

Supplementary Material: Correlation of Rattlers with Thermal Transport and Thermoelectric Performance

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Structure and stability.

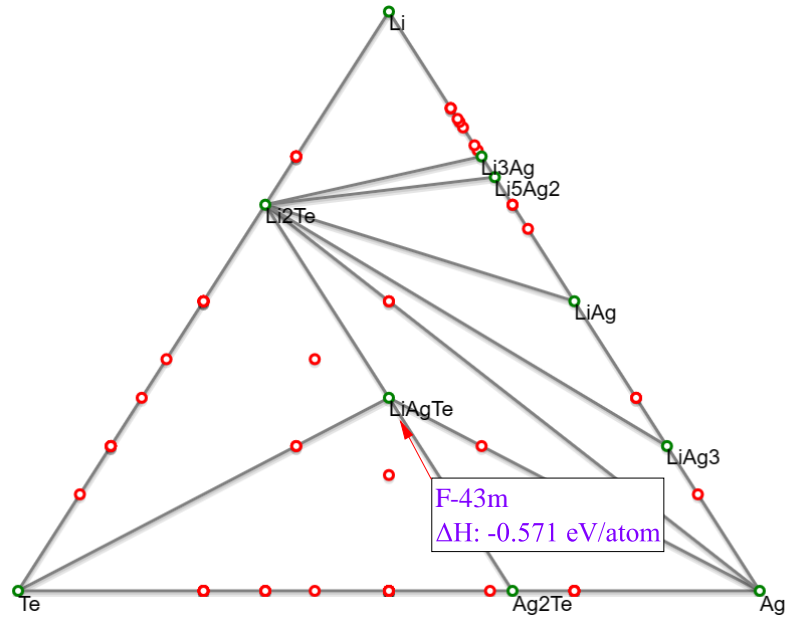


Fig. S1. (Color online). The green circles on the phase diagram of LiAgTe represent the minimum free energy structures of different compositions in the ternary system.

Rattlers and Thermal Transport.

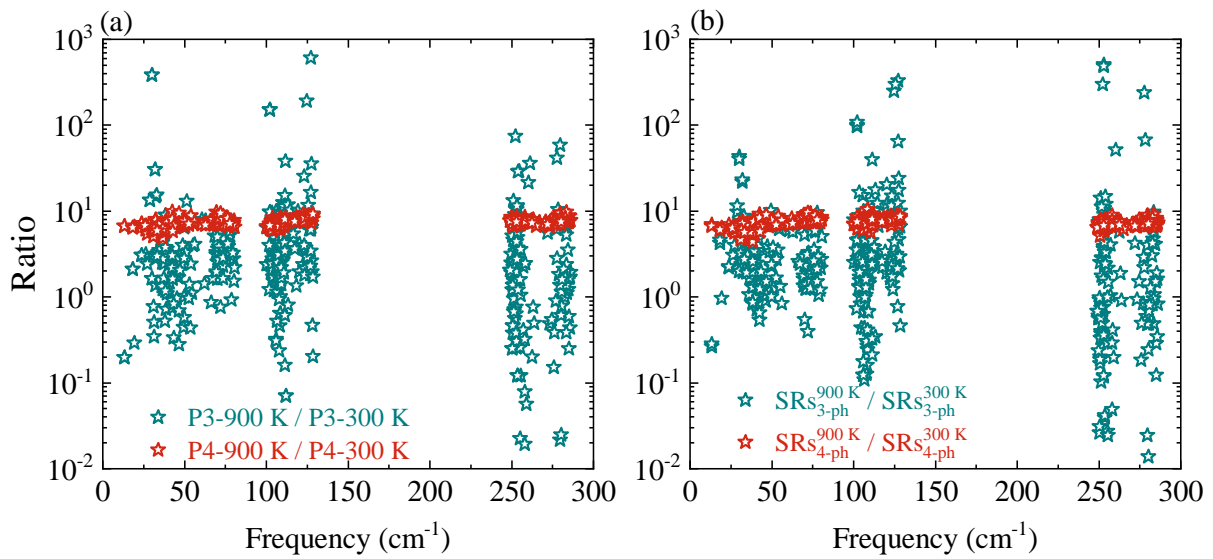


Fig. S2. (Color online). The ratio of the scattering phase space (P3, P4) (a) and scattering index (SRs) (b) of 900 K to 300 K is given.

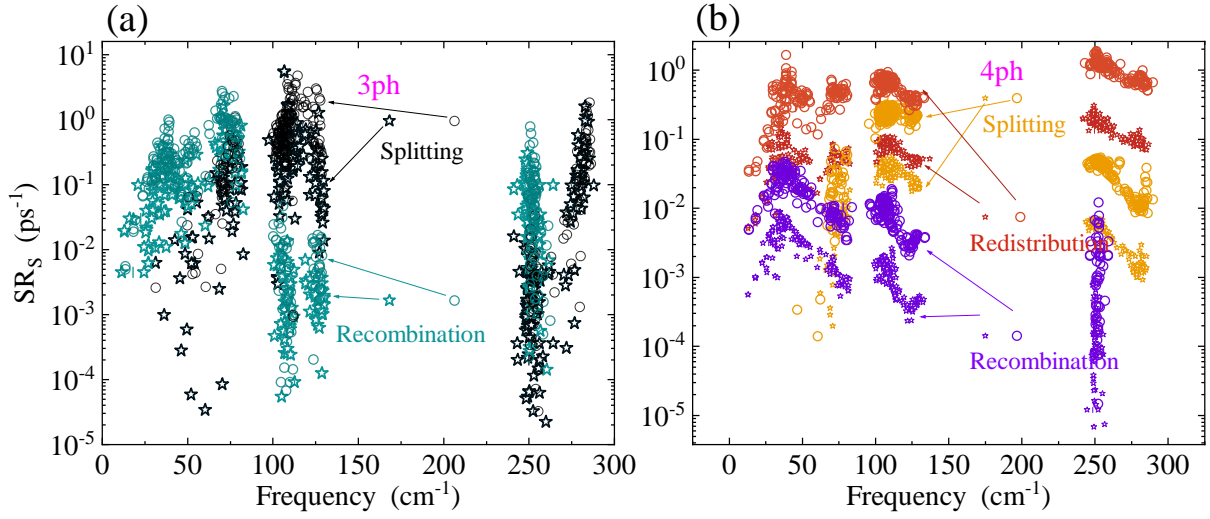


Fig. S3. (Color online). (a). The process of Splitting and Recombination of 3-ph scattering. (b) The process of Splitting, Redistribution and Recombination of 4-ph scattering. The circle scatter and star scatter in (a), (b) correspond to 900K and 300K, respectively.

Rattlers and electronic transport.

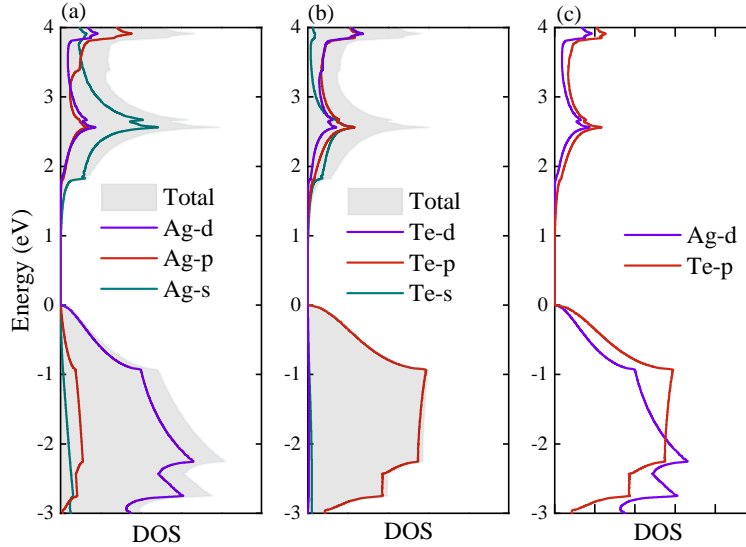


Fig. S4. (Color online). Comparison of the density of states of different orbital electrons of Ag atom (a) and Te atom (b) calculated using pbe functional, as well as the contribution of d-orbital of Ag atom and p-orbital of Te atom (c).

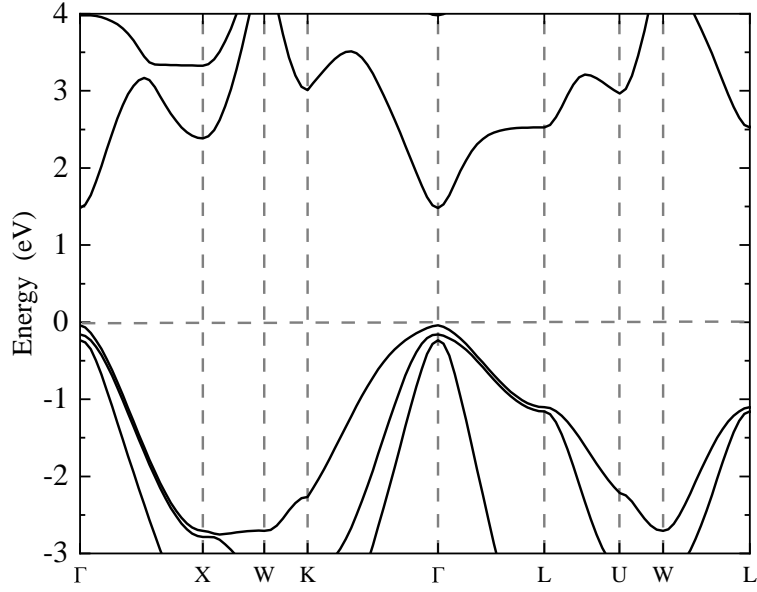


Fig. S5. (Color online). Band structure captured using HSE06.

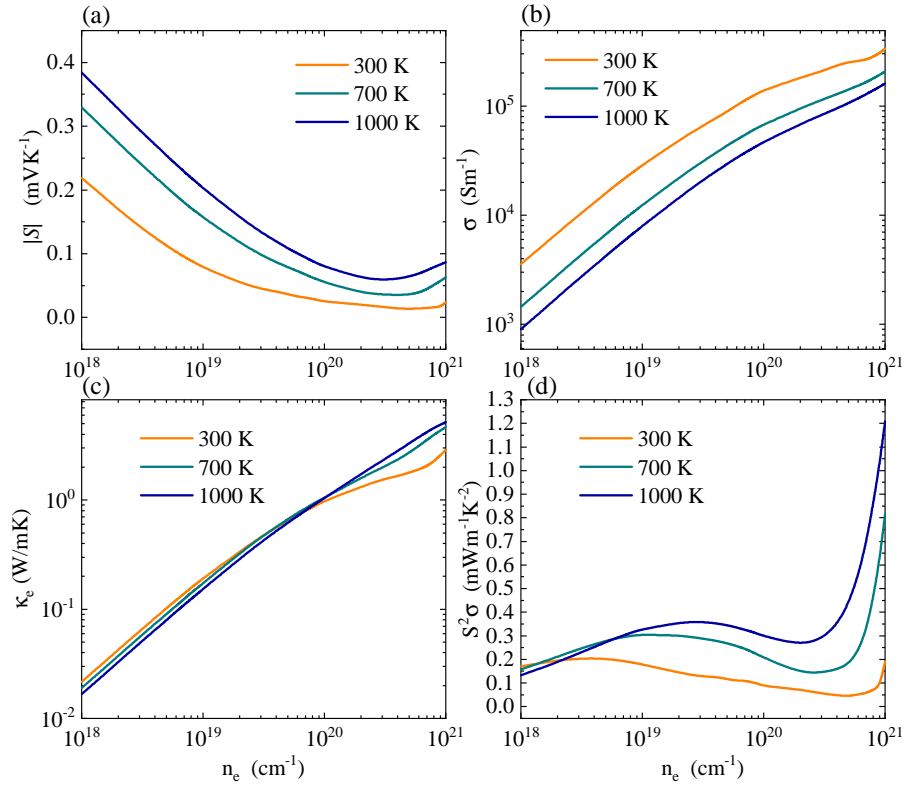


Fig. S6. (Color online). Electronic transport parameters under n-type doping.