Supplementary Information (SI) for Journal of Materials Chemistry A.
This journal is © The Royal Society of Chemistry 2025

Supporting Information

Enhanced P-Type Conductivity in Sb_2Se_3 through Akali and Alkaline Earth Metal Doping

Eunkyung Cho,* Shi-Joon Sung, Kee-Jeong Yang, Jae-Baek Lee, Van-Quy Hoang,

Bashiru Kadiri-English, Dae-Kue Hwang, Jin-Kyu Kang, Dae-Hwan Kim*

Division of Energy and Environmental Technology, DGIST,

Daegu, 42988, Republic of Korea

Email: ekcho@dgist.ac.kr; monolith@dgist.ac.kr

Content

Table S1. Formation energies (ΔH_f, in eV) of secondary phases, as calculated at the HSE06-GD3DJ level of theory.

Dopant	Phase	ΔH_f	Phase	ΔH_f
Na	Na_3SbSe_3	-6.90	Na_3SbSe_3	-6.90
K	KSe	-2.20	KSe	-2.20
Mg	$MgSe_2$	-3.12	MgSe	2.86
Ca	CaSe	-4.71	CaSe	-4.71

Table 2. Elemental chemical potential (μ_i, in eV) and maximum chemical potential values (μ_{max}, in eV) of various dopants in Sb_2Se_3 under two growth conditions, as calculated at the HSE06-GD3DJ level of theory.

Dopant	μ_i	$\mu_{max}^{Se-rich}$	Phase	$\mu_{max}^{Se-poor}$	Phase
Na	-1.62	-3.69	Na_3SbSe_3	-3.46	Na_3SbSe_3
K	-1.33	-3.53	KSe	-3.06	KSe
Mg	-1.90	-5.01	$MgSe_2$	-4.29	MgSe
Ca	-2.14	-6.85	CaSe	-6.39	CaSe

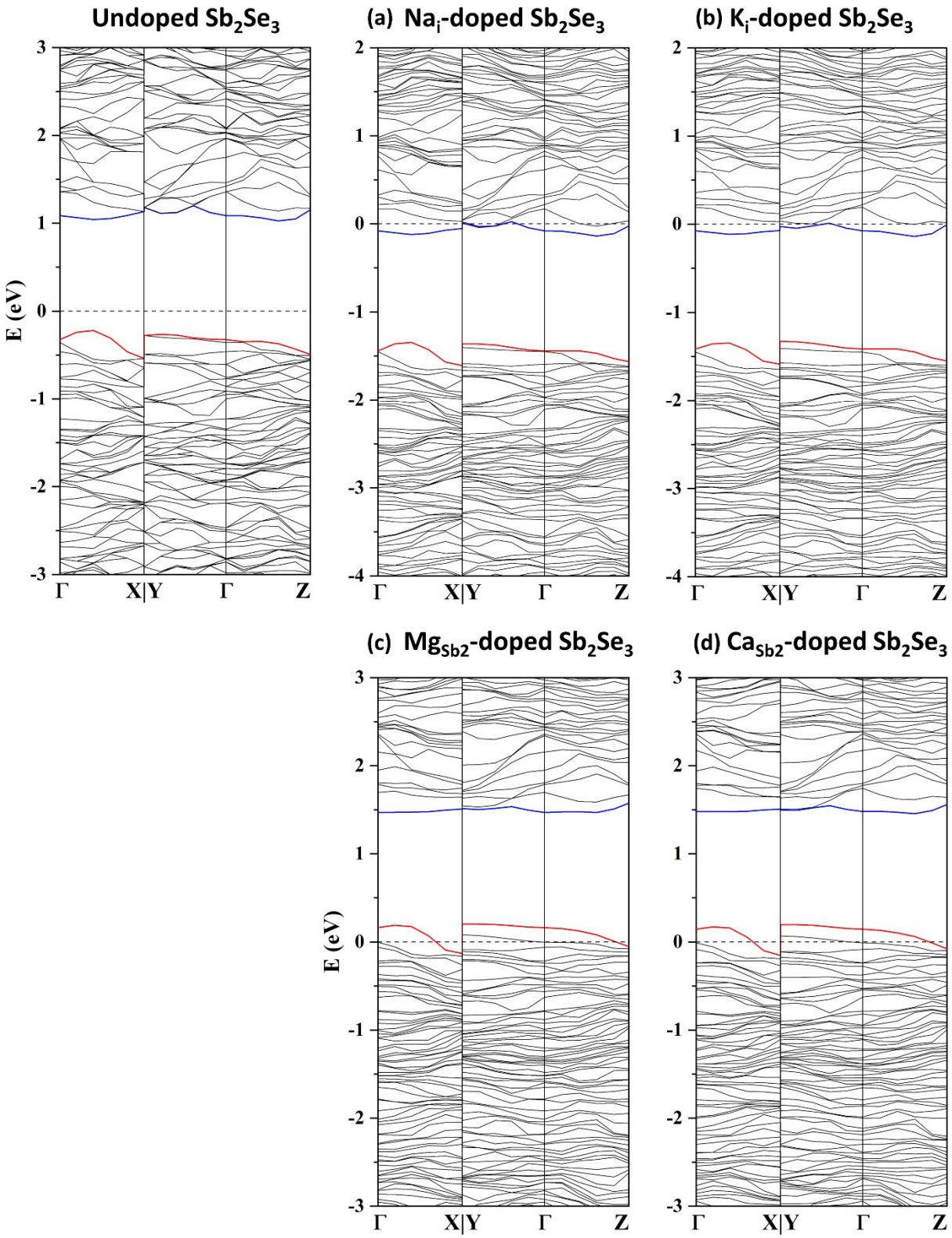

Figure S1. Band structures of (a) Na_i-, (b) K_i-, (c) Mg_{Sb2}-, and (d) Ca_{Sb2}-doped Sb_2Se_3 in comparison to the band structure of undoped Sb_2Se_3, as calculated at the HSE06-GD3DJ level of theory.