

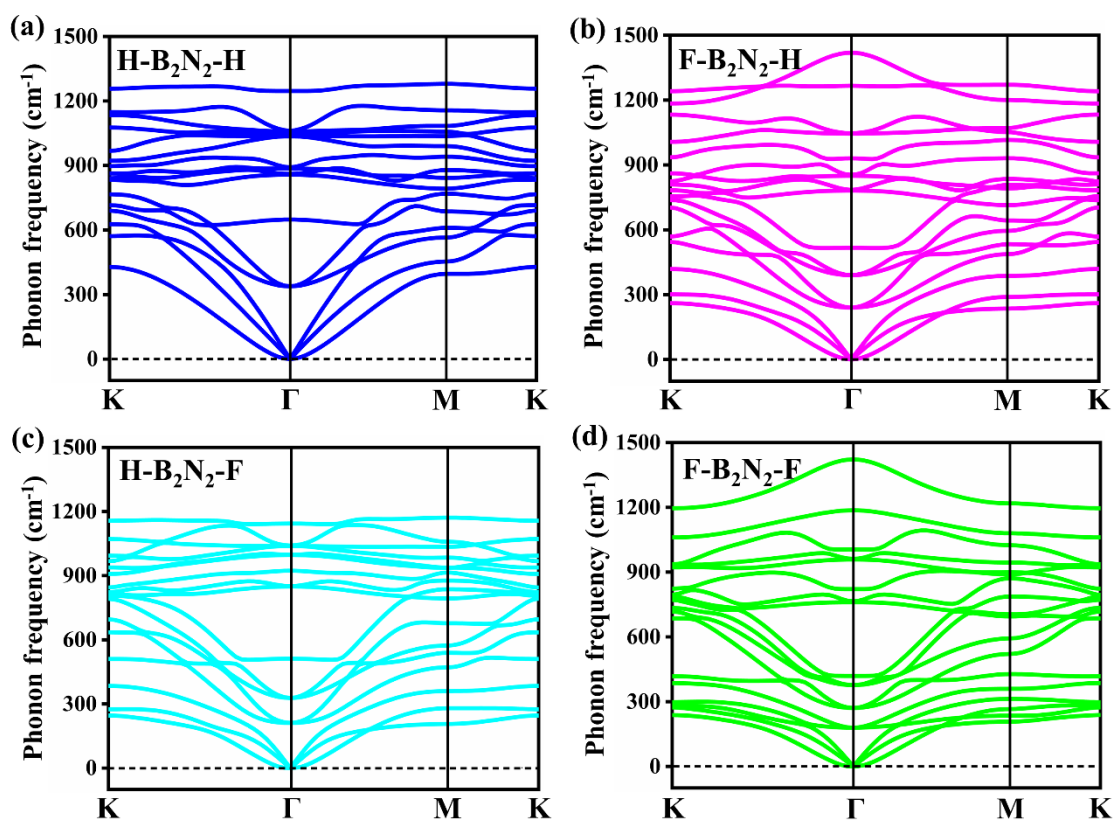
Supporting information for

**Functionalized hexagonal boron nitride bilayers: Desirable electro-optical properties for optoelectronic applications**

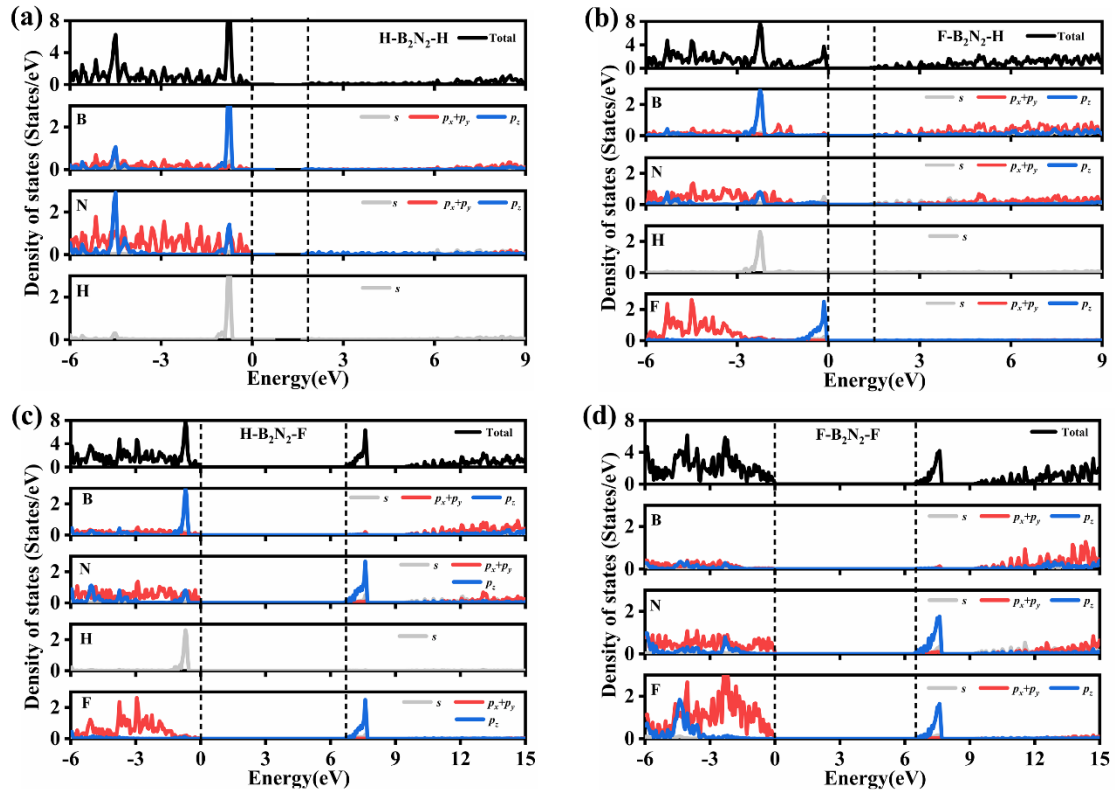
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**Fig. S1** (a)-(d) Phonon spectra of functionalized h-BN bilayers, in which the phonon vibration modes with lower frequencies are provided for the H-B<sub>2</sub>N<sub>2</sub>-H, F-B<sub>2</sub>N<sub>2</sub>-H, H-B<sub>2</sub>N<sub>2</sub>-F, and F-B<sub>2</sub>N<sub>2</sub>-F.



**Fig. S2** The total and projected density of states of the observed systems: (a) H-B<sub>2</sub>N<sub>2</sub>-H, (b) F-B<sub>2</sub>N<sub>2</sub>-H, (c) H-B<sub>2</sub>N<sub>2</sub>-F, and (d) F-B<sub>2</sub>N<sub>2</sub>-F.