Supporting Information

for

Layer-dependent properties of MoS_2 nanosheets with different crystal structures study by DFT calculations

Zong-Yan Zhao*, Qing-Lu Liu

Faculty of Materials Science and Engineering, Kunming University of Science and Technology, Kunming 650093, P. R. China

Table S1. The structure parameters of MoS_2 bulk with different crystal phases

Crystal phase	1T'-MoS_2	2H-MoS_2	3R-MoS_2
Symmetry	Monoclinic (triclinic) $P2_1/m$	Hexagonal $P6_3/mmc$	Trigonal R3m
Lattice constant	a = 5.815 Å, b = 3.243 Å, c = 5.407 Å α = γ = 90°, β = 89.94°	a = b = 3.185 Å, c = 12.389 Å, α = β = 90°, γ = 120°	a = b = 3.192 Å, c = 18.281 Å, α = β = 90°, γ = 120°
Density /g.cm^{-3}	5.212	4.884	4.944
Binding energy /eV.molecule^{-1}	22.235	22.860	22.047
Bond length /Å	S1-Mo: 2.534*1, 2.462*2 S2-Mo: 2.385*1, 2.367*2	2.40731	2.42096
Bond angel /°	79.945, 82.404, 84.060, 86.515, 89.315, 93.331, 106.181	80.384, 82.836	82.477, 97.523
Charge populations	S1: -0.10 S2: -0.12 Mo: 0.23	S: -0.11 Mo: 0.22	S: -0.11 Mo: 0.23

Table S2. Distribution of bond length of the out-side of first layer of MoS_2 with typical layer numbers, in comparison with those of in bulk phase, the unit in Å.

	1T'-MoS_2		2H-MoS_2	3R-MoS_2
	Mo-S1	Mo-S2		
bulk	2.367, 2.385	2.462, 2.534	2.407	2.421
20 Layers	2.384, 2.427	2.476, 2.542	2.400	2.422
10 Layers	2.384, 2.426	2.476, 2.541	2.399	2.422
2 Layers	2.364, 2.404	2.473, 2.518	2.407	2.425
Monolayer	2.384, 2.430	2.469, 2.536	2.408	2.425

Table S3. Layer thickness of the first layer with typical layer numbers, in comparison with those of in bulk phase, the unit in Å.

	1T'-MoS_2	2H-MoS_2	3R-MoS_2
bulk	3.298	3.107	3.140
20 Layers	3.353	3.137	3.145
10 Layers	3.353	3.136	3.144
2 Layers	3.348	3.108	3.150
Monolayer	3.400	3.111	3.152

Table S4. Layer spacing of the first layer with typical layer numbers, in comparison with those of in bulk phase, the unit in Å.

	1T'-MoS_2	2H-MoS_2	3R-MoS_2
bulk	2.108	3.087	2.954
20 Layers	2.525	3.207	2.955
10 Layers	2.528	3.173	2.955
2 Layers	2.515	3.087	3.032

The fitting equations for the surface energy curves:

1T'-MoS_2: $E_{surf} = 0.005 + 22.941\exp(-n / 2.128)$ (eqn. S1)

2H-MoS_2: $E_{surf} = 0.183 - 38.959\exp(-n /1.469)$ (eqn. S2)

3R-MoS_2: $E_{surf} = 0.233 - 0.195\exp(-n / 5.658)$ (eqn. S3)

The fitting equations for the cleaving energy curves:

1T'-MoS_2: $E_{cleav} = 0.288 - 0.063\exp(-n / 0.817)$ (eqn. S4)

2H-MoS_2: $E_{cleav} = 0.304 - 0.032\exp(-n / 0.995)$ (eqn. S5)

3R-MoS_2: $E_{cleav} = 0.351 - 0.243\exp(-n / 0.466)$ (eqn. S6)

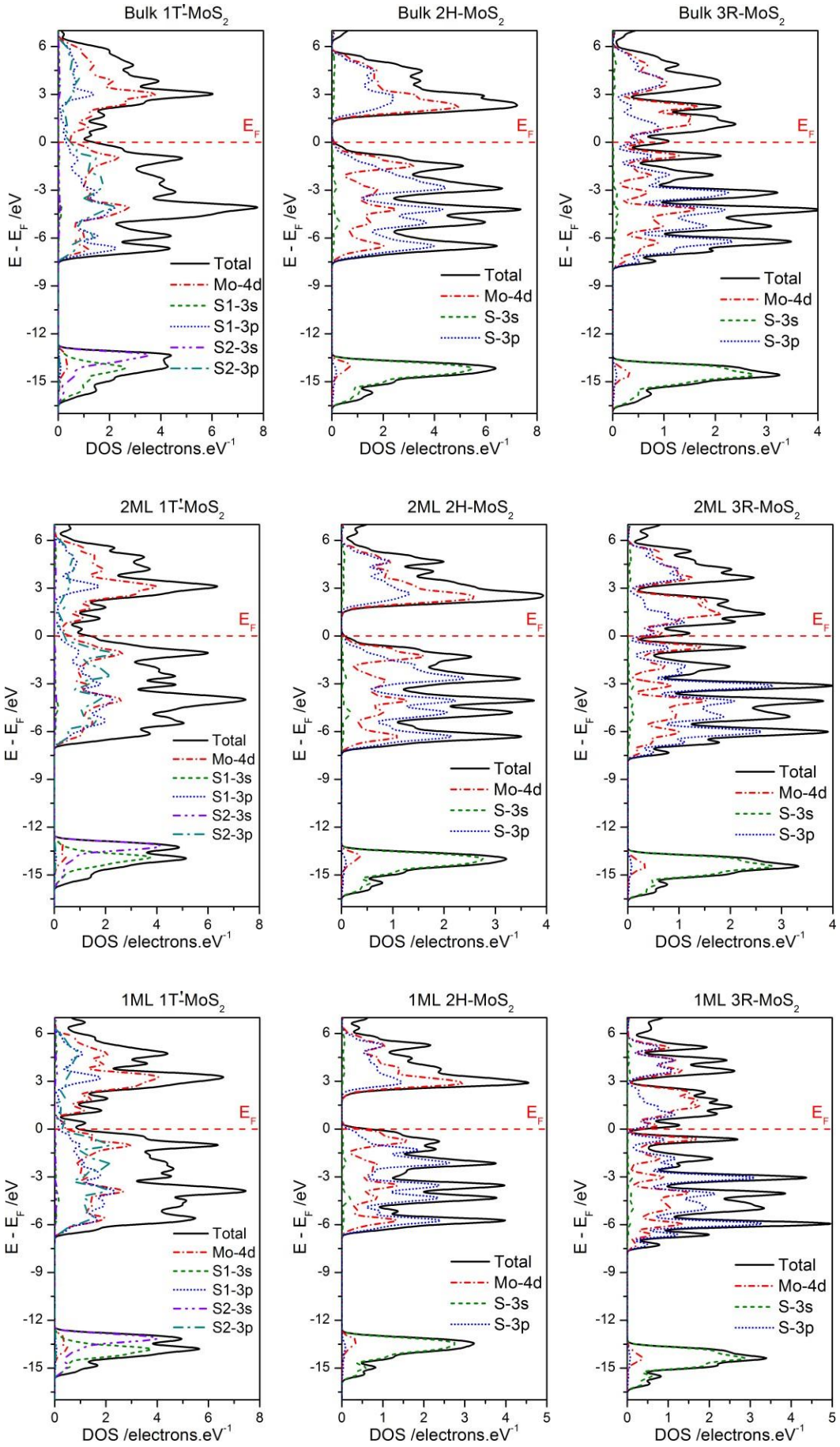

Figure S1. Calculated density of states of MoS_2 bulk, bilayer, and monolayer with different crystal phases

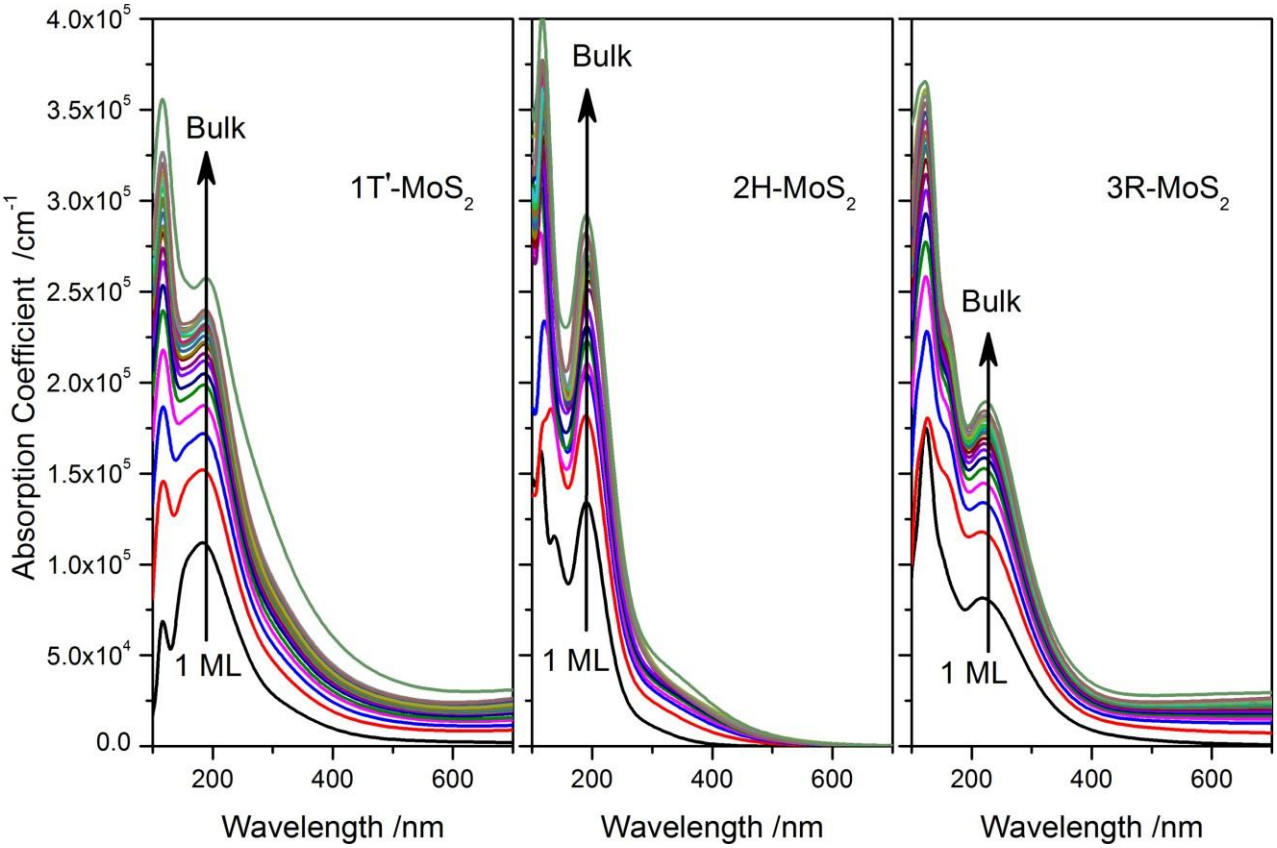

Figure S2. Calculated absorption spectrum of MoS_2 nanosheets with different crystal phases

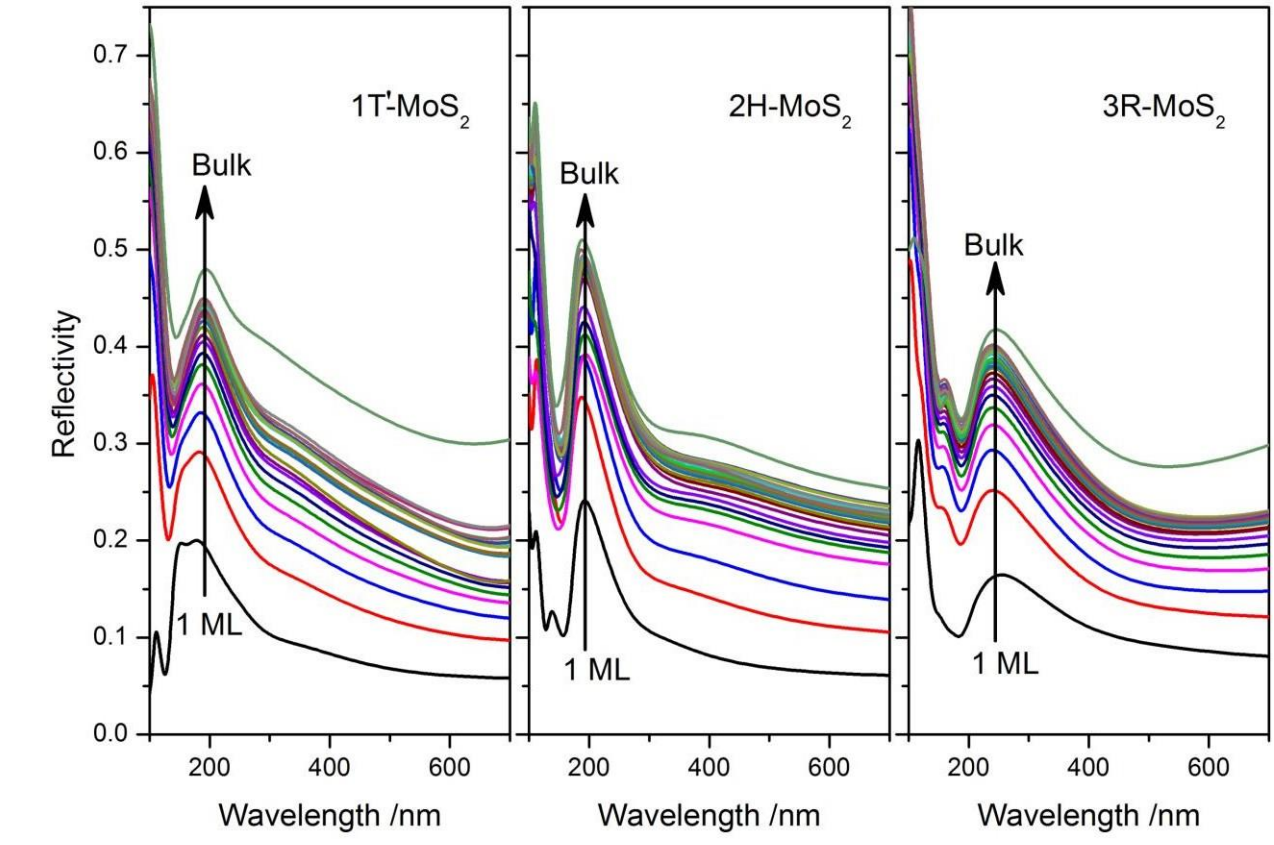

Figure S3. Calculated reflectivity spectrum of MoS_2 nanosheets with different crystal phases