Electronic Supplementary Material (ESI) for RSC Advances.

Thermoelectric properties of highly-mismatched alloys GaN_xAs_{1-x} from first- to second-principles methods: Energy Conversion

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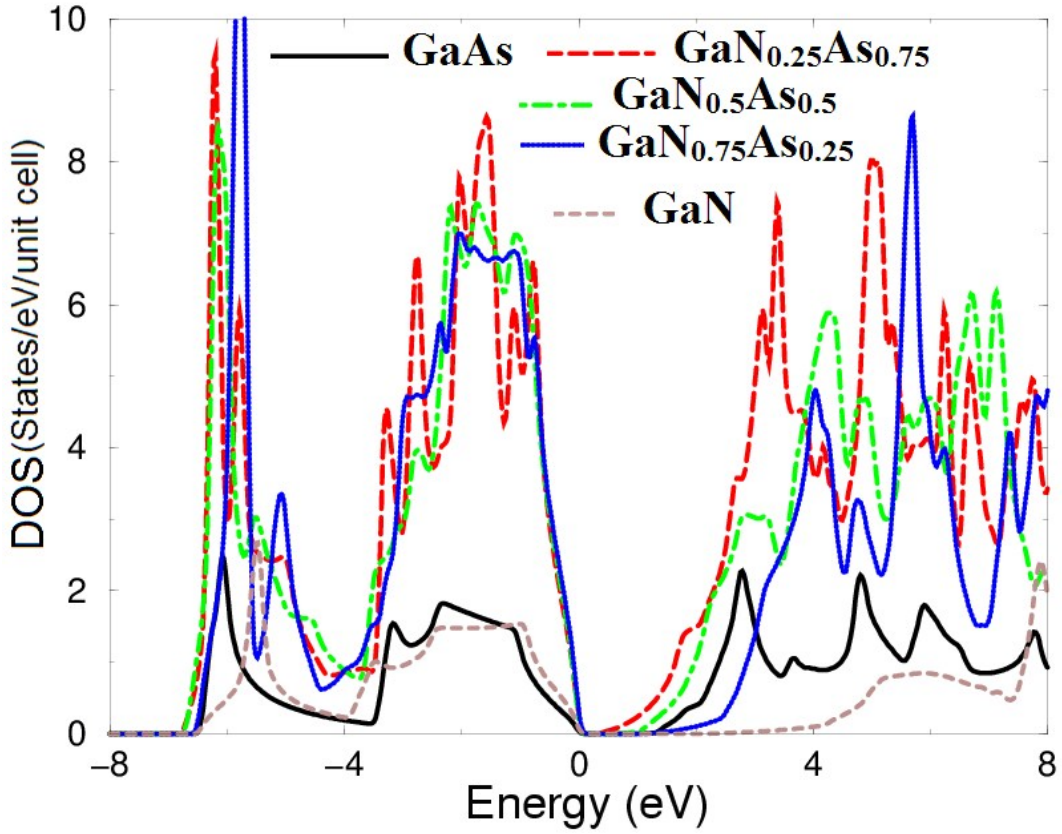
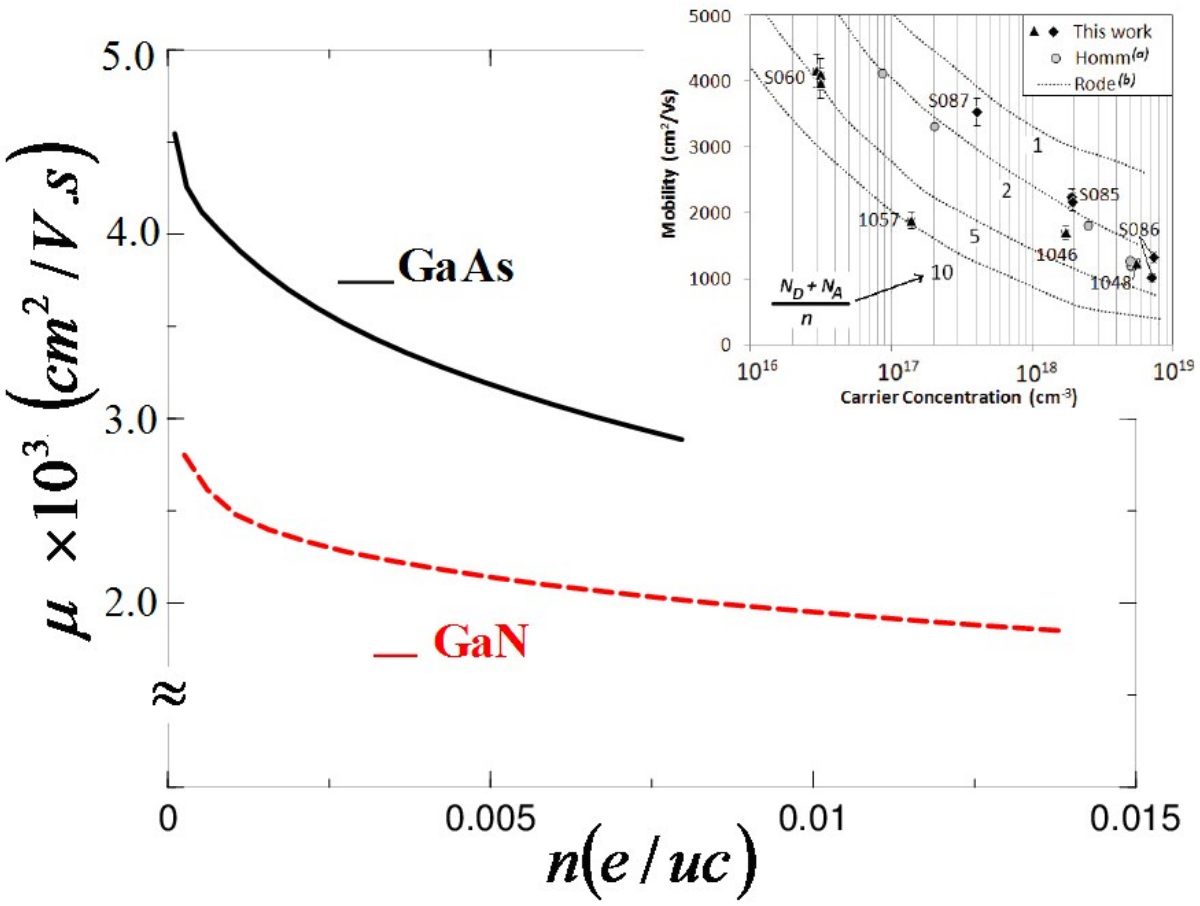
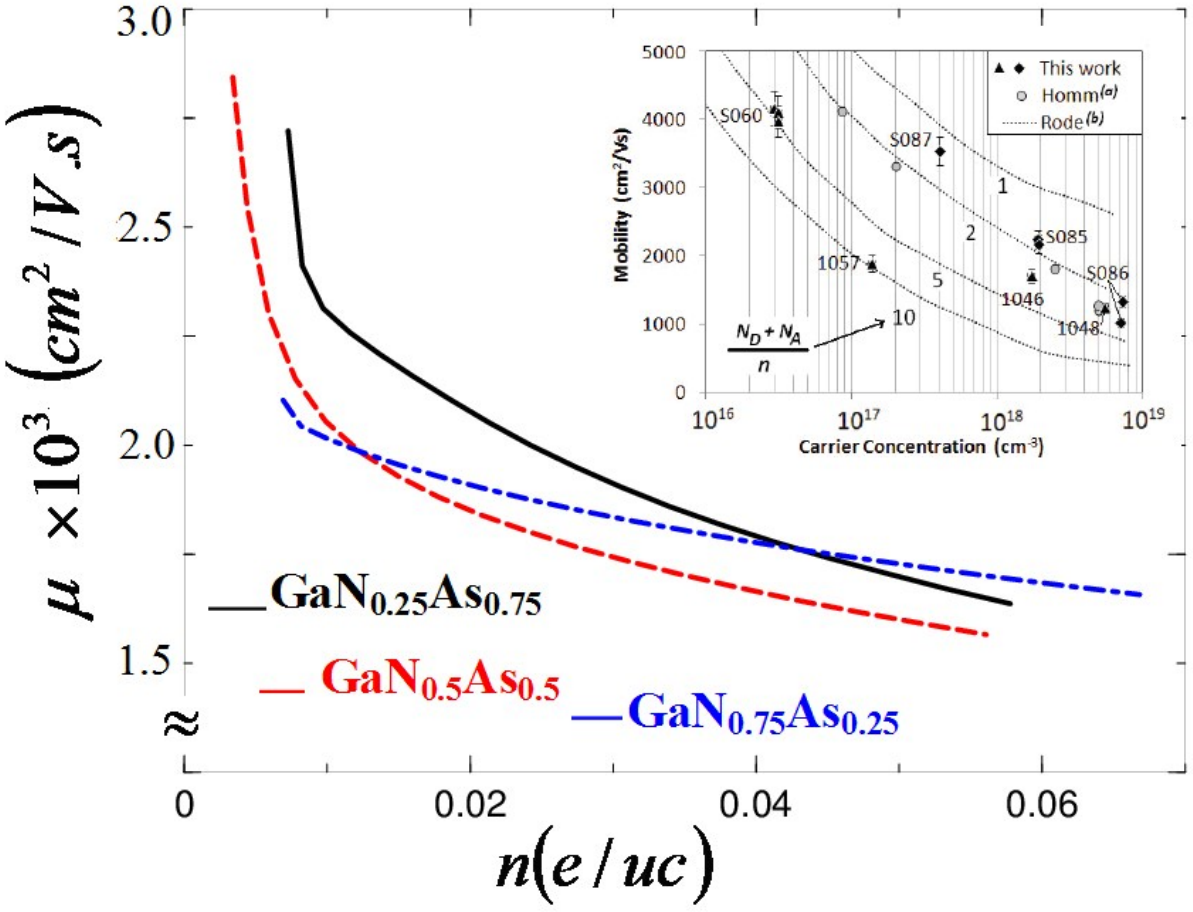


Fig. S1:


5.0
4.0
3.0
2.0
μ ×10³ (cm² /V .s)
GaAs
GaN
0
0.005
0.01
0.015
n(e / uc)
5000
4000
3000
2000
1000
0
Mobility (cm²/Vs)
This work
Homm(a)
Rode(b)
S060
S087
S085
S086
1057
1046
1048
1
2
5
10
N_D + N_A
n
10¹⁶
10¹⁷
10¹⁸
10¹⁹
Carrier Concentration (cm⁻³)

(a)



(b)

Fig. S2:

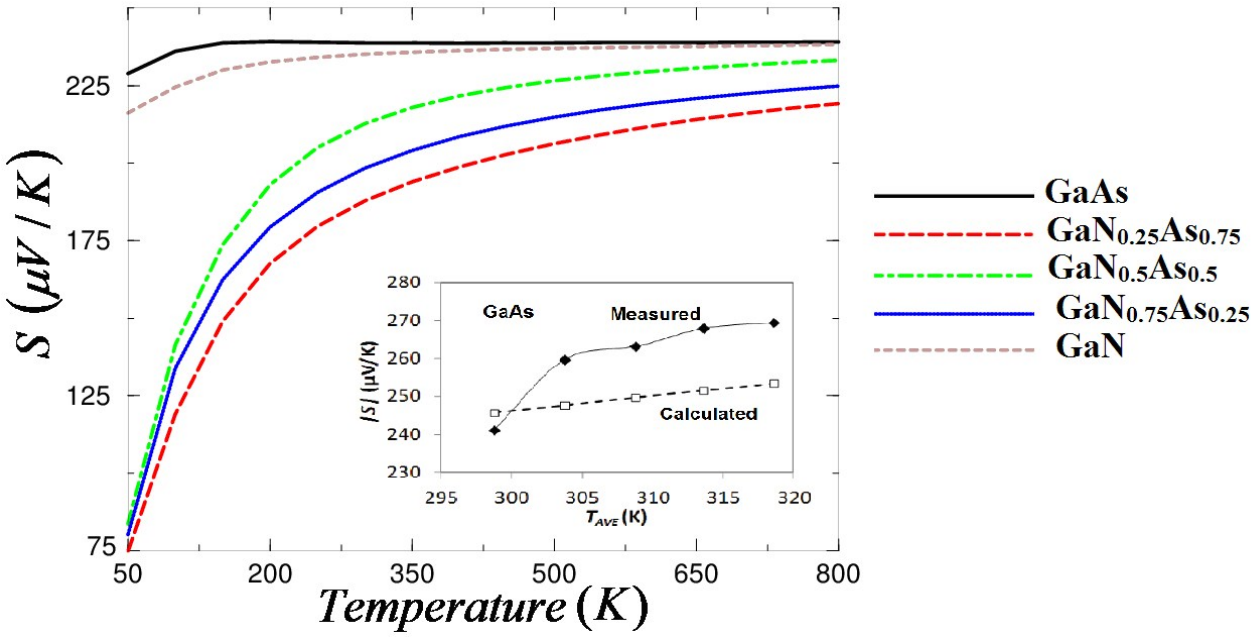


Fig. S3:

Supplementary materials

Fig. S1: Calculated density of states for GaN_xAs_{1-x} (x=0.0, 0.25, 0.5, 0.75 and 1.0) alloys. Which clearly show that replacing As atoms by N atoms cause significant influence in the density of states.

Fig. S2: (a, b) Calculated carrier's mobility vs. carrier's concentration of GaN_xAs_{1-x} (x=0.0, 0.25, 0.5, 0.75 and 1.0) alloys. We have compared our results with the previous experimental data for GaAs [58-60] good agreement was found.

Fig. S3: Calculated Seebeck coefficient vs. temperature. We have compared our calculated S of GaN_xAs_{1-x} (x=0.0, 0.25, 0.5, 0.75 and 1.0) alloys to the measured and calculated S for GaAs [58]. It has been found that the increase in the calculated S for GaN_xAs_{1-x} (x=0.0, 0.25, 0.5, 0.75 and 1.0) with increasing the temperature is consistent with previously measured and calculated S of GaAs [58], good agreement was found.

References:

[58] https://escholarship.org/uc/item/2h7846vd.pdf

[59] G. Homm, P. J. Klar, J. Teubert, and W. Heimbrodt. Seebeck coefficients of n-type (Ga,In)(N,As), (B,Ga,In)As, and GaAs. Applied Physics Letters, 93:042107, 2008.

[60] D. L. Rode and S. Knight. Electron transport in GaAs. Physical Review B, 3(8):2534, 1971.