

**Electrical Contact Property and Control Effects for Stable
T(H)-TaS₂/C₃B Metal-Semiconductor Heterojunction**

*Cao Shengguo, Li Zhanhai, Han Jianing, Zhang Zhenhua**

Supplementary Information

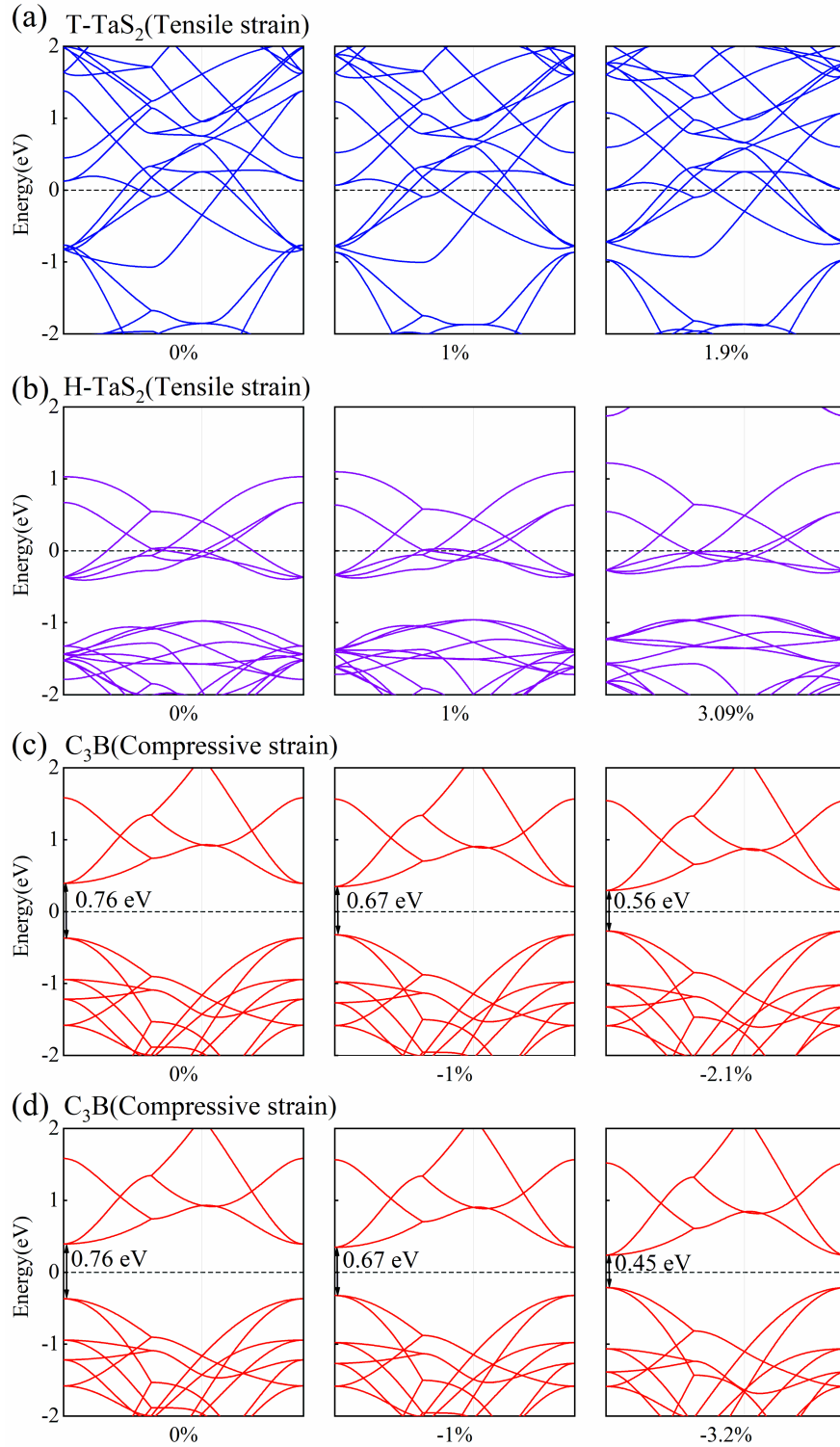


Fig. S1 (a) and (b) the band structure of T-TaS₂ and H-TaS₂ monolayers under different tensile strains, where the largest tensile strains just correspond to fully match the T(H)-TaS₂ and H-TaS₂ monolayers to the intrinsic C₃B monolayer, respectively. (c) and (d) the band structure of C₃B under different compressive strains, where the largest compressive strains just correspond to fully match the C₃B monolayer to the intrinsic T-TaS₂ and H-TaS₂, respectively.

Table S1 Mismatch rate, interlayer distance, and binding energy for various stack configurations.

Heterojunction	Mismatch rate(%)	Stack configuration	Interlayer distances(\AA)	Binding energy($\text{meV}/\text{\AA}^2$)
T-TaS ₂ /C ₃ B	1.90	A ₁	3.32	-45.64
		A ₂	3.33	-44.89
		A ₃	3.33	-44.89
		A ₄	3.34	-44.88
H-TaS ₂ /C ₃ B	3.09	B ₁	3.33	-43.62
		B ₂	3.33	-43.62
		B ₃	3.33	-43.63
		B ₄	3.33	-43.62

Table S2 Tunnel barrier height (Φ_{TB}), half width of the tunneling barrier(W_{TB}), tunneling probability (T_{TB}) and comprehensive factor (C) of heterojunctions

	$W_{TB}(\text{\AA})$	$\Phi_{TB}(\text{eV})$	$T_{TB}(\%)$	$C(\text{eV}\text{\AA}^{-2})$
T-TaS ₂ /C ₃ B	1.28	19.17	2.58%	31.40
H-TaS ₂ /C ₃ B	1.22	17.56	3.57%	26.14

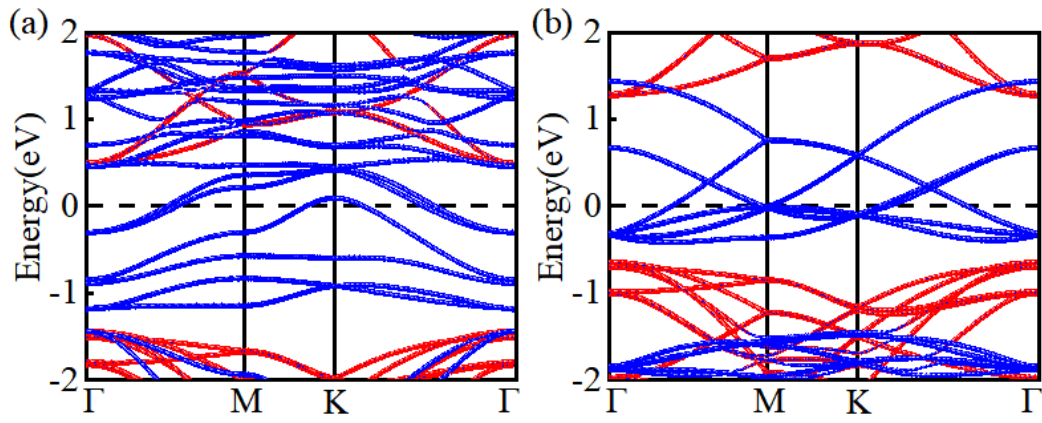


Fig. S2 Projected band structure for heterojunctions by HSE06 calculations: (a) T-TaS₂/C₃B, (b) H-TaS₂/C₃B, where red, blue and purple represent the projected band structure of the C₃B, T-TaS₂, and H-TaS₂ monolayer, respectively.

* Corresponding author.

E-mail: zhzhang@csust.edu.cn