Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

for

Ternary selenides $A_2Sb_4Se_8$ (A = K, Rb, Cs) as an n-type thermoelectric material with high power factor and low lattice thermal conductivity: Importance of the conformationally flexible Sb-Se-Se-Sb bridges

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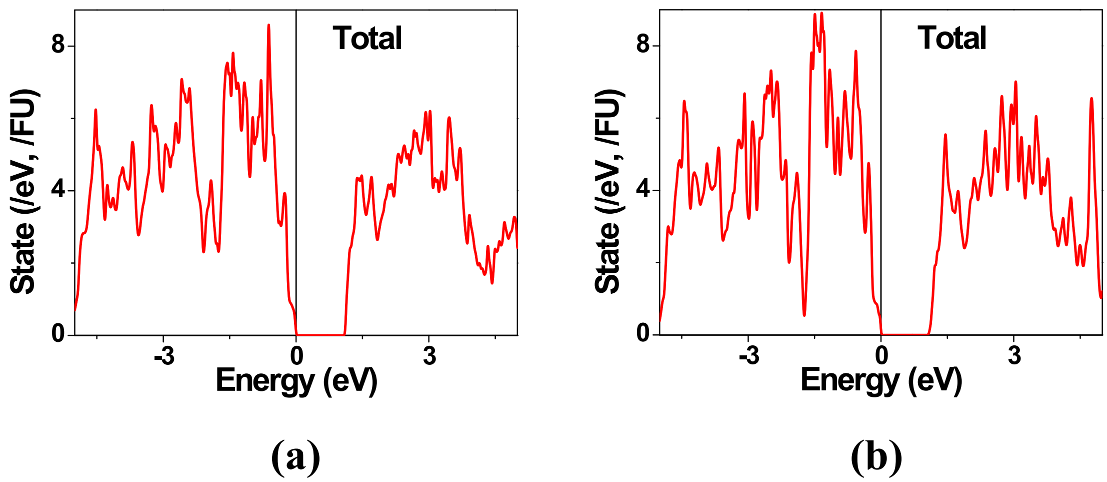

Figure S1. Total DOS plots calculated for (a) $Rb_2Sb_4Se_8$ and (b) $Cs_2Sb_4Se_8$.

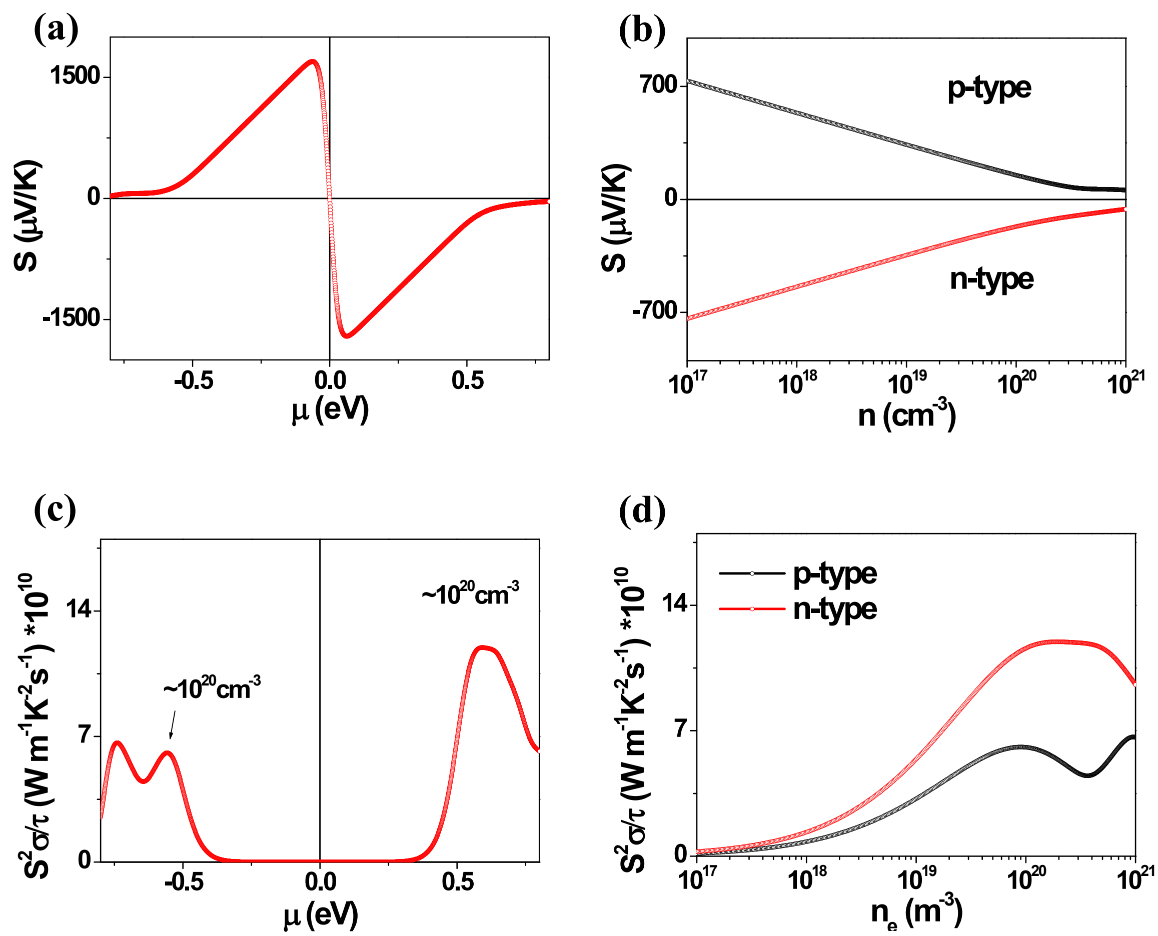

Figure S2. Thermodynamic properties of $Rb_2Sb_4Se_8$ calculated at 300 K: (a) Seebeck coefficient S as function of the chemical potential μ. (b) Seebeck coefficient S as function of the carrier density n. (c) Power factor $S^2\sigma/\tau$ as function of the chemical potential μ. (d) Power factor $S^2\sigma/\tau$ as function of the carrier density n.

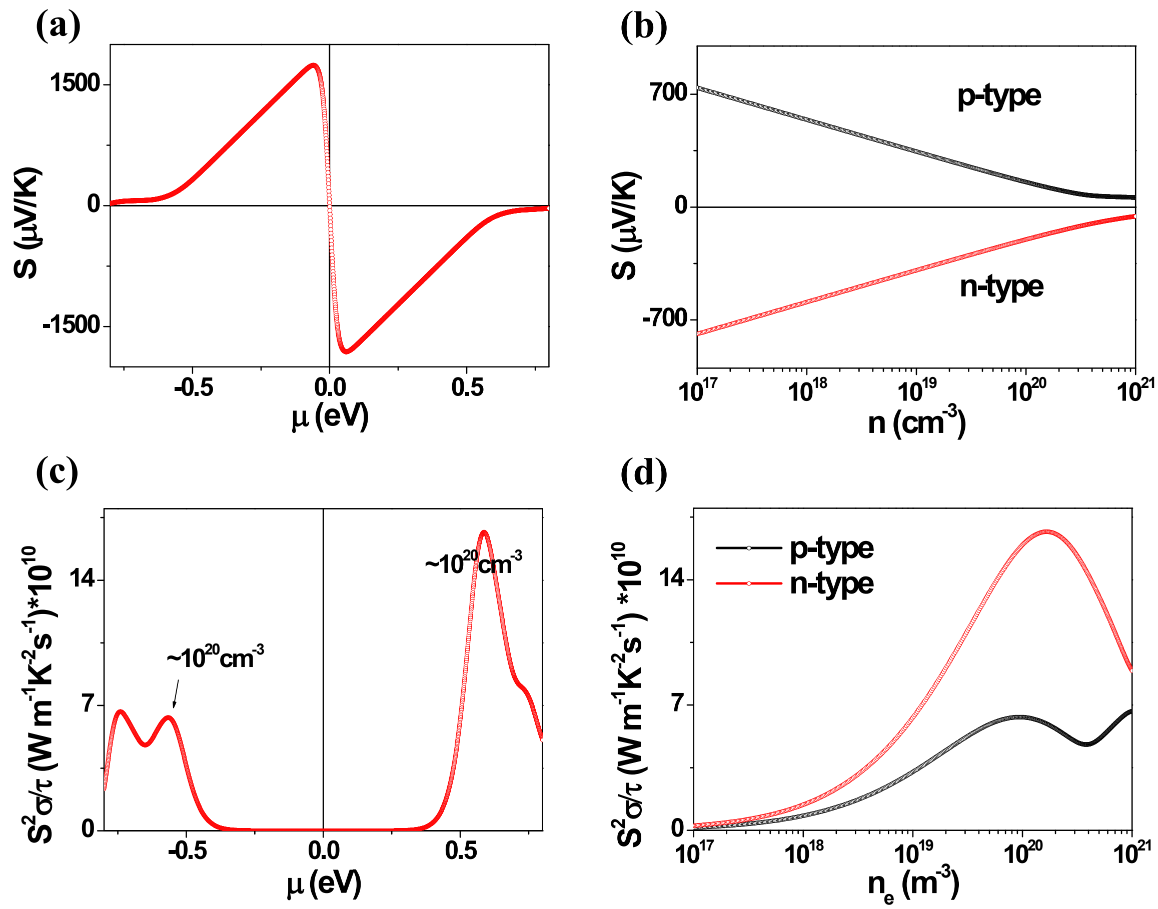

Figure S3. Thermodynamic properties of $Cs_2Sb_4Se_8$ calculated at 300 K: (a) Seebeck coefficient S as function of the chemical potential μ. (b) Seebeck coefficient S as function of the carrier density n. (c) Power factor $S^2\sigma/\tau$ as function of the chemical potential μ. (d) Power factor $S^2\sigma/\tau$ as function of the carrier density n.

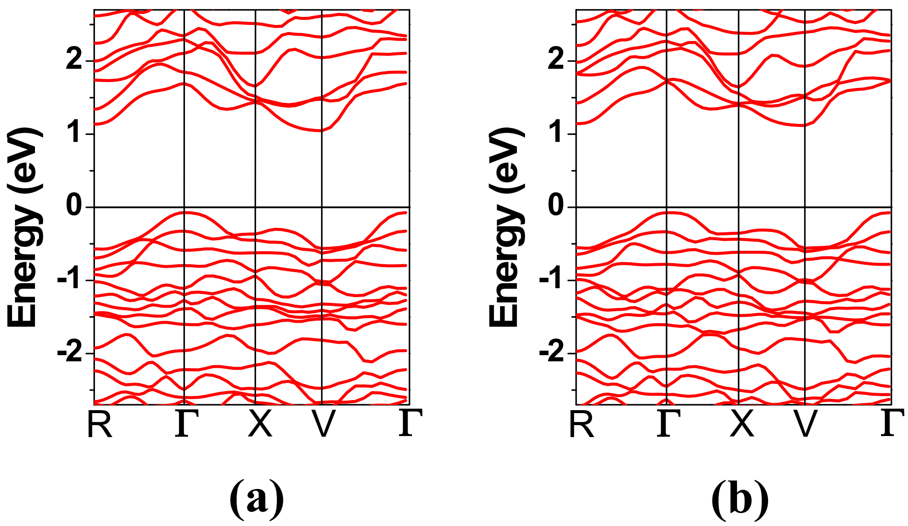

Figure S4. Band dispersion relations calculated for (a) $Rb_2Sb_4Se_8$ and (b) $Cs_2Sb_4Se_8$.

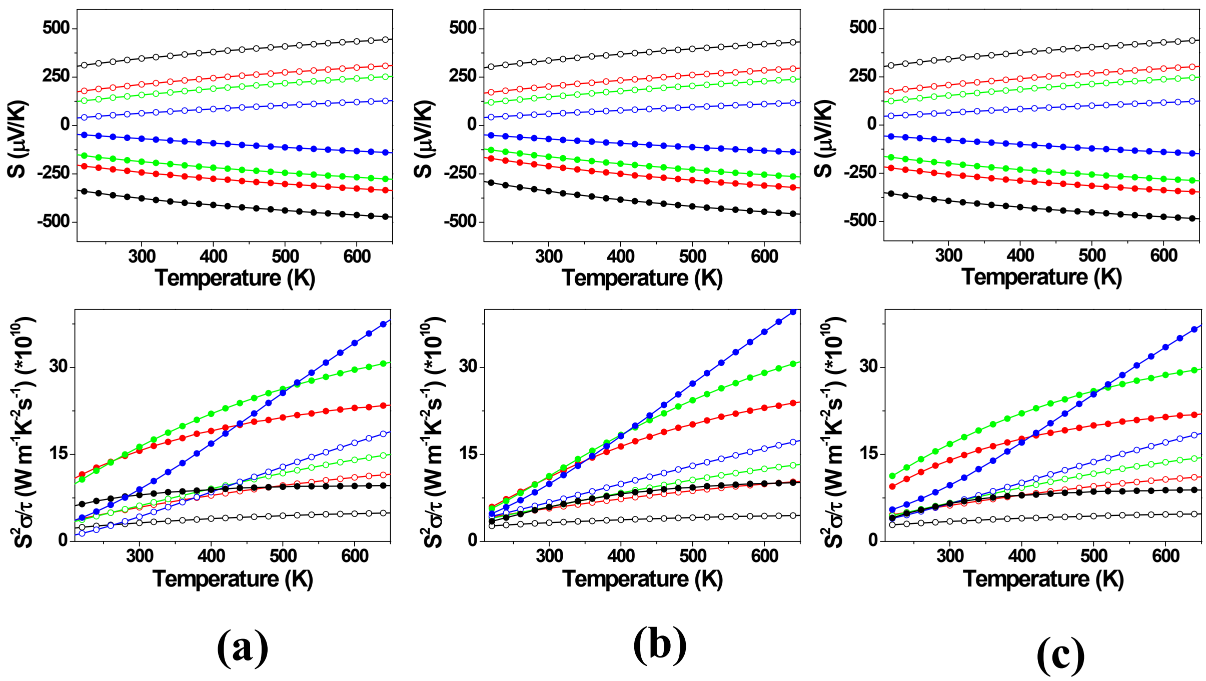

Figure S5. The temperature dependence of the Seebeck coefficients S (upper panels) and the power factor $S^2\sigma/\tau$ (down panels) plots calculated for (a) $K_2Sb_4Se_8$, (b) $Rb_2Sb_4Se_8$, and (c) $Cs_2Sb_4Se_8$. The black, red, green, and blue circles refer to carrier concentration 1×10^{19}, 5×10^{19}, 1×10^{20}, and 5×10^{20} cm^{-3}, respectively. The open and filled circles indicate hole- and electron-type carriers.