

Supporting Information

Tuning Electronic Structures of $\text{Sc}_2\text{CO}_2/\text{MoS}_2$ Polar-Nonpolar van der Waals Heterojunctions: Interplay of Internal and External Electric Field

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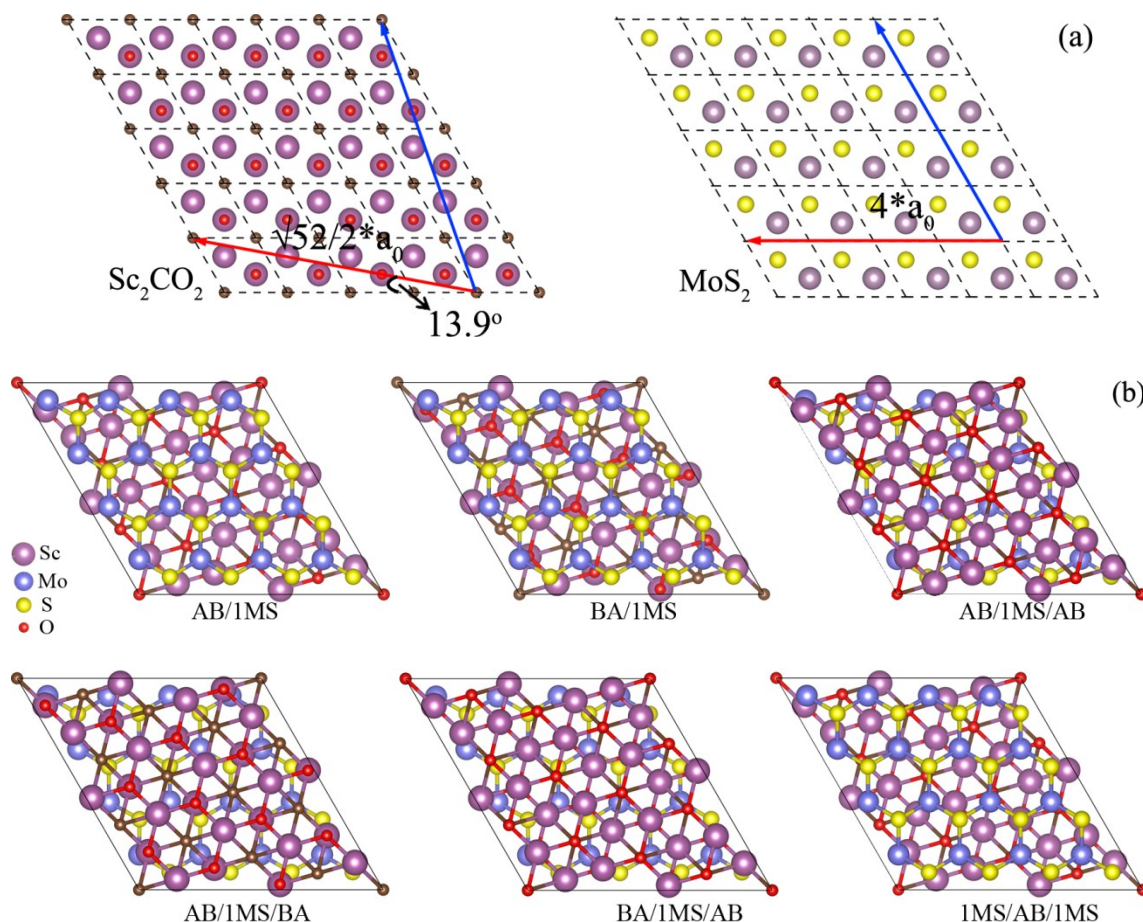
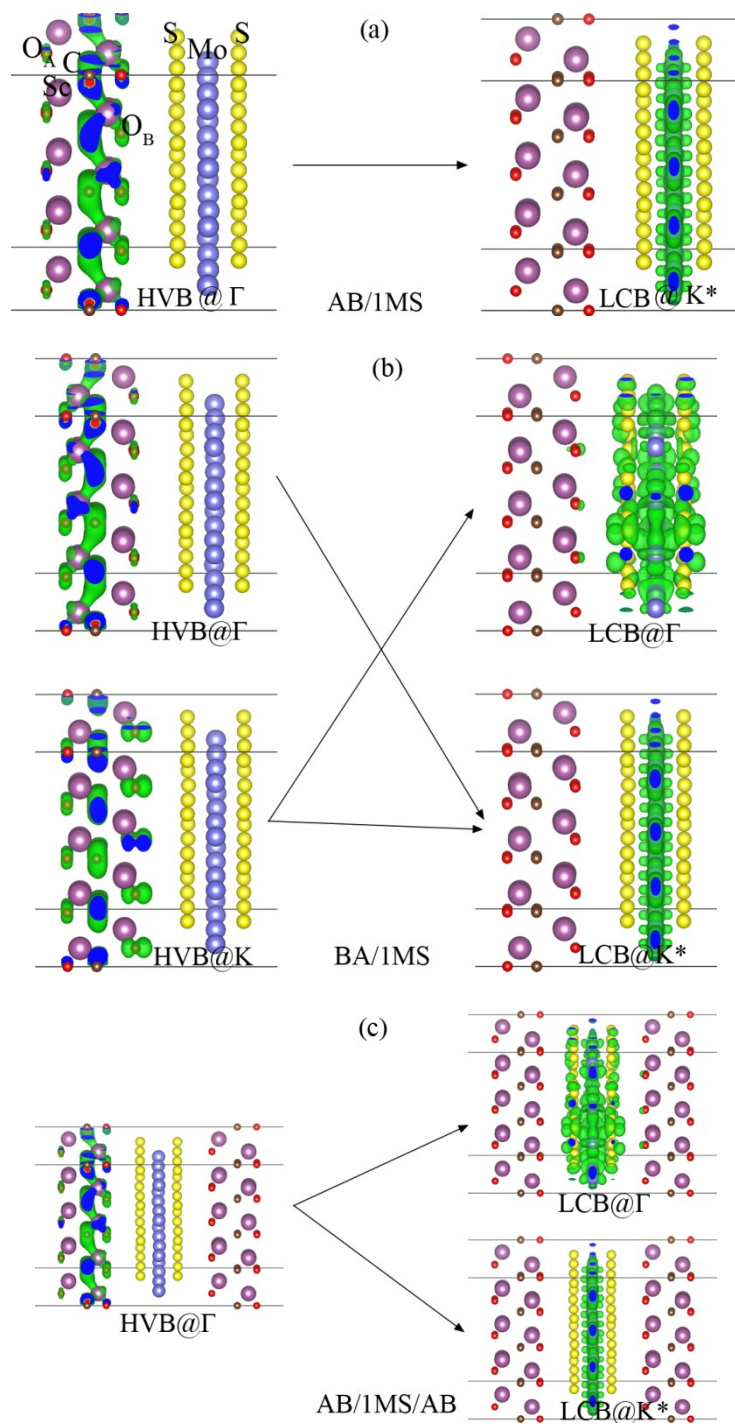


Fig. S1 (a) The supercell (red and blue lines) of Sc_2CO_2 and MoS_2 that used in $\text{Sc}_2\text{CO}_2/\text{MoS}_2$ heterojunctions. (b) Top views of $\text{Sc}_2\text{CO}_2/\text{MoS}_2$ heterojunctions.



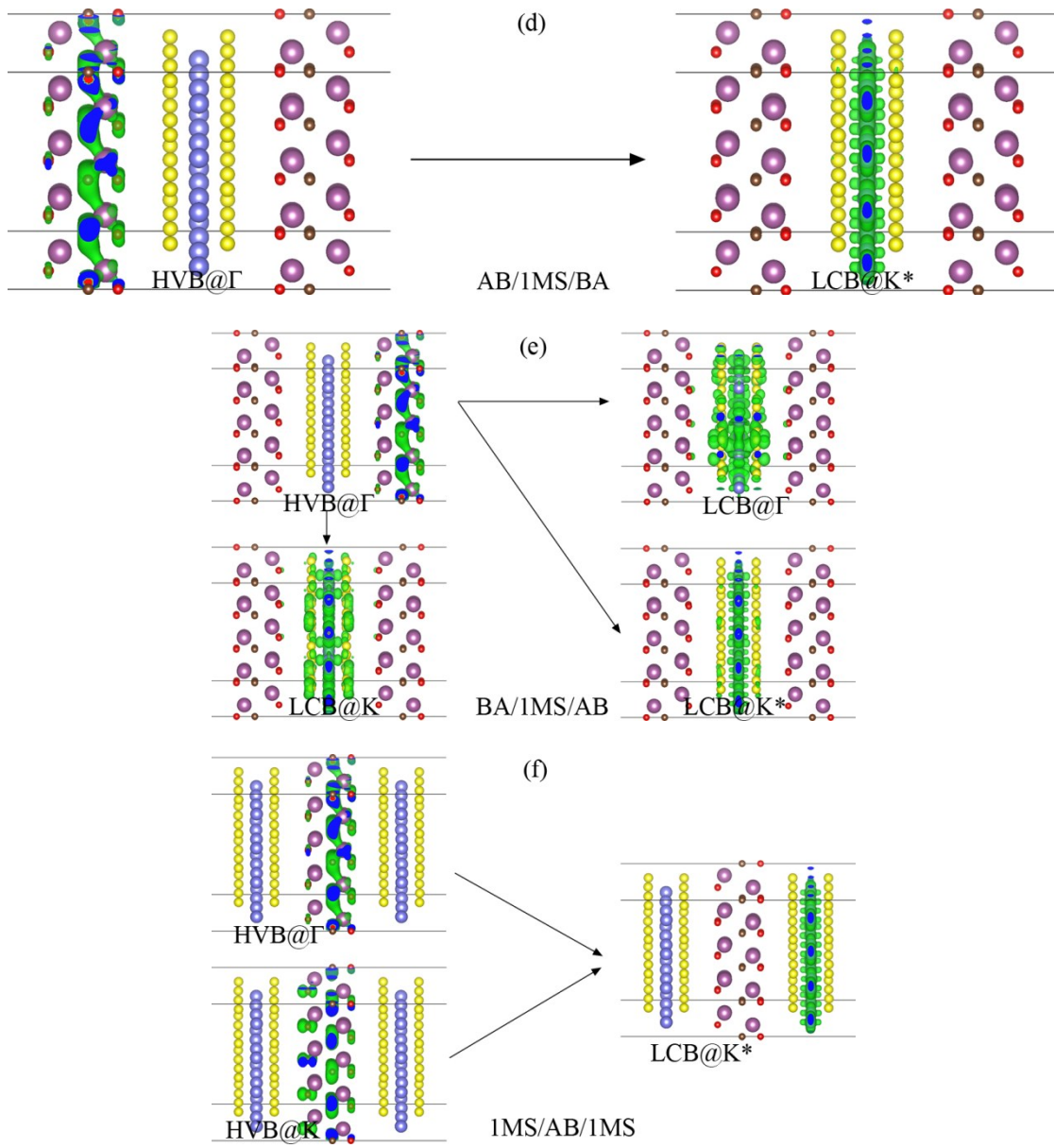


Fig. S2 Charge densities of VBM and CBM for $\text{Sc}_2\text{CO}_2/\text{MoS}_2$ heterojunctions, and the transitions under the external electric field.

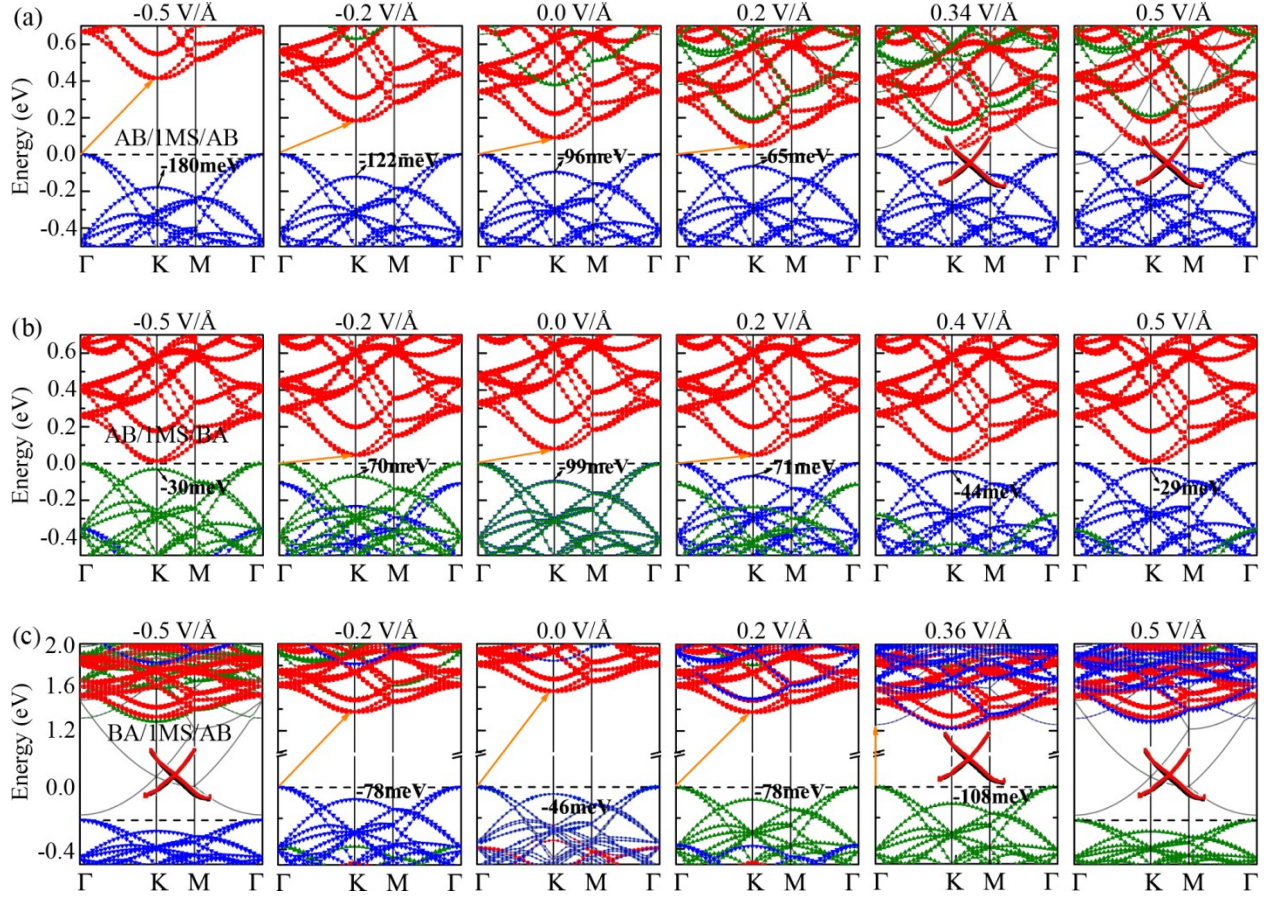


Fig. S3 The dependence of band structure on external electric field. (a) AB/1MS/AB; (b) AB/1MS/BA and (c) BA/1MS/AB. Red cross: unphysical states.

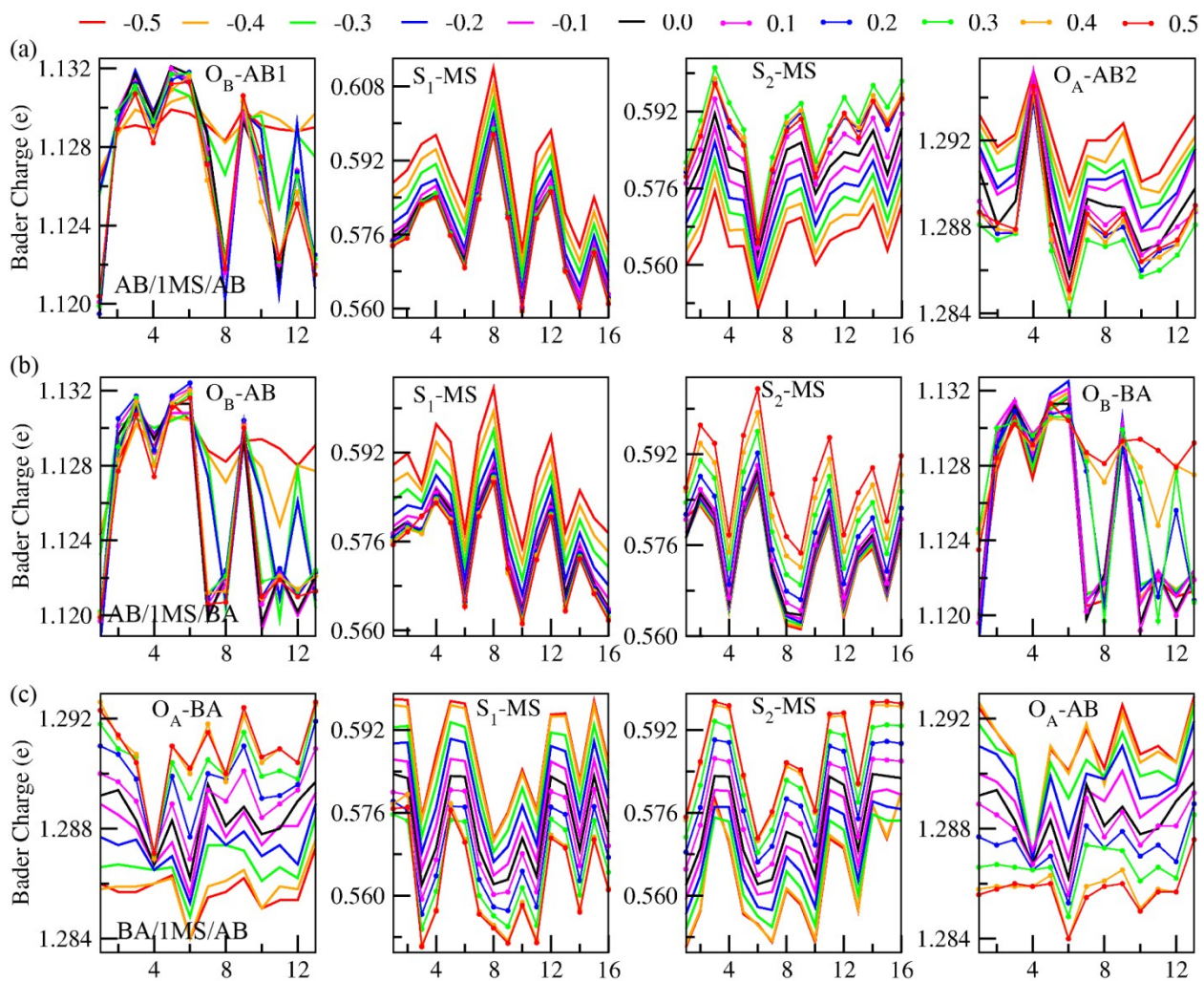


Fig. S4 Charge distribution at interface of AB/IMS/AB, AB/IMS/BA and BA/IMS/AB heterojunctions.

Table S1. The dependence of lattice parameter a (upper, Å) and interlayer distance (lower, Å) on external electric field (V/Å).

	−0.5	−0.4	−0.3	−0.2	−0.1	0.0	0.1	0.2	0.3	0.4	0.5
AB/1M S	12.428	12.429	12.430	12.434	12.436	12.439	12.441	12.443	12.445	12.447	12.450
	2.850	2.848	2.846	2.845	2.844	2.843	2.843	2.843	2.843	2.844	2.845
BA/1M S	12.459	12.455	12.453	12.451	12.449	12.445	12.444	12.442	12.441	12.437	12.436
	2.937	2.934	2.930	2.925	2.922	2.918	2.915	2.911	2.908	2.905	2.903
AB/1M S/AB	12.392	12.394	12.396	12.395	12.398	12.397	12.399	12.402	12.405	12.404	12.406
	2.880/ 2.941	2.879/ 2.944	2.878/ 2.947	2.876/ 2.950	2.875/ 2.952	2.874/ 2.953	2.873/ 2.956	2.873/ 2.960	2.873/ 2.966	2.873/ 2.962	2.873/ 2.963
AB/1M S/BA	12.395	12.394	12.393	12.393	12.393	12.392	12.393	12.392	12.394	12.394	12.395
	2.885/ 2.879	2.884/ 2.879	2.882/ 2.879	2.881/ 2.880	2.879/ 2.880	2.879/ 2.881	2.878/ 2.881	2.878/ 2.883	2.877/ 2.884	2.877/ 2.885	2.876/ 2.886
BA/1M S/AB	12.407	12.406	12.406	12.405	12.404	12.403	12.404	12.405	12.406	12.406	12.407
	2.934/ 2.917	2.933/ 2.918	2.930/ 2.922	2.927/ 2.925	2.924/ 2.927	2.921/ 2.928	2.920/ 2.932	2.918/ 2.935	2.916/ 2.938	2.913/ 2.943	2.913/ 2.942
1MS/A B/1MS	12.485	12.486	12.487	12.486	12.487	12.487	12.489	12.491	12.493	12.495	12.495
	2.989/ 2.854	2.993/ 2.853	2.996/ 2.851	2.999/ 2.849	3.001/ 2.848	3.003/ 2.846	3.006/ 2.846	3.009/ 2.846	3.013/ 2.846	3.016/ 2.847	3.017/ 2.846