Supplementary Material for "Theoretical studies of valleytronic, optical and piezoelectric properties in Janus $MoBXY_2$ (X = N, P; Y = S, Se, Te) monolayers"

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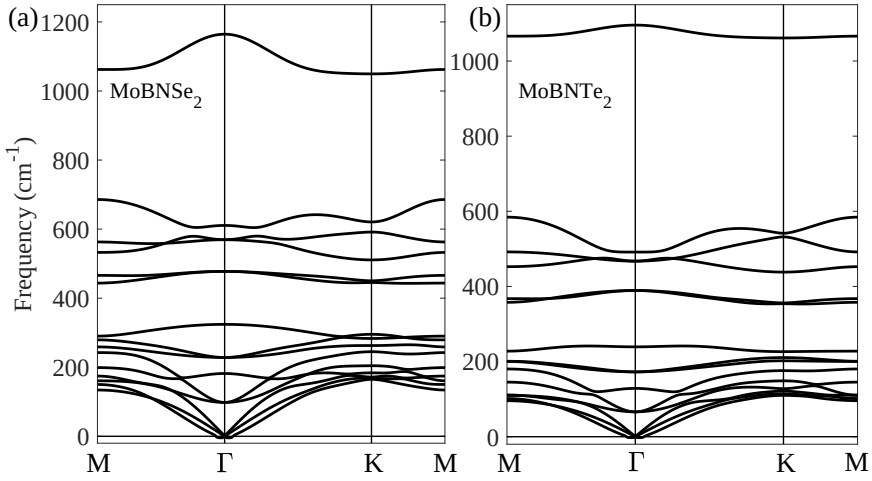

FIG. S1: Phonon dispersion spectrum of monolayer $MoBNSe_2$ (a) and $MoBNTe_2$ (b).

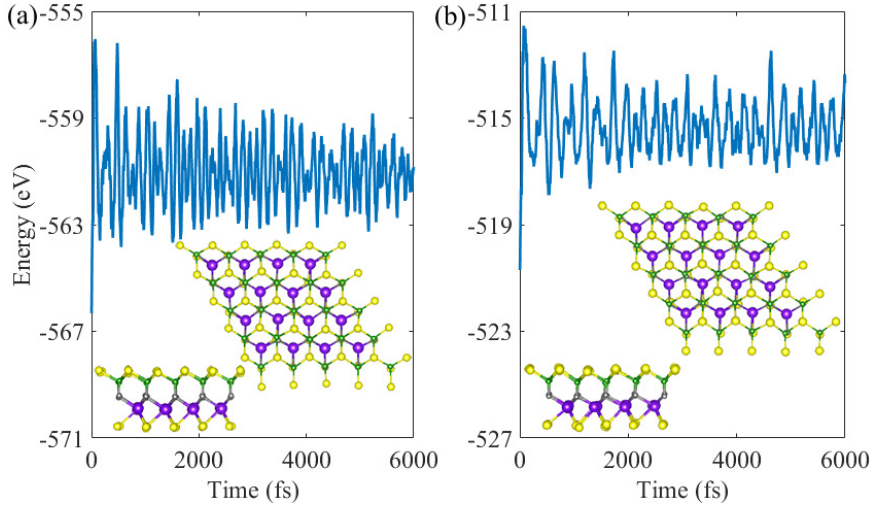

FIG. S2: Total energy fluctuations of $MoBNSe_2$ (a) and $MoBNTe_2$ (b) during AIMD simulations, with snapshots after 6 ps at 500 K shown in the insets.

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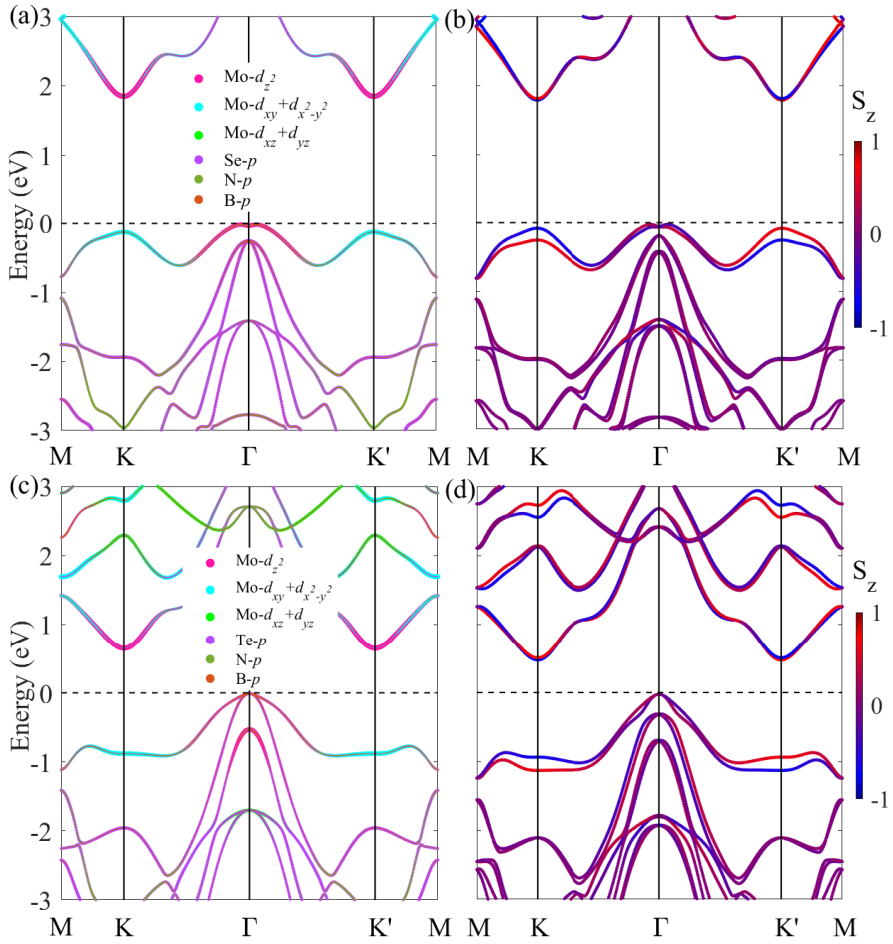

FIG. S3: Orbital-resolved band structures of monolayer $MoBNSe_2$ (a) and $MoBNTe_2$ (c) without considering SOC. Spin-resolved band structures of monolayer $MoBNSe_2$ (b) and $MoBNTe_2$ (d) with considering SOC, where red and blue lines indicate spin-up and spin-down states.