Single-Layer MoS₂: A Two-Dimensional Material with Negative Poisson's Ratio

Yucheng Zhu [1], Xiaofei Cao [1], Yuan Tan [1], Yao Wang [2], Jun Hu [1,*], Baotong Li [3] and Zhong Chen [4]

[1] School of Chemical Engineering, Northwest University, Xi'an 710069, China
[2] Engineering Research Center of Alternative Energy Materials and Devices, Ministry of Education, Sichuan University, Chengdu 610065, China; wangyao516@scu.edu.cn
[3] Key Laboratory of Education Ministry for Modern Design and Rotor-Bearing System, Xi'an Jiaotong University, Xi'an 710049, China
[4] School of Materials Science and Engineering, Nanyang Technological University, Singapore 639798, Singapore
* Correspondence: hujun@nwu.edu.cn

Table S1. The calculated elastic constants (units of GPa) of 2D MoS₂ and MoTe₂.

2D Materials	C_{11}	C_{12}	C_{22}	C_{66}
MoS₂(P6₃/mmc)	176	44	176	66
MoS₂(R3̄m)	179.3	-13.5	179.3	99.7
MoS₂(F4̄3m)	119.4	53.2	112.6	33.1
WS₂(R3̄m)	194	43	194	76
MoTe₂(P6₃/mmc)	106	26	106	40
MoTe₂(P6₃/mmc)	108.6	30.4	108.6	38

Table S2. Structural information of three configurations of MoS_2.

	Lattice Parameters(Å)	Fractional Coordinates of Atoms
$MoS_2(P6_3/mmc)$	a=3.190	Mo1(0.6667 0.3333 0.75)
	b=3.190	Mo2(0.3333 0.6667 0.25)
	c=14.879	S1(0.3333 0.6667 0.8552)
		S2(0.6667 0.3333 0.3552)
		S3(0.3333 0.6667 0.6448)
		S4(0.6667 0.3333 0.1448)
$MoS_2(R\overline{3}m)$	a=3.190	Mo1(0 0 0)
	b=3.190	Mo2(0.6667 0.3333 0.3333)
	c=18.976	Mo3(0.3333 0.6667 0.6667)
		S1(0 0 0.2488)
		S2(0.6667 0.3333 0.0845)
		S3(0.6667 0.3333 0.5822)
		S4(0.3333 0.6667 0.4178)
		S5(0.3333 0.6667 0.9155)
		S6(0 0 0.7511)
$MoS_2(F\overline{4}3m)$	a=6.788	Mo1(0.4235 0.8588 0.8588)
	b=6.788	Mo2(0.8588 0.8588 0.4235)
	c=6.788	Mo3(0.8588 0.8588 0.8588)
		Mo4(0.8588 0.4235 0.8588)
		S1(0.1185 0.1185 0.1185)
		S2(0.1185 0.6446 0.1185)
		S3(0.1185 0.1185 0.6446)
		S4(0.1553 0.6149 0.6149)
		S5(0.6149 0.1553 0.6149)
		S6(0.6149 0.6149 0.6149)
		S7(0.6149 0.6149 0.1553)
		S8(0.6446 0.1185 0.1185)
$WS_2(R\overline{3}m)$	a=3.19	W1(0 0 0)
	b=3.19	S1(0.3333 0.6667 0.07)
	c=21.36	S2(0 0 0.26)

Figure S1. The band structure and the DOS of MoS_2. The energy band structure describes the energy that electrons are forbidden or allowed to carry, which is caused by the diffraction of quantum

dynamics electron waves in a periodic lattice. The energy band structure of a material determines various properties, especially its electronic and optical properties.
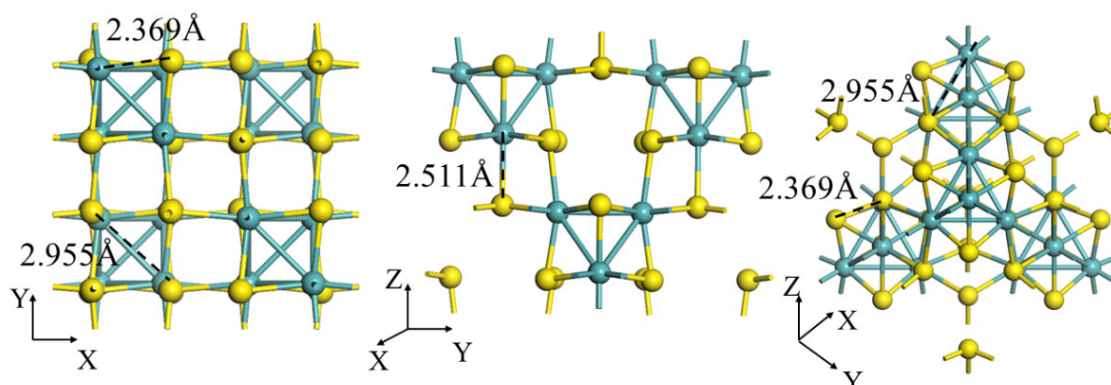

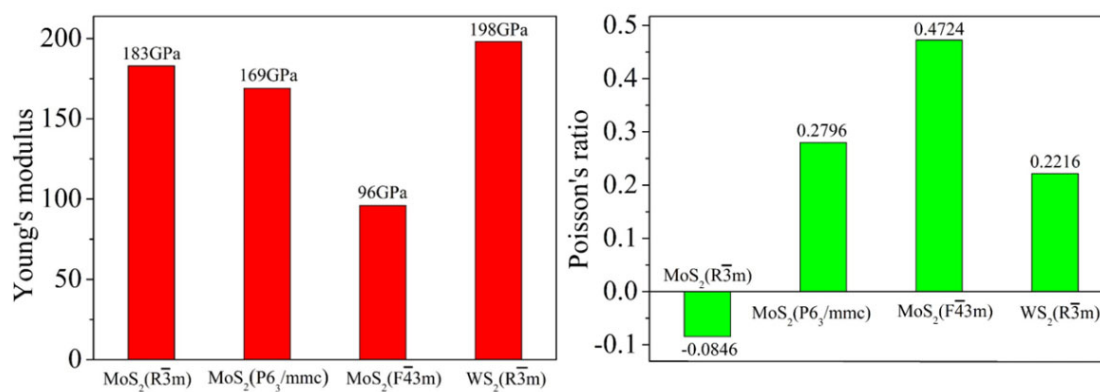**Figure S2.** MoS$_2$ (space group F$\bar{4}$3m).

Figure S3. Comparison graphs of Young's modulus and Poisson's ratio for the four materials.
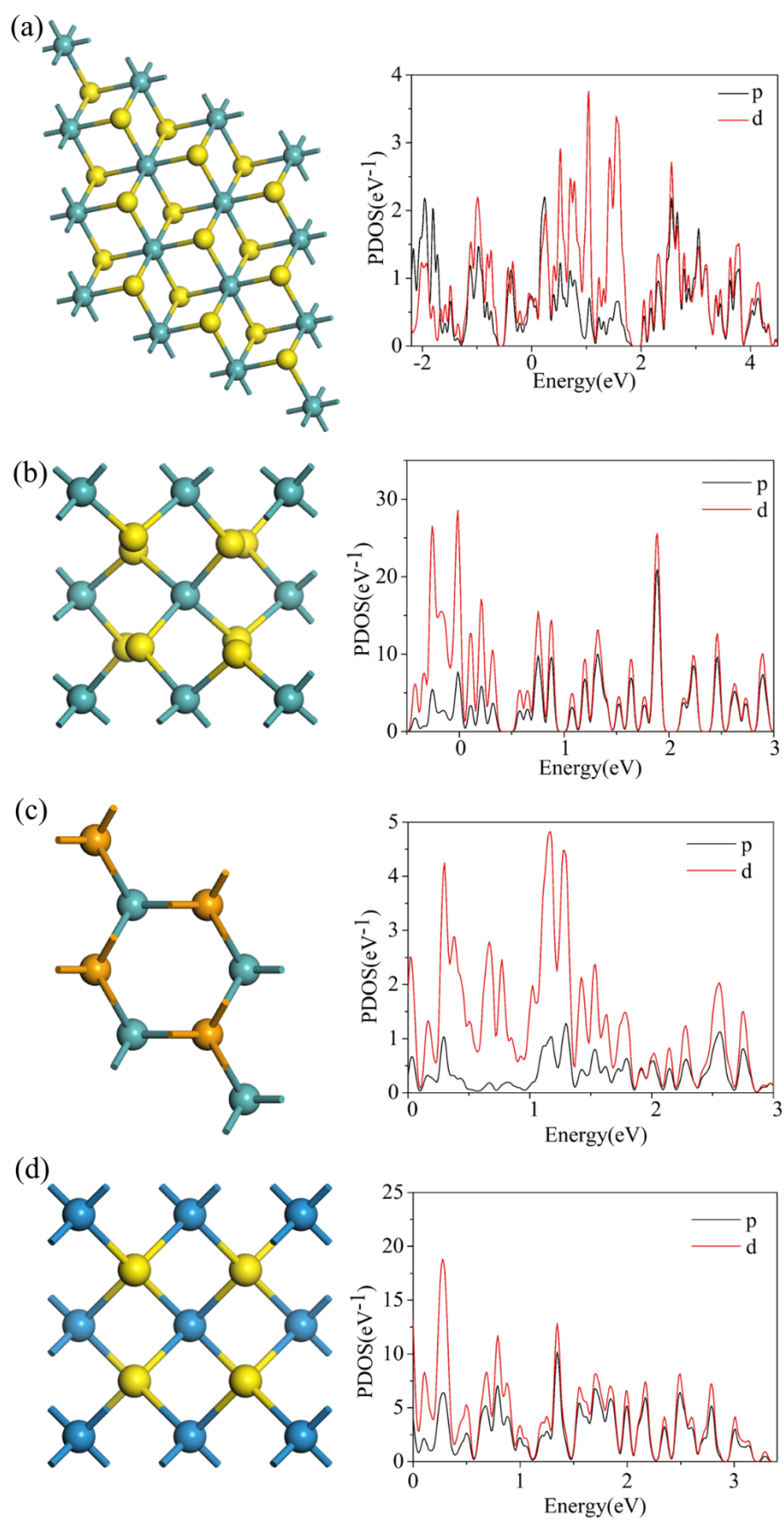
Figure S4. Four negative Poisson's ratio materials and their PDOS plots. (a) MoS₂ (space group P$\bar{3}$m1). (b) MoS₂ (space group I$\bar{4}$2d). (c) MoSe (space group P$\bar{6}$m2). (d) WS₂ (space group I$\bar{4}$2d).
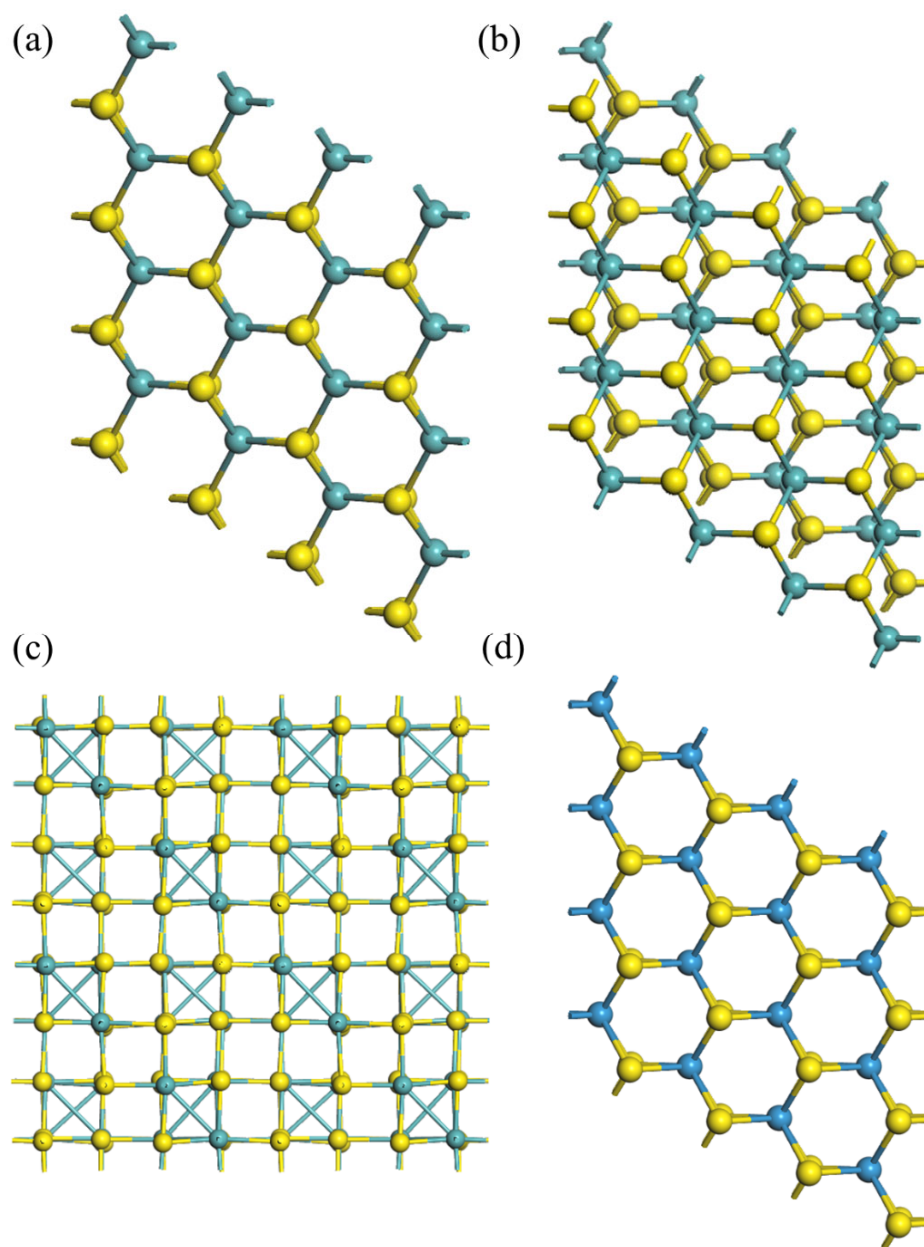
Figure S5. Structural snapshots (side view) of the (a) MoS_2 (space group $R\bar{3}m$) (b) MoS_2 (space group $P6_3/mmc$) (c) MoS_2 (space group $F\bar{4}3m$) and (d) WS_2 (space group $R\bar{3}m$) with the evolution of the average potential energy and temperature per atom in AIMD simulations at 500 K and 6 ps.