Journal Name

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Supplementary Information for

Electronic, magnetic and optical properties of $MnPX_3$ (X = S, Se) monolayers with and without chalcogen defects: A first-principle study

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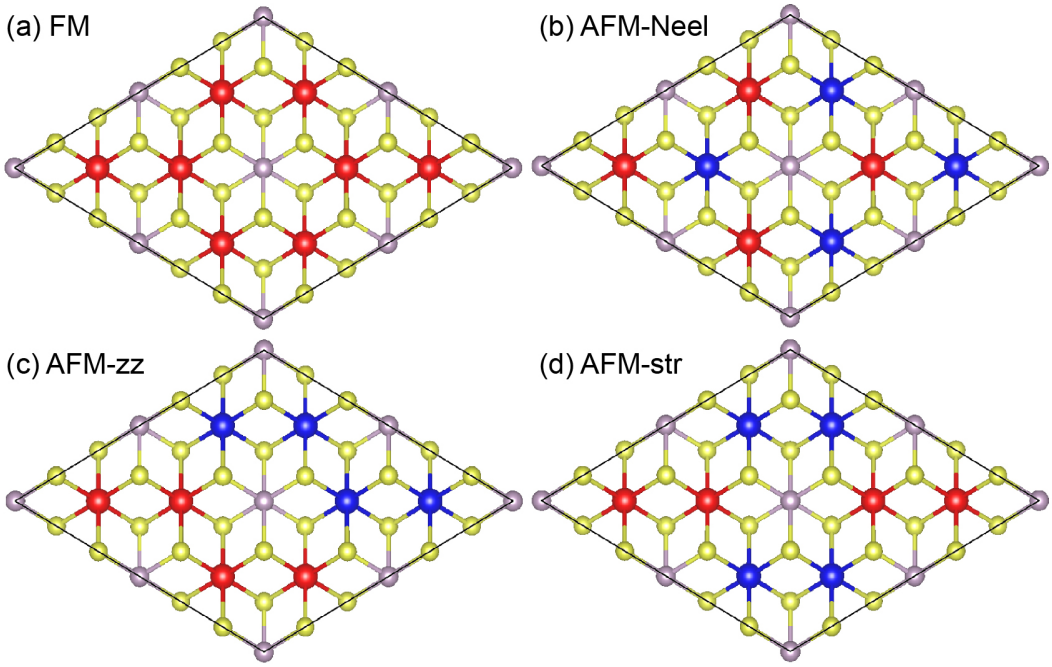

Fig. S1. Four different magnetic configurations of $MnPX_3$: (a) FM, (b) AFM-Néel, (c) AFM-zig-zag, and (d) AFM-stripy. Up and down spin moments orientations for Mn ions are coded by red and blue spheres, respectively.

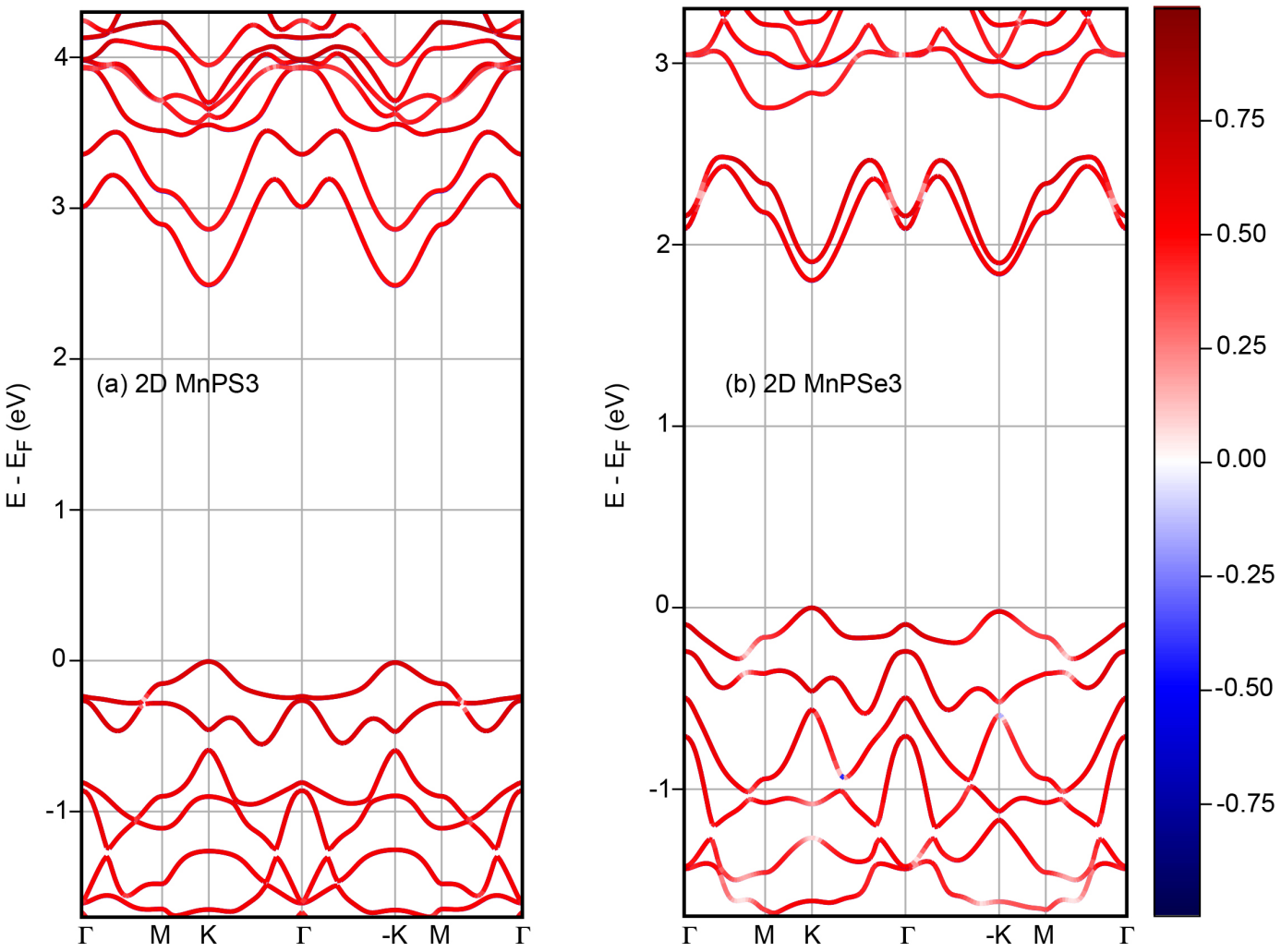

Fig. S2. Band structures of (a) 2D $MnPS_3$ and (b) 2D $MnPSe_3$ with SOC taken into account. The red and blue colors denote the spin up and down states, respectively.

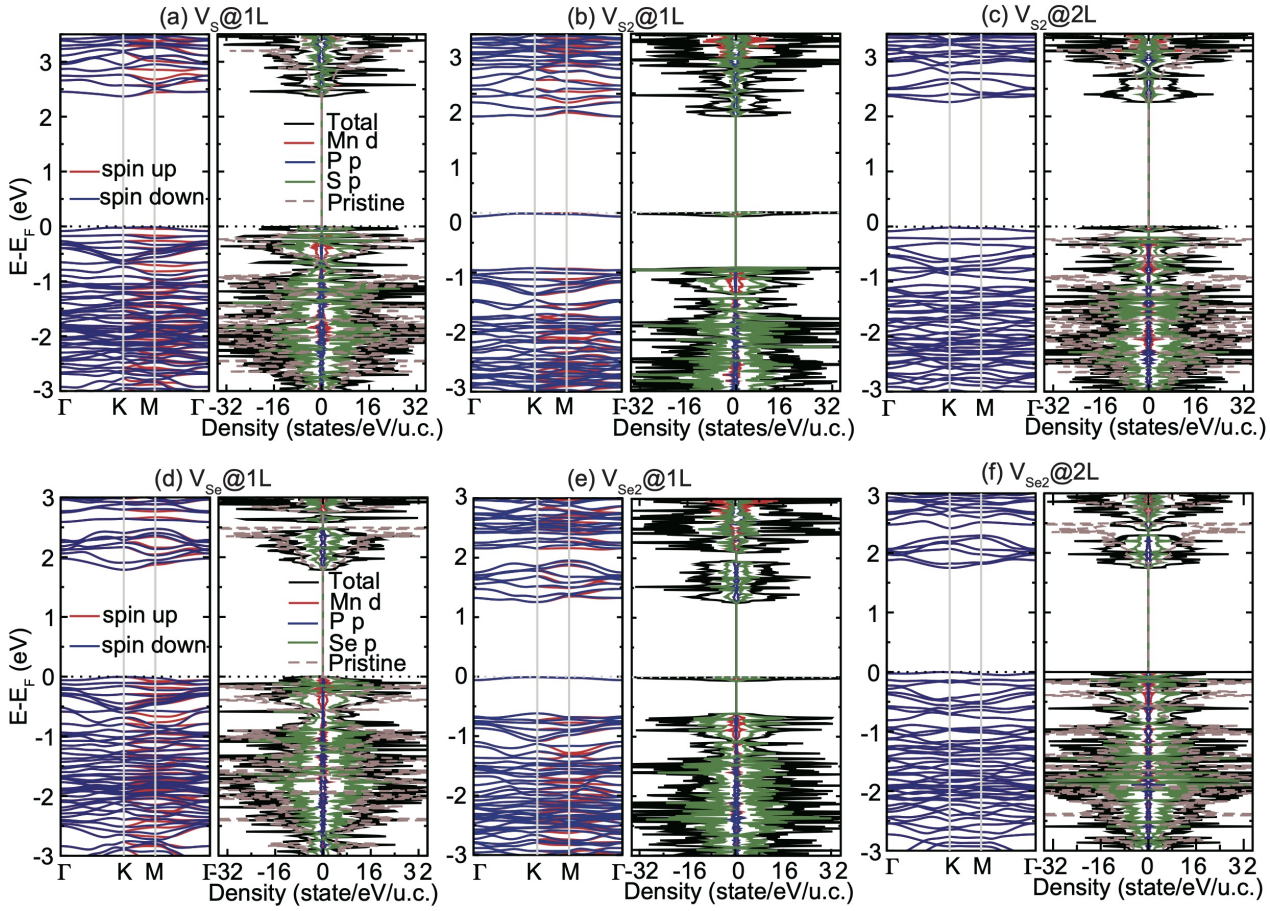

Fig. S3. Band structures, total and partial DOS for 2D $MnPS_3$ (upper panels) and 2D $MnPSe_3$ (lower panels) vacancy systems.

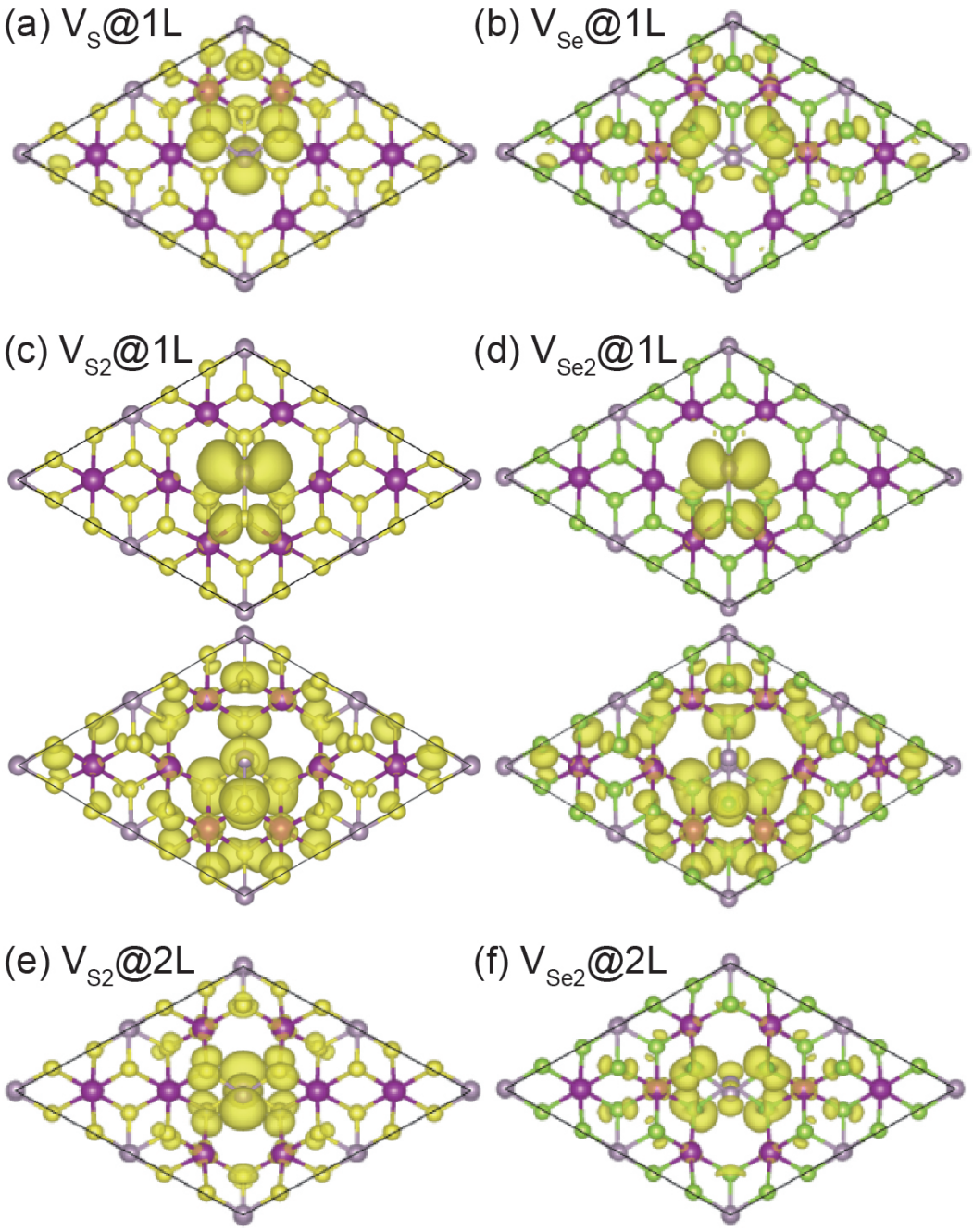

Fig. S4. Partial charge densities (iso-surface value $= 2 \times 10^{-3} e/\text{Å}^3$) of 2D $MnPS_3$ (left panels) and 2D $MnPSe_3$ (right panels) vacancy systems.