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Supporting Information

Strain-induced semimetal-to-semiconductor transition and indirect-to-direct band gap transition in monolayer 1T-TiS_2

Chengyong Xu, Paul A. Brown, and Kevin L. Shuford*

Department of Chemistry and Biochemistry, Baylor University, One Bear Place #97348, Waco, TX 76798-7348

E-mail: kevin_shuford@baylor.edu

Monolayer TiS_2

Table 1: The effect of strain on the geometry and band gap of monolayer 1T-TiS_2. Negative (Positive) strain means compression (tensile). d_{Ti-S} is the bond length between nearest Ti and S atoms, h_{S-S} represents the interlayer height between upper and lower S atomic planes, and CT means charge transfer from Ti to S atoms. Negative band gap indicates overlapping of valence and conduction bands. VB-CB denotes the transition point from valence to conduction bands, and Ind/Dir refers to whether the transition of VB-CB is indirect or direct.

strain (%)	d_{Ti-S} (Å)	h_{S-S} (Å)	CT (e)	band gap (eV)	VB-CB	Ind/Dir
-10	2.368	3.150	1.528	—	—	—
-9	2.373	3.120	1.546	—	—	—
-8	2.378	3.091	1.566	—	—	—
-7	2.382	3.058	1.608	-1.004	Γ-M	Ind
-6	2.387	3.024	1.613	-0.833	Γ-M	Ind
-5	2.394	2.999	1.626	-0.670	Γ-M	Ind
-4	2.400	2.968	1.639	-0.521	Γ-M	Ind
-3	2.407	2.939	1.656	-0.379	Γ-M	Ind
-2	2.413	2.909	1.673	-0.246	Γ-M	Ind
-1	2.420	2.879	1.685	-0.121	Γ-M	Ind
0	2.427	2.851	1.702	-0.005	Γ-M	Ind
+1	2.435	2.822	1.721	0.106	Γ-M	Ind
+2	2.443	2.794	1.732	0.211	Γ-M	Ind
+3	2.451	2.766	1.742	0.309	Γ-M	Ind
+4	2.459	2.737	1.741	0.401	Γ-M	Ind
+5	2.467	2.708	1.746	0.487	Γ-M	Ind
+6	2.476	2.677	1.752	0.567	Γ-Γ	Dir
+7	2.484	2.646	1.759	0.594	Γ-Γ	Dir
+8	2.492	2.614	1.762	0.618	Γ-Γ	Dir
+9	2.500	2.581	1.769	0.641	Γ-Γ	Dir
+10	2.508	2.547	1.771	0.601	I-Γ	Ind
+11	2.516	2.511	1.779	0.550	I-Γ	Ind
+12	2.524	2.474	1.777	0.507	I-Γ	Ind
+13	2.532	2.436	1.777	0.470	I-Γ	Ind
+14	2.540	2.396	1.779	0.440	I-Γ	Ind
+15	2.548	2.354	1.778	0.431	I-Γ	Ind
+16	2.555	2.311	1.775	0.400	I-Γ	Ind
+17	2.563	2.267	1.778	0.389	I-Γ	Ind
+18	2.571	2.222	1.773	0.383	I-Γ	Ind
+19	2.578	2.174	1.771	0.384	I-Γ	Ind
+20	2.586	2.125	1.768	0.389	I-Γ	Ind

Bulk TiS_2

Bulk TiS_2 crystallizes in the 1T-CdI_2 structure with a $P\bar{3}m1$ space group symmetry. The geometric and electronic properties of bulk TiS_2 have been calculated using VASP[1] with projector augmented wave pseudopotentials.[2] The zero-damping DFT-D3 method of Grimme[3] was adopted to describe the van der Waals interaction between adjacent TiS_2 layers. The optimization and energy calculation of bulk TiS_2 were performed on a dense k-point mesh of 25×25×15 and 35×35×15, respectively. We obtained lattice constants for bulk TiS_2 of $a = 3.4$ Å and $c = 5.7$ Å, in good agreement with other reports.[4–6] The band structure and density of states for bulk 1T-TiS_2 are shown in 1. The Fermi level (E_F) crosses the valence band and conduction band simultaneously, indicating a semimetallic nature.

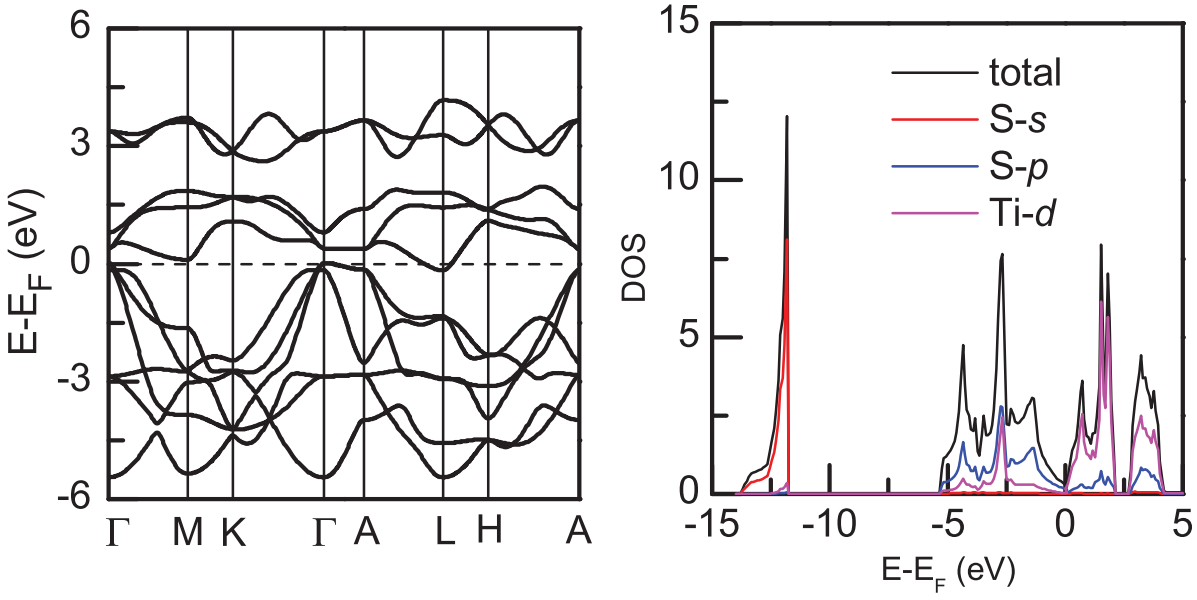

Figure 1: Band structure and density of states of bulk 1T-TiS_2.

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