Supporting Information:

Systematic Search for Highly Symmetric Transition Metal Dichalcogenide Multilayers

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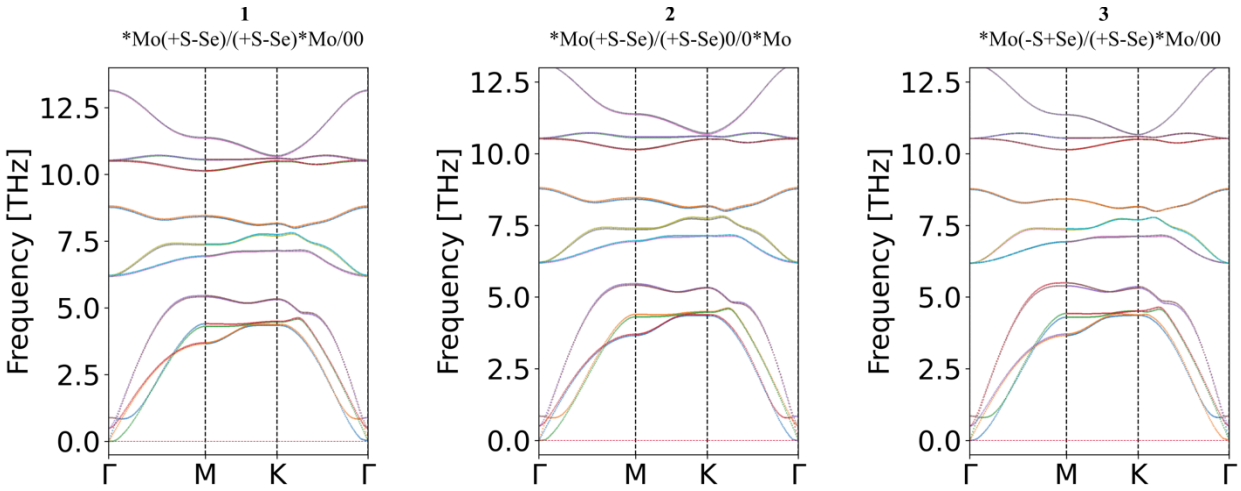

Figure S1. Phonon band structures of the three lowest-energy MoSSe bilayers.

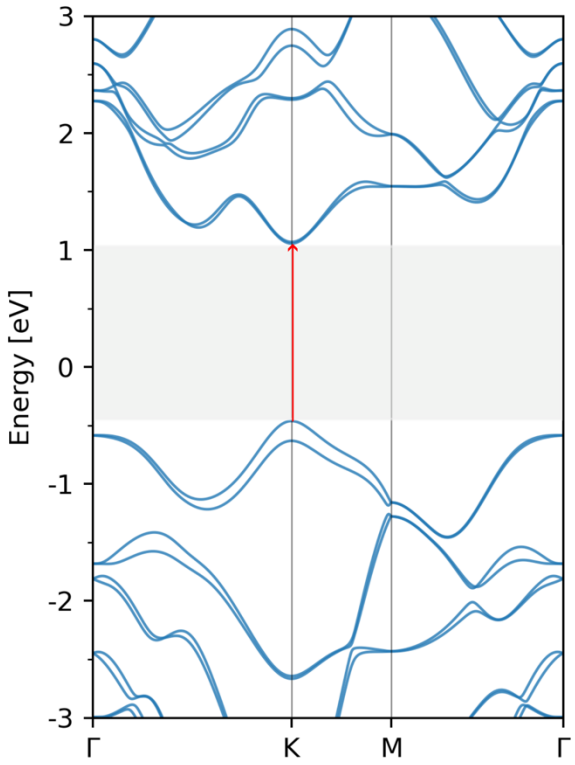

Figure S2. Electronic band structure of the MoSSe monolayer.

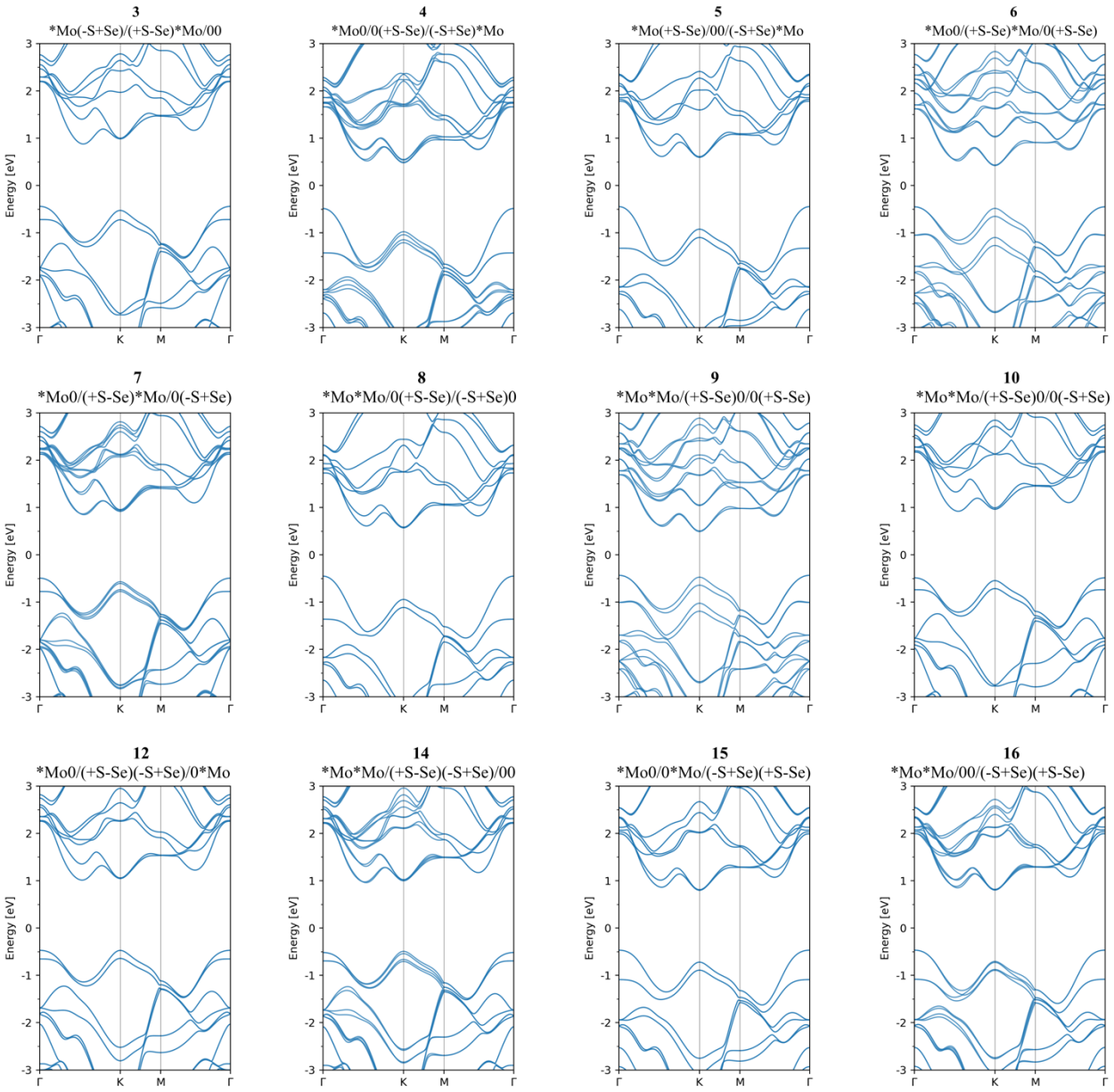

Figure S3. Electronic band structures of the MoSSe bilayers.

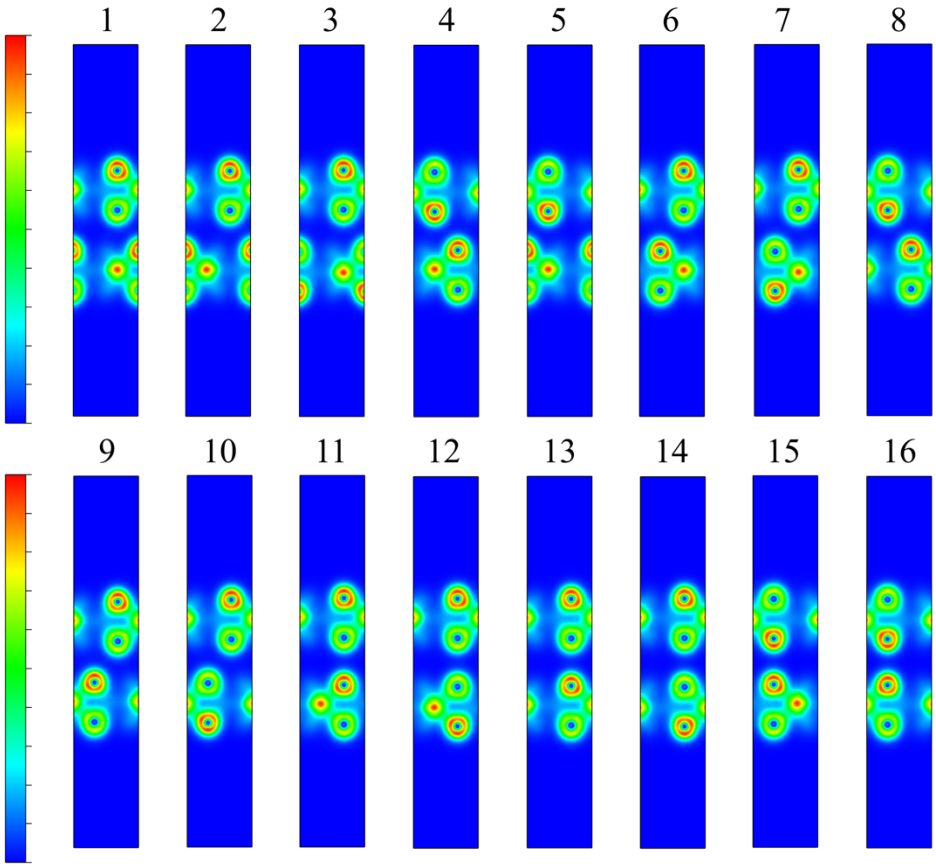

Figure S4. Charge density maps of the MoSSe bilayers.

Table S1. Interlayer distances (Å), *d*, and relative energies (meV/atom), *ΔE*, for MoSSe bilayer stackings computed at the PBE-D3 and optB86b-vdW levels of theory.

PBE-D3		**optB86b-vdW**	
d	***ΔE***	***d***	***ΔE***
1.16	3.11	0.28	3.11
0.96	3.08	0.00	3.07
0.00	3.21	0.64	3.20
3.34	2.99	0.66	2.98
3.93	3.04	1.27	3.04
1.95	3.12	1.23	3.13
1.06	3.24	1.84	3.22
5.14	3.04	2.49	3.01
4.04	3.19	3.34	3.17
4.17	3.35	5.20	3.34
13.08	3.65	12.18	3.67
12.20	3.74	12.42	3.78
13.69	3.67	12.76	3.71
12.87	3.77	13.06	3.80
15.13	3.56	13.07	3.60
15.70	3.59	13.62	3.63