Supplementary Information

Intermediate bands and p orbital tuning the band structure of $BiFeO_3$ for photovoltaic application

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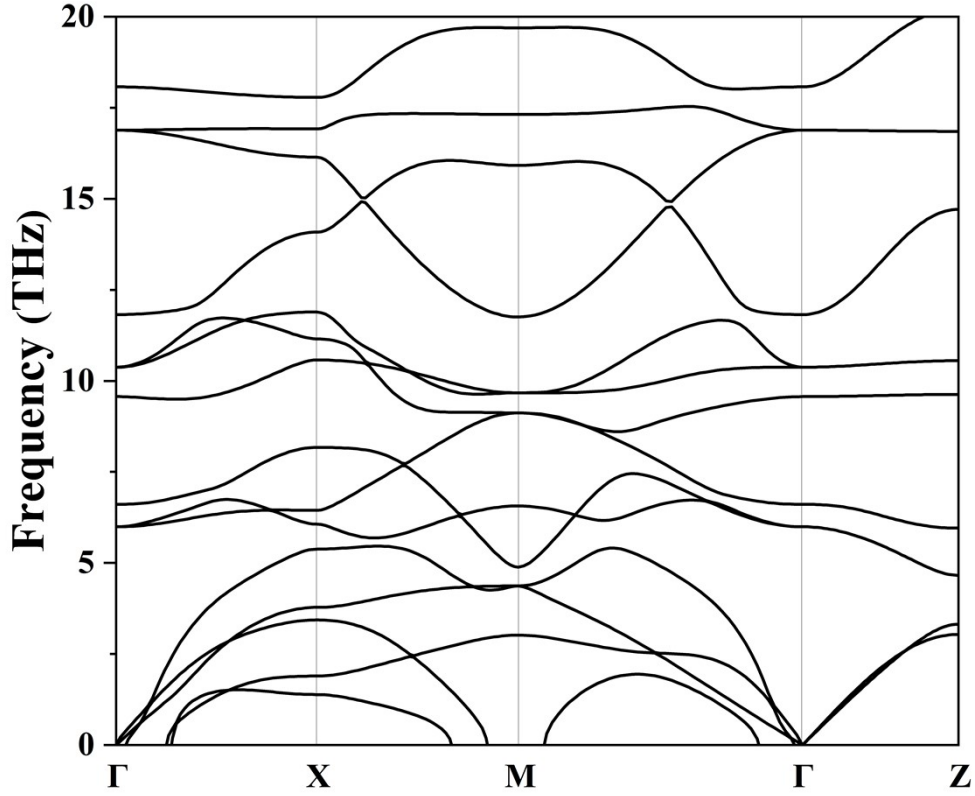

Fig. S1. Phonon spectrum of 80-atom 2×2×1 P4*mm* $BiFeO_3$.

The input files for phonon calculation of pure BFO include INCAR, KPOINTS, POSCAR, and POTCAR.


INCAR.zip


KPOINTS.zip


POSCAR.zip


POTCAR.zip