

## Support Information

### Band alignment of one-dimensional transition-metal dichalcogenide heterotubes

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Table S1. The diameter (in the unit of Å) of both inner and outer ac MoS<sub>2</sub>@WS<sub>2</sub> and WS<sub>2</sub>@MoS<sub>2</sub> heterotubes.

MoS <sub>2</sub> @WS <sub>2</sub>		WS <sub>2</sub> @MoS <sub>2</sub>	
D_Inner	D_Outer	D_Inner	D_Outer
14.304	26.667	14.336	26.588
15.972	28.353	16.029	28.321
17.638	30.085	17.698	30.055
19.286	31.786	19.348	31.756
21.000	33.597	21.064	33.574
22.700	35.350	22.765	35.334
24.385	37.068	24.447	37.045
26.088	38.799	26.145	38.779

Table S2. The diameter (in the unit of Å) of both inner and outer zz MoS<sub>2</sub>@WS<sub>2</sub> and WS<sub>2</sub>@MoS<sub>2</sub> heterotubes.

MoS <sub>2</sub> @WS <sub>2</sub>		WS <sub>2</sub> @MoS <sub>2</sub>	
D_Inner	D_Outer	D_Inner12.264	D_Outer24.148
13.191	25.180	13.231	25.154
14.132	26.165	14.169	26.141
15.083	27.175	15.133	27.143
16.019	28.171	16.088	28.157
16.996	29.139	17.029	29.109
17.966	30.120	17.992	30.097
21.783	34.086	21.862	34.044
22.924	35.283	22.975	35.241
23.810	36.101	23.835	36.077
24.814	37.135	24.842	37.110

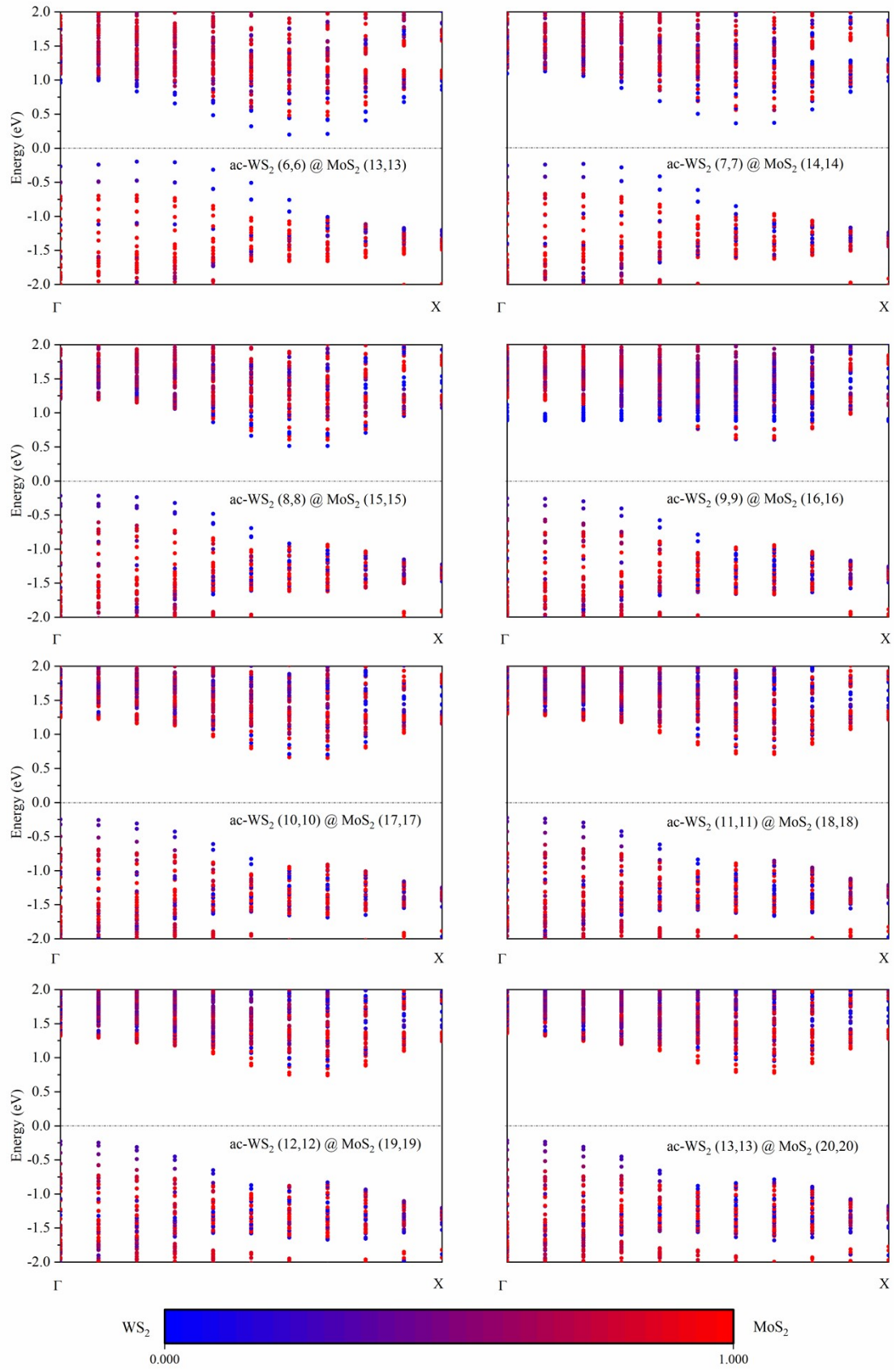


FIG. S1. Band structures of 1D AC WS<sub>2</sub>@MoS<sub>2</sub> heterotubes.

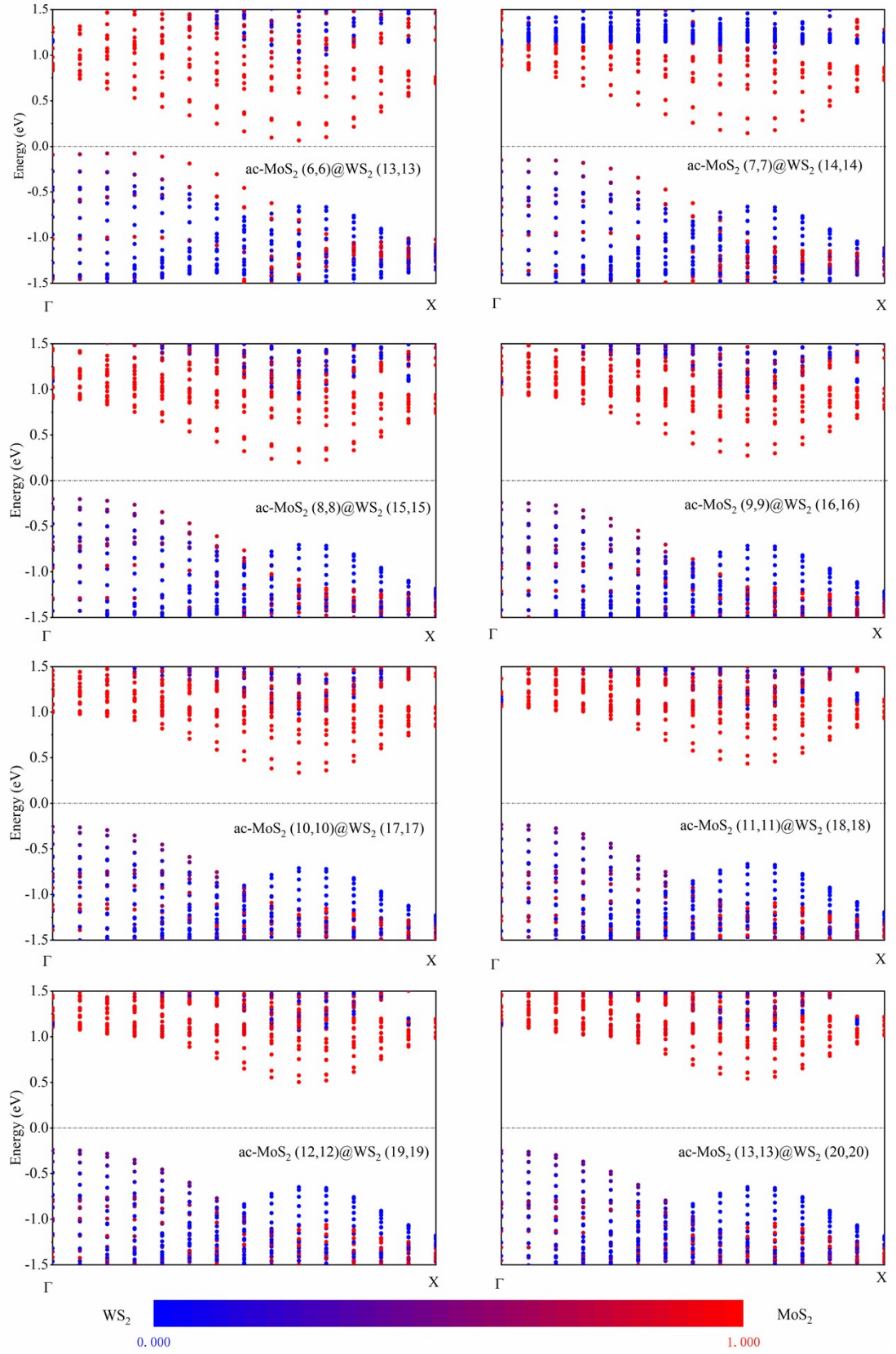


FIG. S2. Band structures of 1D AC  $\text{MoS}_2@WS_2$  heterotubes.

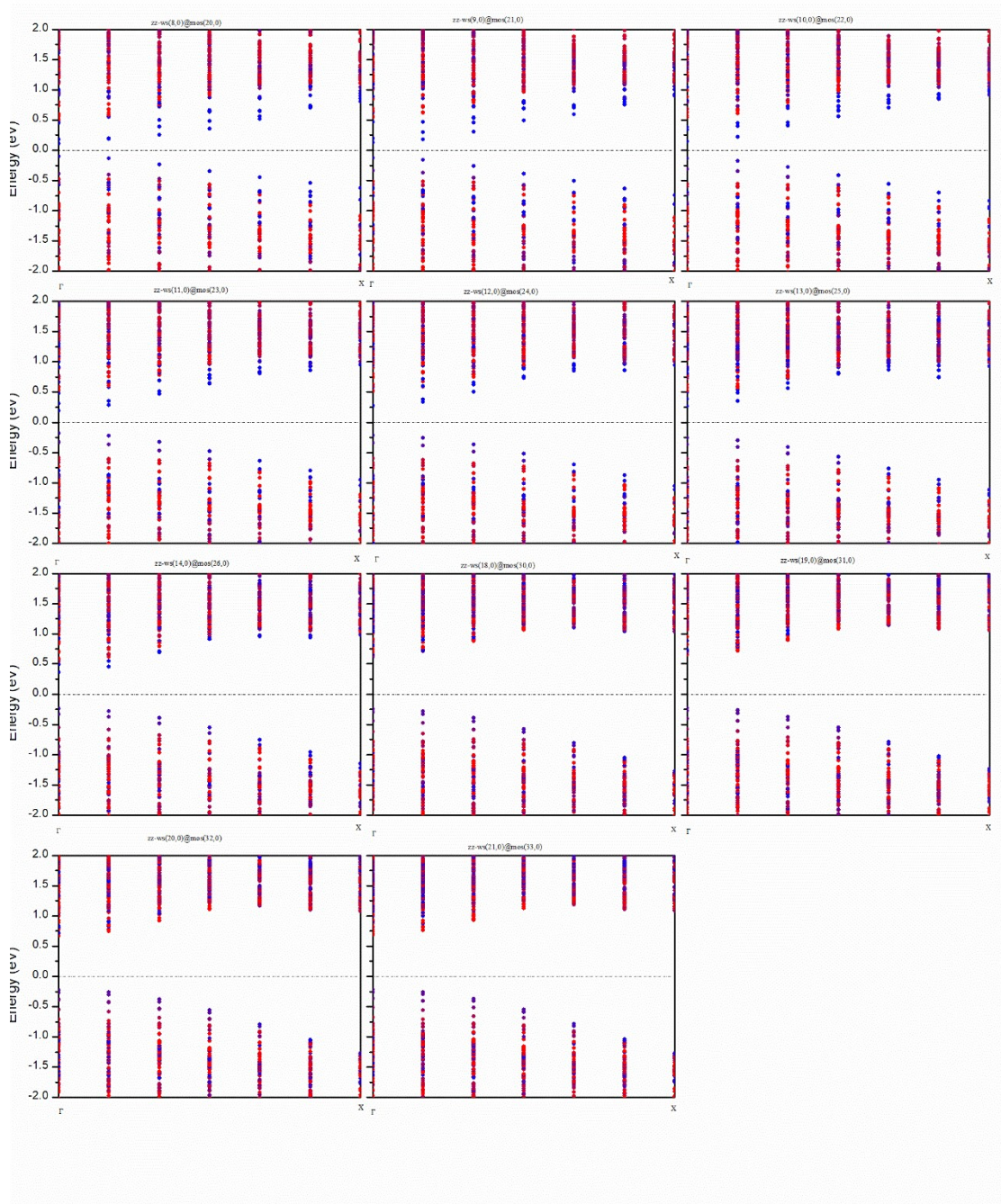


FIG. S3. Band structures of 1D ZZ WS<sub>2</sub>@MoS<sub>2</sub> heterotubes.



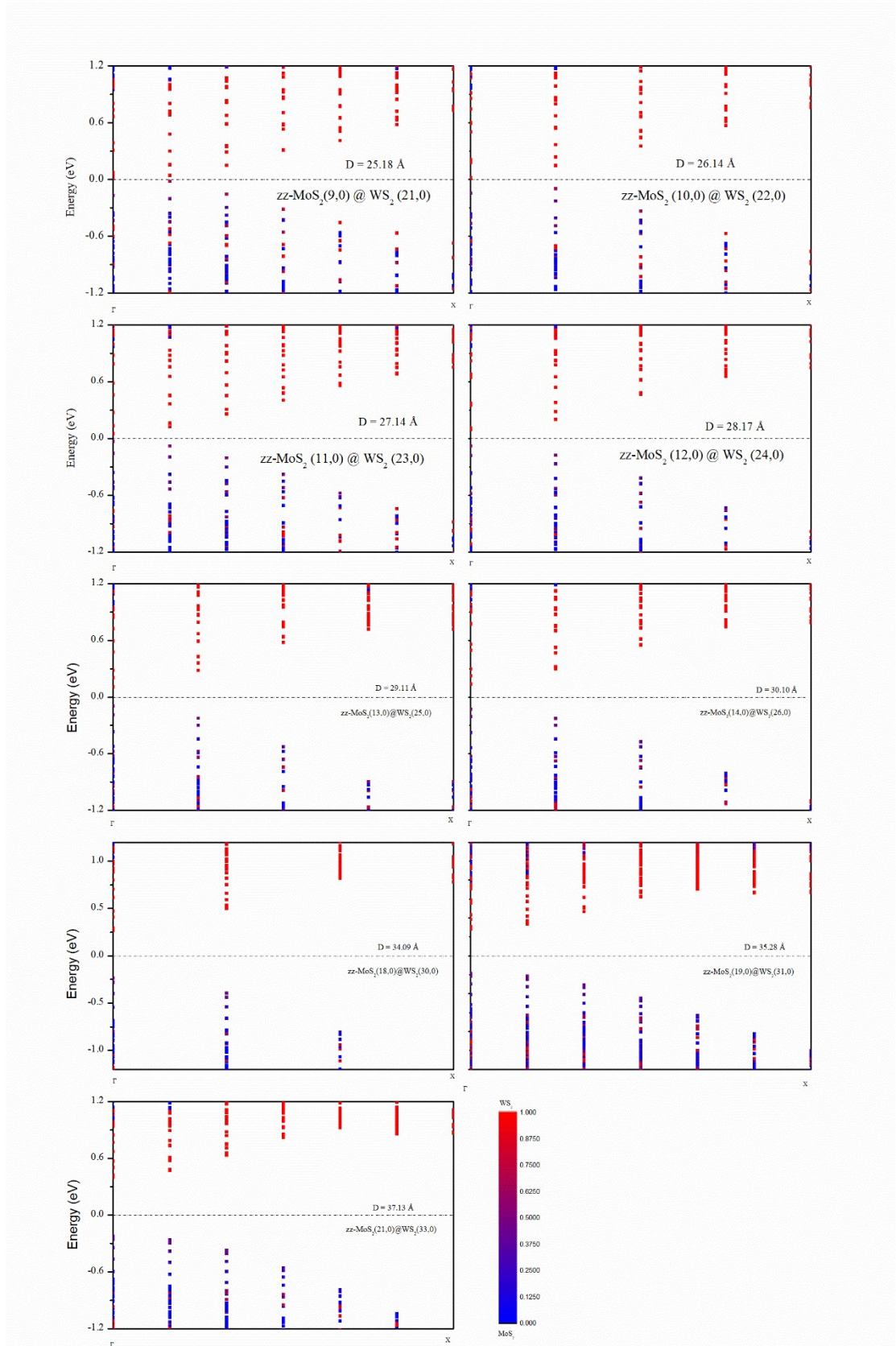


FIG. S4. Band structures of 1D ZZ  $\text{MoS}_2@WS_2$  heterotubes.

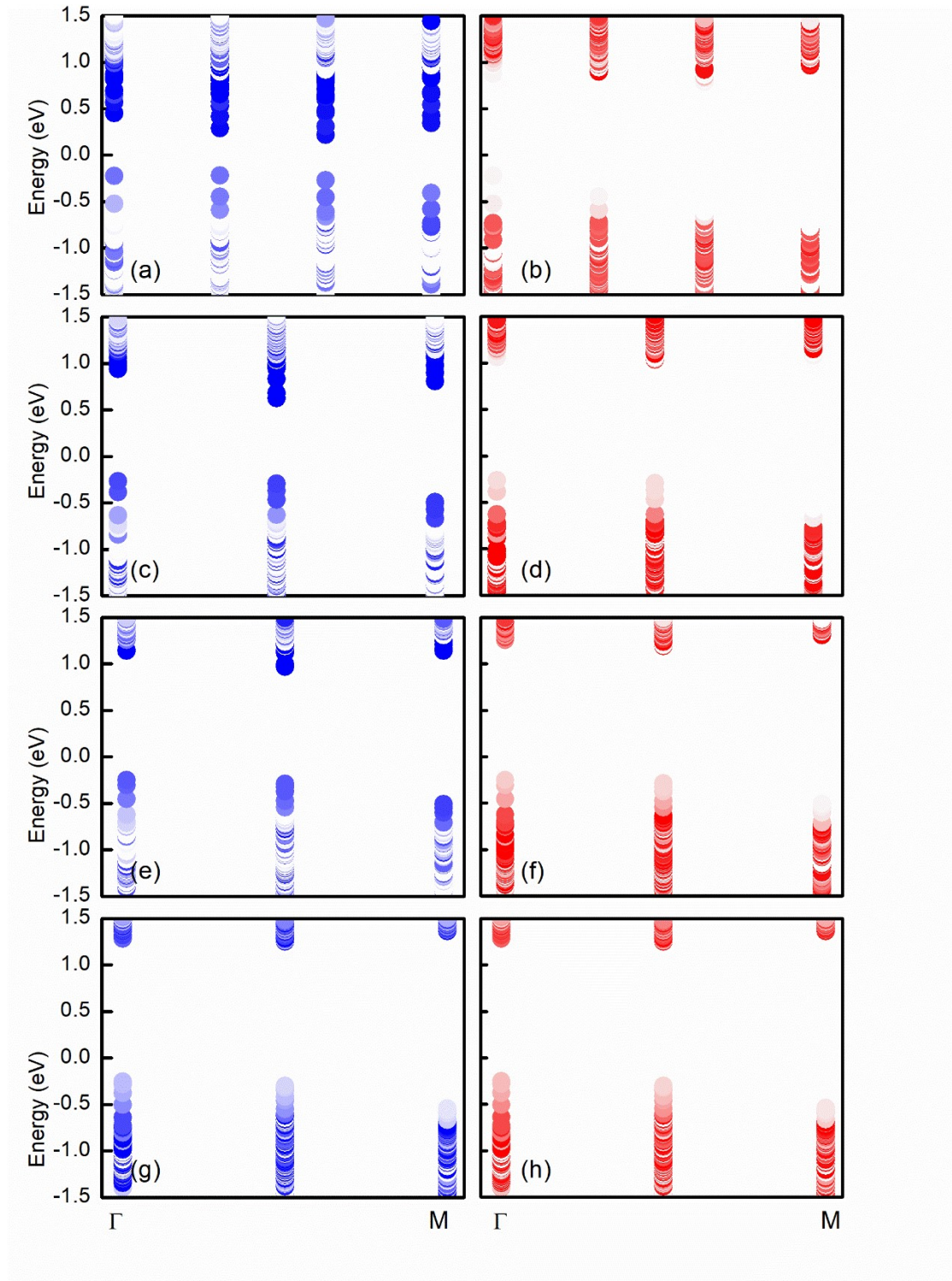


FIG. S5. Band structures of 1D chiral  $(41|41)$   $\text{WS}_2@MoS_2$  heterotubes.



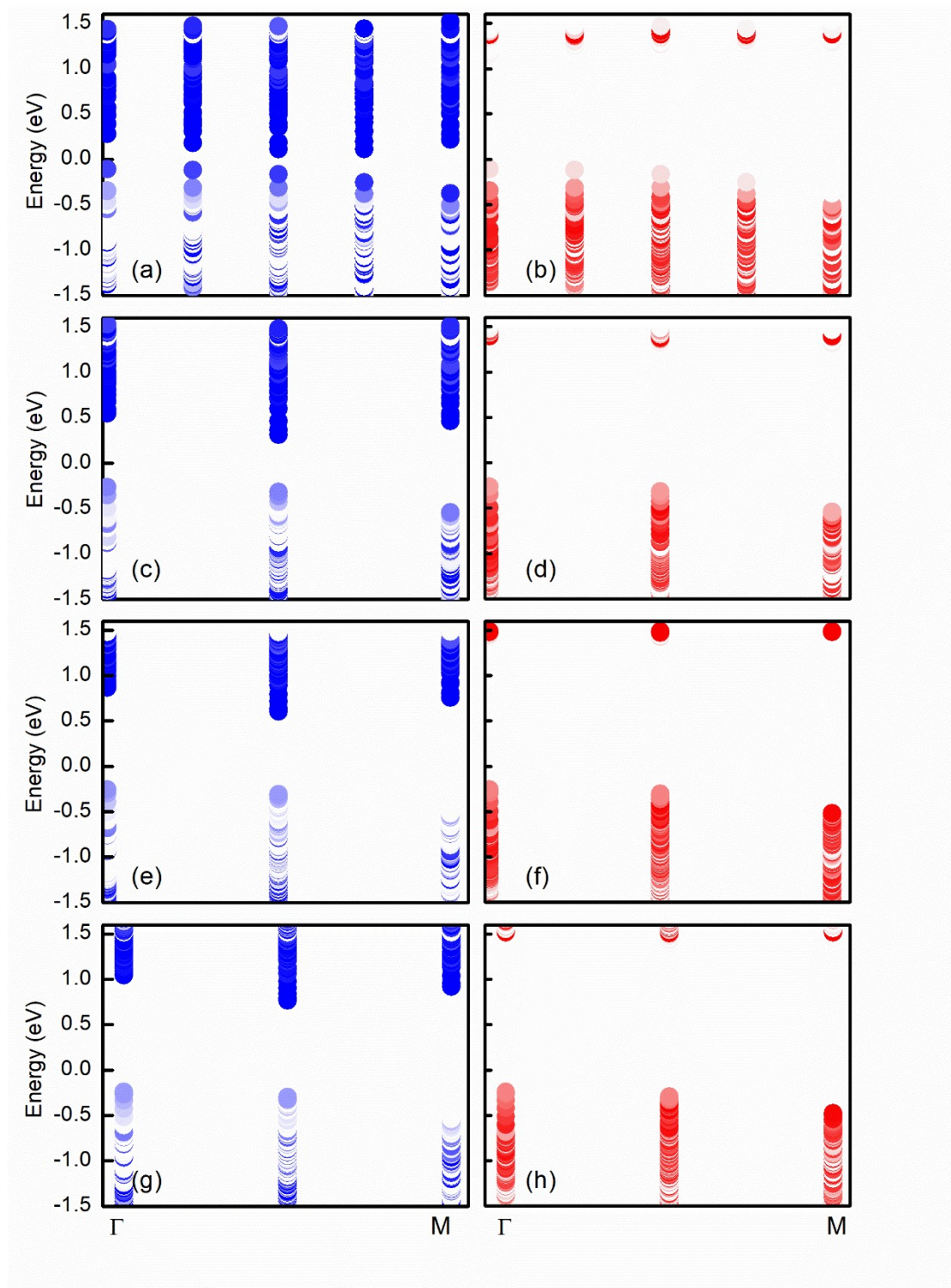


FIG. S6. Band structures of 1D chiral (41|41) MoS<sub>2</sub>@WS<sub>2</sub> heterotubes.