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

SUPPLEMENTARY INFORMATION

Predicting high thermoelectric performance of ABX ternary compounds NaMgX (X=P, Sb, As) with weak electron-phonon coupling and strong bonding anharmonicity

A. J. Hong[1], J. J. Gong[1], L. Li[1], Z. B. Yan[1], Z. F. Ren[2], and J. –M. Liu[1]

[1]*Laboratory of Solid State Microstructures and Innovation Center of Advanced Microstructures, Nanjing University, Nanjing 210093, China*

[2]*Department of Physics and TcSUH, University of Houston, Houston, TX 77204, USA*

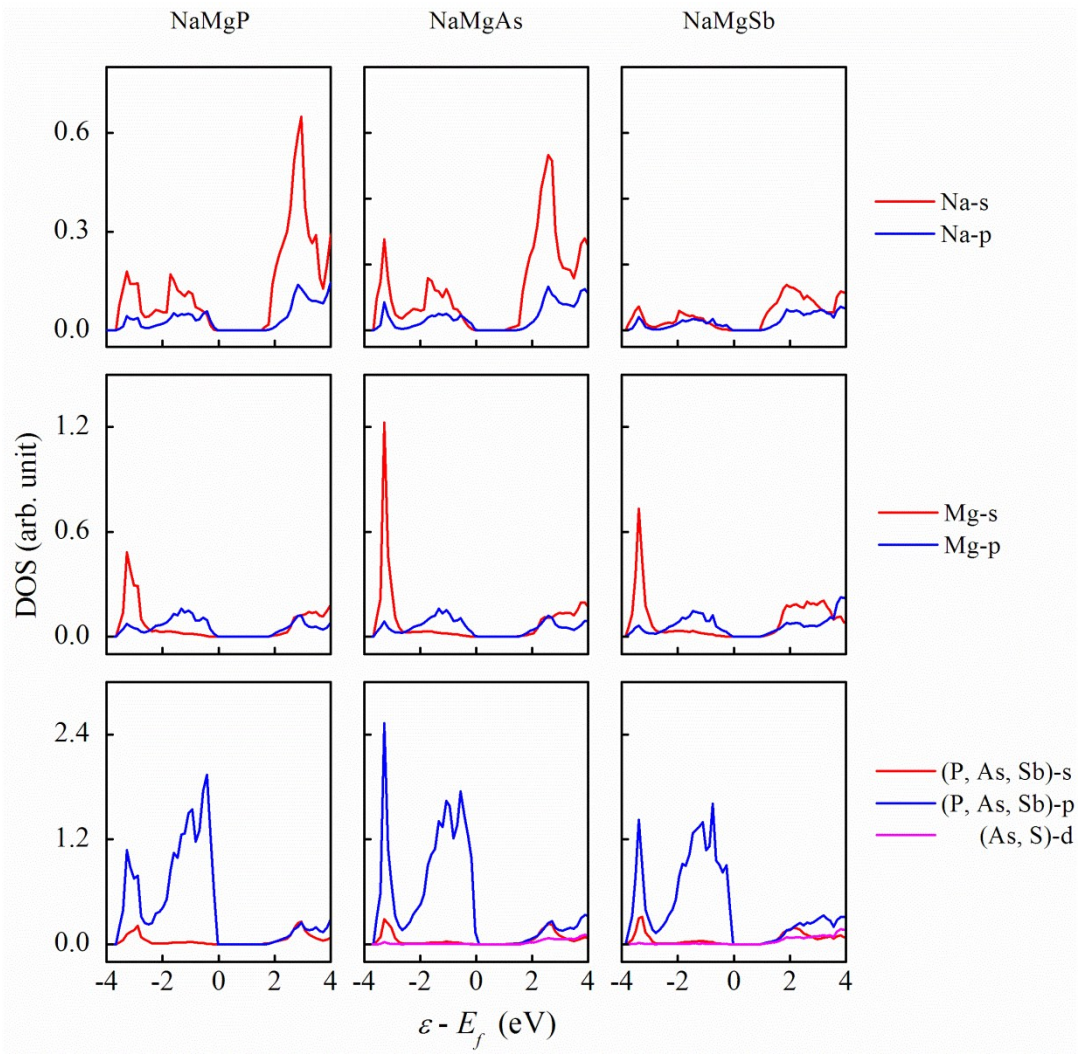

Figure S1. (Color online) Na-s/p, Mg-s/p, and X-s/p/d partial densities of states for NaMgX (X=P, Sb, As).

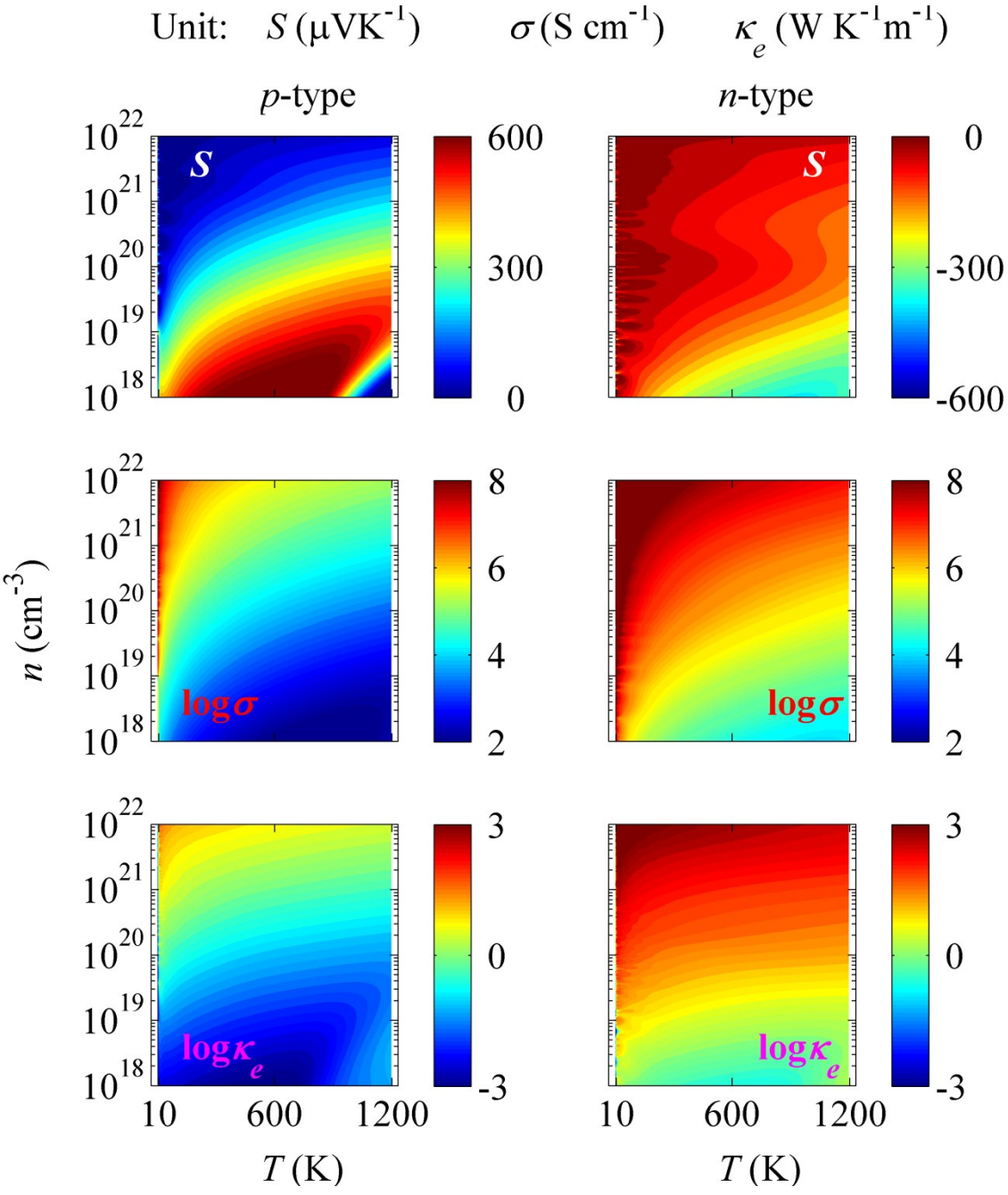

Figure S2. (Color online) The calculated S (top row), $\log\sigma$ (middle row), and $\log\kappa_e$ (bottom row) in the (T, n) plane for carrier-doped NaMgP compound. Left panel: p-type and right panel: n-type. Here *log* is the natural algorithm.

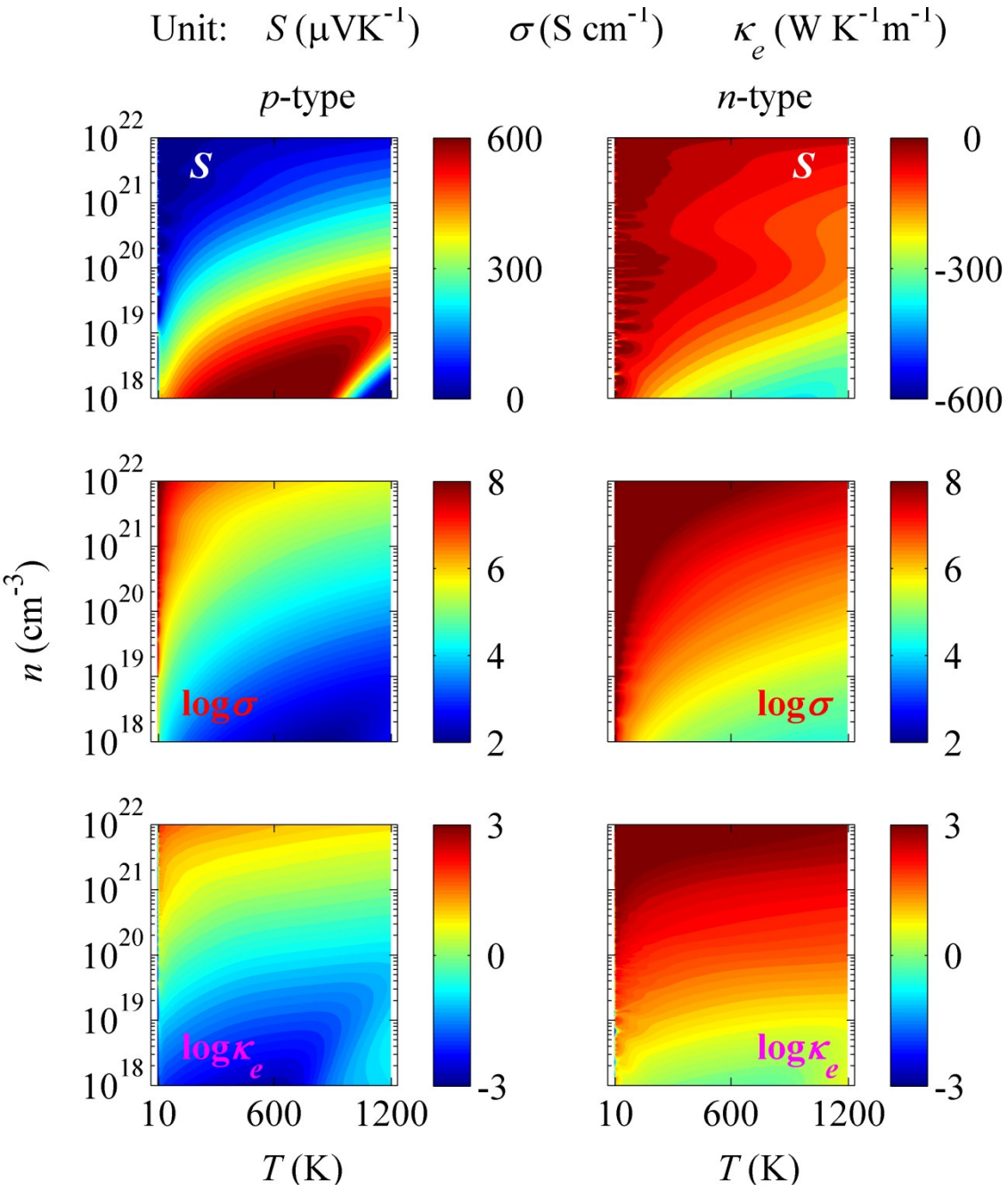

Figure S3. (Color online) The calculated S (top row), logσ (middle row), and logκ_e (bottom row) in the (T, n) plane for carrier-doped NaMgAs compound. Left panel: p-type and right panel: n-type. Here *log* is the natural algorithm.