	0	0.368
Ti	0	0	0.417	Ti	0	0	0.471	Ti	0	0	0.421
S	1/3	2/3	0.375	S	1/3	2/3	0.191	Ti	0	0	0.474
S	2/3	1/3	0.458	S	1/3	2/3	0.250	S	1/3	2/3	0.171
				S	1/3	2/3	0.309	S	1/3	2/3	0.224
4 layers				S	1/3	2/3	0.368	S	1/3	2/3	0.276
c=45.52 Å				S	1/3	2/3	0.426	S	1/3	2/3	0.329
Ti	0	0	0.438	S	1/3	2/3	0.485	S	1/3	2/3	0.382
Ti	0	0	0.313	S	1/3	2/3	0.838	S	1/3	2/3	0.434
S	1/3	2/3	0.469	S	2/3	1/3	0.221	S	1/3	2/3	0.487
S	1/3	2/3	0.344	S	2/3	1/3	0.279	S	1/3	2/3	0.855
S	2/3	1/3	0.406	S	2/3	1/3	0.338	S	2/3	1/3	0.197
S	2/3	1/3	0.281	S	2/3	1/3	0.397	S	2/3	1/3	0.250
				S	2/3	1/3	0.456	S	2/3	1/3	0.303
8 layers								S	2/3	1/3	0.355
c=68.28 Å								S	2/3	1/3	0.408
Ti	0	0	0.231					S	2/3	1/3	0.461
Ti	0	0	0.308								
Ti	0	0	0.385								
Ti	0	0	0.462								
S	1/3	2/3	0.250								
S	1/3	2/3	0.327								
S	1/3	2/3	0.404								
S	1/3	2/3	0.481								
S	1/3	2/3	0.788								
S	2/3	1/3	0.288								
S	2/3	1/3	0.365								
S	2/3	1/3	0.442								