Supplementary Information: Electron doping as a handle to increase the Curie temperature in ferrimagnetic $Mn_3Si_2X_6$ (X=Se, Te)

Lei Qiao,^{1,2} Paolo Barone,³ Baishun Yang,²

Phil D.C. King,⁴ Wei Ren,^{1,*} and Silvia Picozzi^{2,†}

¹Physics Department, International Center of Quantum and Molecular Structures,

Materials Genome Institute, State Key Laboratory of Advanced Special Steel,

Shanghai Key Laboratory of High Temperature Superconductors,

Shanghai University, Shanghai 200444, China

²Consiglio Nazionale delle Ricerche (CNR-SPIN),

Unità di Ricerca presso Terzi c/o Università "G. D'Annunzio", 66100 Chieti, Italy

³Consiglio Nazionale delle Ricerche (CNR-SPIN), Area della Ricerca di Tor Vergata,

Via del Fosso del Cavaliere 100, I-00133 Rome, Italy ⁴SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews KY16 9SS, UK



FIG. S1. Band structures of (a) MSS and (b) MST calculated with different directions of magnetic moments (SOC included). The dotted line 001 and the solid line 100 represent the band structure calculated with out-of-plane magnetization and in-plane magnetization, respectively. The band splitting Δ at the Γ point for the valence band maximum is 0.163 eV in MSS and 0.378 eV in MST.



FIG. S2. Band structures and the corresponding projected DOS of (a) MSS and (b) MST, at different doping concentration, *i.e.* undoped (left column), 0.4 (middle column) and 0.8 (right column) e/unit-cell.

^{*} renwei@shu.edu.cn

 $^{^\}dagger$ silvia.picozzi@spin.cnr.it



FIG. S3. T_{C} of MSS and MST obtained from MF method.



FIG. S4. Susceptibility, calculated via MC simulations, of (a) MSS and (b) MST as a function of temperature for different doping levels.