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

Electronic Supplementary Information

I. ELECTRONIC TRANSPORT PROPERTIES OF N-TYPE Bi_2O_2S BULK AND MONO LAYER

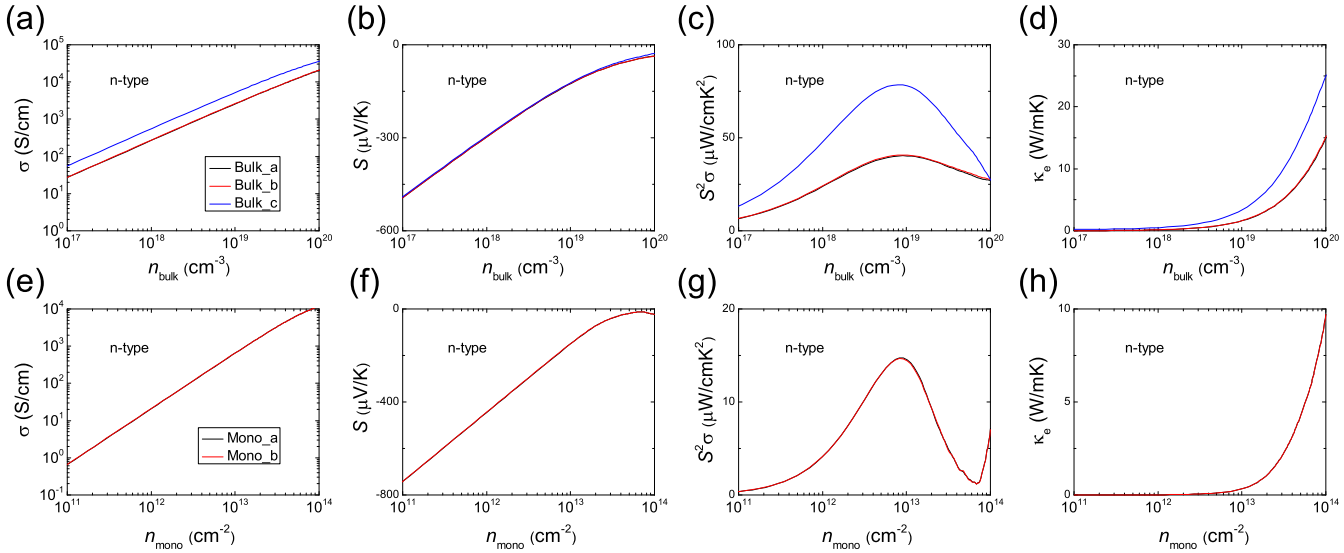

FIG. S1. The calculated electronic transport properties as a function of carrier concentration n for n-type Bi_2O_2S bulk (a, b, c, d) and n-type mono layer (e, f, g, h) at 300 K: the electrical conductivity σ, Seebeck coefficient S, power factor $S^2\sigma$ and electronic thermal conductivity κ_e.

II. PHONON TRANSPORT PROPERTIES FOR Bi_2O_2S BULK AND MONO LAYER

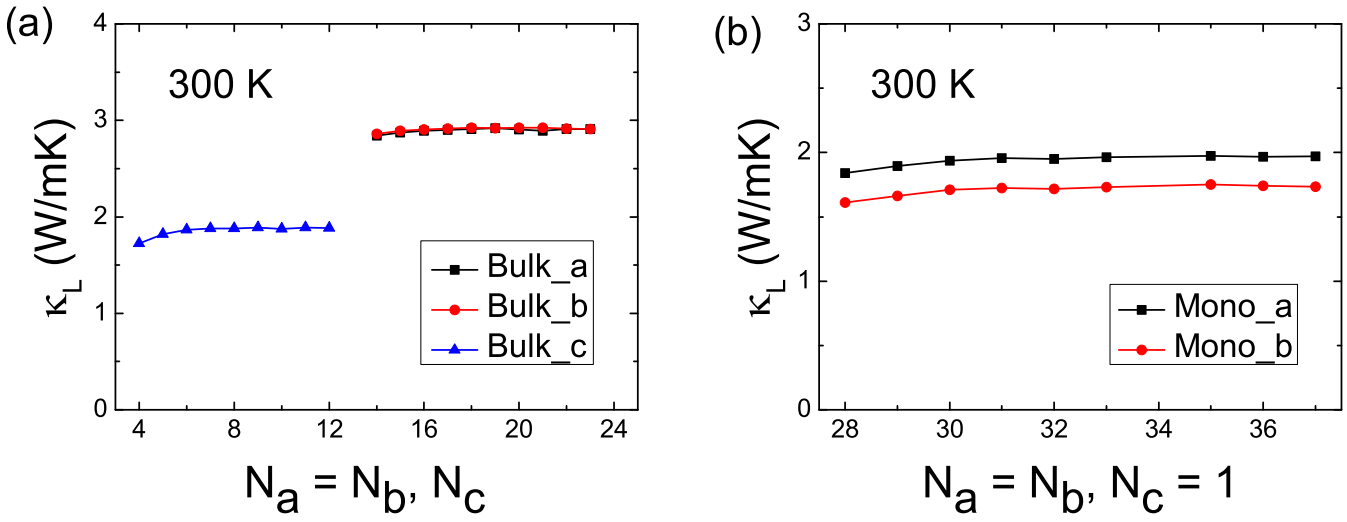

FIG. S2. The lattice thermal conductivity of Bi_2O_2S bulk (a) and mono layer (b) for different numbers of **q** points ($N_a \times N_b \times N_c$) at 300 K. The lattice thermal conductivity of $N_a = N_b = 34$ for Bi_2O_2S mono layer is outputless.

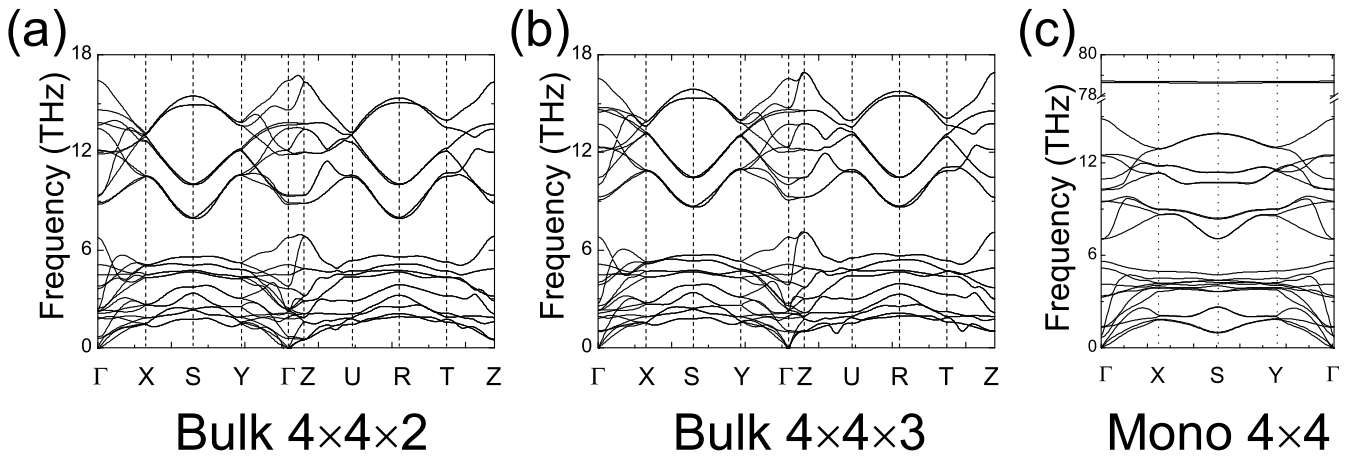

FIG. S3. The phonon dispersion relations with supercell size 4×4×2 (a) and 4×4×3 (b) for Bi_2O_2S bulk. The phonon dispersion relations with supercell size 4×4 (c) for Bi_2O_2S mono layer.

III. TRANSPORT PROPERTIES OF BI_2O_2S BILAYER

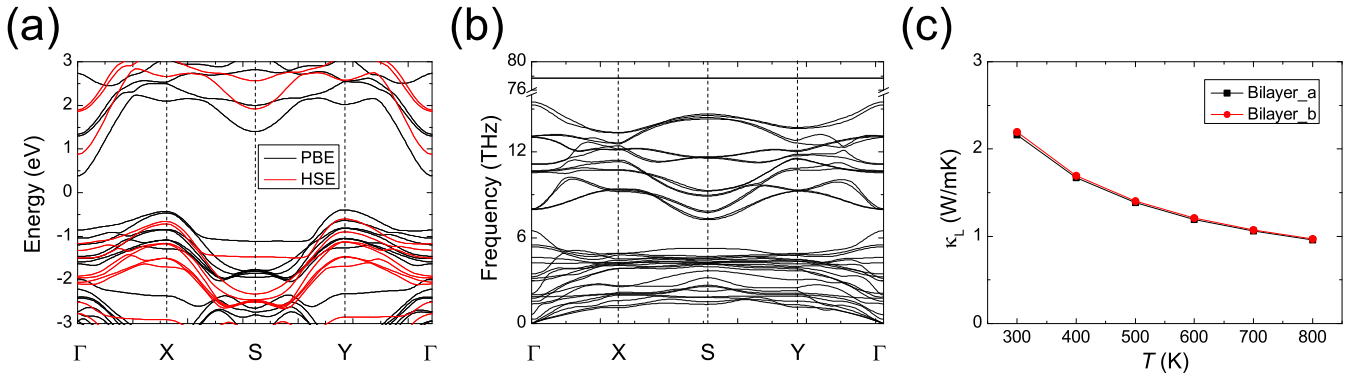

FIG. S4. (a) The band structure of Bi_2O_2S bilayer. The Fermi energy is set to 0 eV. (b) The phonon dispersion relations. (c) The calculated lattice thermal conductivity for Bi_2O_2S bilayer.

TABLE S1. The carrier relaxation time for Bi_2O_2S bilayer at 300 K in the *a* and *b* directions. The corresponding DOS effective mass m^*_{dos}, elastic constant *C* and DP constant *E* are also listed.

Carrier type	$m^*_{dos}(m_e)$	*C* (eV/Å)	*E* (eV/strain)	τ (10^{-14}s)
Electron	0.47	14.79 (*a*)	-11.96 (*a*)	2.79 (*a*)
		14.53 (*b*)	-11.70 (*b*)	2.86 (*b*)
Hole	-1.91	14.79 (*a*)	-9.88 (*a*)	1.00 (*a*)
		14.53 (*b*)	-7.90 (*b*)	1.54 (*b*)

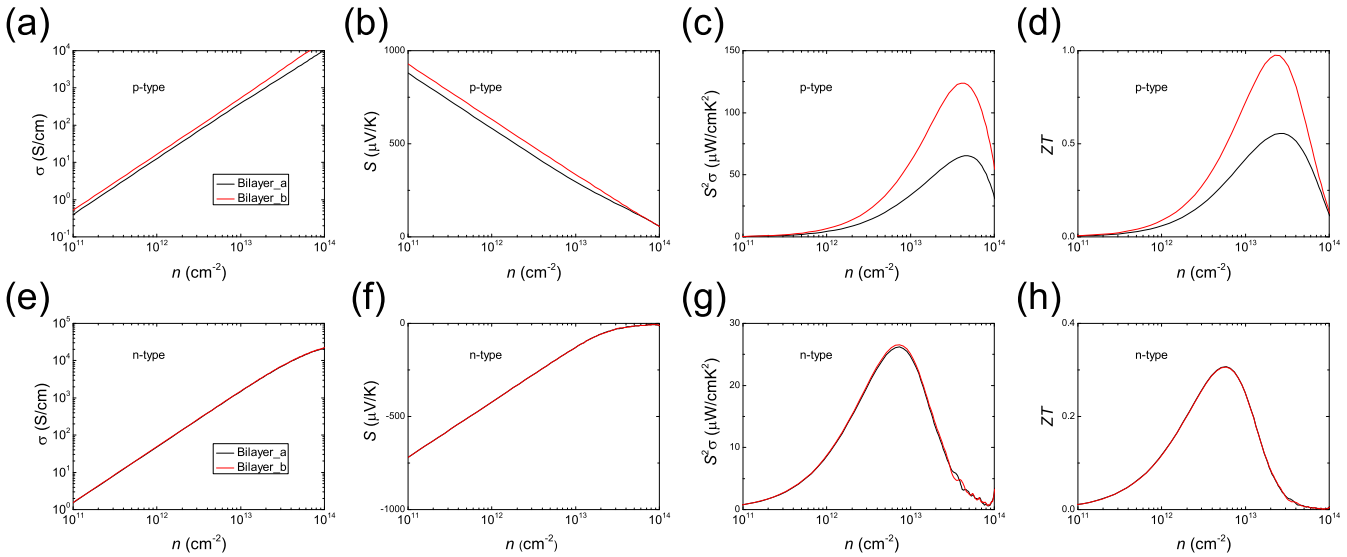

FIG. S5. The calculated transport properties as a function of carrier concentration n for p-type (a, b, c, d) and n-type (e, f, g, h) Bi_2O_2S bilayer at 300 K: the electrical conductivity σ, Seebeck coefficient S, power factor $S^2\sigma$ and ZT value.