Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Electronic Supplementary Information

"Investigation of n-type Doping Strategies for Mg_3Sb_2"

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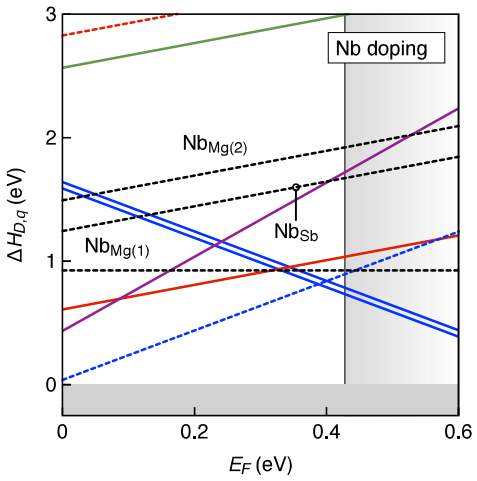

Figure S1: Defect energetics of n-type doping of Mg_3Sb_2 with Nb, under Mg-rich ($\Delta\mu_{Mg}$ = 0 eV) and most dopant-rich conditions as accommodated by the stability of Mg_3Sb_2 in the Nb-Mg-Sb chemical potential phase space. The native defects are also shown for reference.

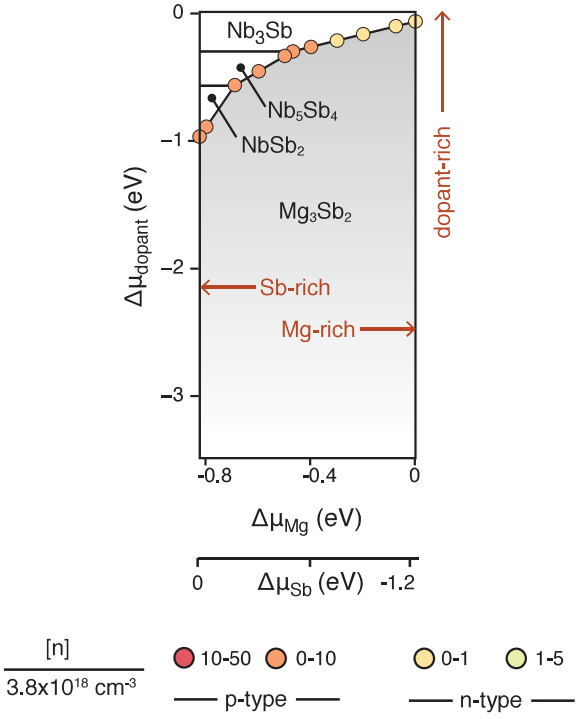

Figure S2: Phase stability of Mg_3Sb_2 in the ternary Nb-Mg-Sb chemical potential phase space. The shaded area represents the region of phase stability of Mg_3Sb_2. The x-axis is bounded by Mg-rich/Sb-poor ($\Delta\mu_{Mg}$ = 0 eV, $\Delta\mu_{Sb}$ = -1.28 eV) and Mg-poor/Sb-rich ($\Delta\mu_{Mg}$ = -0.83 eV, $\Delta\mu_{Sb}$ = 0 eV) conditions. The y-axis denotes $\Delta\mu_{Nb}$, ranging from Nb-rich (0 eV) and below. The markers at the Mg_3Sb_2 phase boundary are the free carrier concentrations calculated at 900K, normalized by the free electron concentration in self-doped n-type Mg_3Sb_2 grown under Mg-rich conditions (3.8×10^{18} cm^{-3}). Red and orange markers denote free hole concentrations while other colors free electron concentrations.

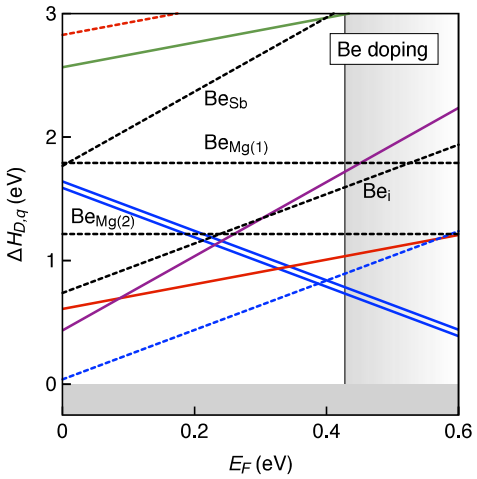

Figure S3: Defect energetics of n-type doping of Mg_3Sb_2 with Be, under Mg-rich ($\Delta\mu_{Mg} = 0$ eV) and most dopant-rich conditions as accommodated by the stability of Mg_3Sb_2 in the Be-Mg-Sb chemical potential phase space. The native defects are also shown for reference.